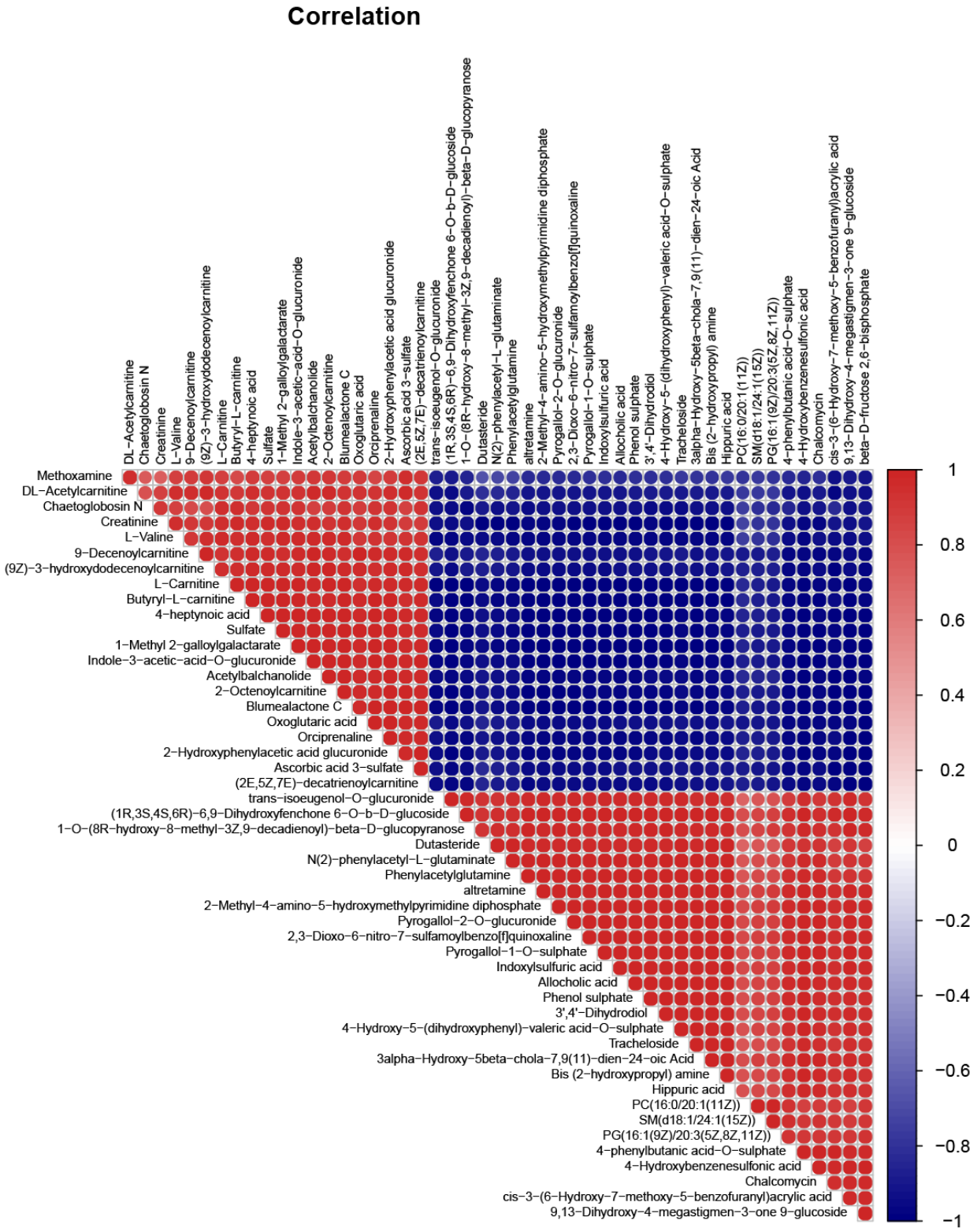
Supplementary file Table S1. Information of the three participations

Name	Sex	Age	Smoking years	Nation
Participation 1	Male	58	16	Han
Participation 2	Male	46	10	Han
Participation 3	Male	42	12	Han

Supplementary file Figure S1. Correlation analysis heatmap of the top 50 significantly differential expressed metabolites between LN and HN groups



Red represents positive correlation, and blue represents negative correlation. There was a significant correlation among 50 differential metabolites.

Supplementary file Table S2. Raw negative data obtained from sequencing

ID	m/z	Retention time (min)	Ion mode	Metabolites	Compound ID	Super Class	Class	Sub Class	level	kegg	Score	Fragmentation Score	Adducts	Formula	Mass Error (ppm)	CK1	CK2	CK3	HN1	HN2	HN3	LN1	LN2	LN3
4.79_151.0401m/z	151.0401147	4.792316667	neg	3-Cresotinic acid	6661	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives		C14088	59	97.7	M-H	C8H8O3	0.309310423	3988.903632	4292.847518	4677.456248	4962.132168	4956.103801	5003.075784	4631.990888	4906.8231	5234.225656
5.22_167.0350m/z	167.0350416	5.222166667	neg	Vanillic acid	HMDB0000484	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	***	C06672	58.7	96.5	M-H	C8H8O4	0.352842483	5472.604211	5730.643319	5914.011913	568.7488299	512.836852	686.763145	5061.884992	5215.861842	5471.473995
4.92_194.0460m/z	194.0459594	4.92485	neg	Salicyluric acid	617	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*	C07588	58.6	95.6	M-H	C9H9NO4	0.400099959	31219.45981	34804.0261	34938.75925	4255.661137	4286.678612	4416.639838	7151.178015	7937.766494	7730.460374
4.39_264.1110n	263.1037232	4.3893	neg	Phenylacetylglutamine	HMDB0006344	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***	C04148	57.9	90.9	M-H, 2M-H, M-H2O-H	C13H16N2O4	-0.028048749	1296934.967	1401733.886	1353489.988	885556.1803	854312.3244	845983.9958	1427805.186	1689978.386	1536547.731
1.70_283.0686m/z	283.0685973	1.6992	neg	Xanthosine	3408	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	**	C01762	57.6	92.6	M-H	C10H12N4O6	0.667546165	22195.50084	23849.25854	22938.99232	17596.77964	17616.69789	16586.69279	18699.98984	16637.35793	20917.84473
3.98_188.0354m/z	188.0354098	3.97985	neg	Kynurenic acid	HMDB0000715	Organoheterocyclic compounds	Quinolines and derivatives	Quinoline carboxylic acids	***	C01717	57.4	89.6	M-H	C10H7NO3	0.492515169	11416.75666	12639.53737	12327.92896	16534.81474	16041.80554	16033.48902	13424.18093	15402.98868	14731.3503
5.73_541.2660m/z	541.265998	5.727283333	neg	Cortolone-3-glucuronide	HMDB0010320	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	*		57.2	90.3	M-H	C27H42O11	1.036962921	123329.377	139921.4341	109479.9291	130085.9335	179957.7227	156685.4862	142056.9616	182114.6084	181757.4575
5.73_591.2801m/z	539.2500672	5.709933333	neg	Tetrahydroaldosterone-3-glucuronide	HMDB0010357	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	*		57	91.3	M-H	C27H40O11	0.521036279	3443712.964	3491488.1809	2925769.9232	309698.6487	414356.91	383306.9577	301396.3394	398647.2635	421864.7832
4.70_172.0980m/z	172.0980228	4.703166667	neg	N-Acetylleucine	HMDB0011756	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***	C02710	56.8	87.1	M-H	C8H15NO3	0.611812152	11354.63742	10910.77498	11889.61897	14475.30345	13871.25213	13887.25413	15632.12355	16389.41836	15875.22343
4.37_159.0663m/z	159.0663257	4.367166667	neg	3-Methyladipic acid	HMDB0000555	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	***		56.6	84.8	M-H	C7H12O4	0.270040869	27988.21385	31259.14337	33018.61132	44853.87341	30255.03439	32473.61499	23792.72381	26712.07358	26390.67325
0.90_168.0284m/z	167.0210934	0.904683333	neg	Uric acid	HMDB0000289	Organoheterocyclic compounds	Imidazopyrimidines	Purines and pyrimidines	***	C00366	56.5	86.4	M-H, 2M-H	C5H4N4O3	0.177727895	470483.5341	489558.9714	527552.7328	446759.0644	592840.7439	459363.8536	526170.4012	428046.3046	541895.5898
4.28_213.0097n	212.0024497	4.278183333	neg	Indoxylsulfuric acid	253	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		56.2	84.8	M-H, 2M-H	C8H7NO4S	0.692021131	873409.2118	944600.9147	934250.8591	63673.55765	57224.44981	55912.32839	768364.9263	855781.0175	805114.1193
4.43_153.0194m/z	153.0193914	4.432683333	neg	Gentisic acid	618	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	**	C00628	56.1	83.4	M-H	C7H6O4	0.384209097	13690.72623	14863.8246	15215.5791	3062.853938	2921.209785	3040.564189	11515.41546	13178.63626	12030.24058
4.00_172.9914m/z	172.9914257	4.002233333	neg	Phenol sulphate	HMDB0060015	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	***	C02180	56	90.8	M-H	C6H6O4S	0.128824485	238836.0847	256838.9891	268094.1966	73576.74837	69812.46795	70739.06463	216549.9843	242558.9318	234102.8175
3.69_196.0597n	195.0524192	3.685866667	neg	1,7-Dimethyluric acid	61971	Organoheterocyclic compounds	Imidazopyrimidines	Purines and pyrimidines	**	C16356	55.7	85.9	M-H, 2M-H	C7H8N4O3	0.282946136	130418.4228	146418.8467	145458.1603	228664.9315	228872.8626	169391.3807	168980.5279	184748.3524	183741.8337
5.01_166.0631n	165.0557731	5.014716667	neg	Dihydro-3-coumaric acid	4152	Phenylpropanoids and polyketides	Phenylpropanoic acids	Unclassified	**	C11457	55.5	80.2	M-H2O-H, M-H	C9H10O3	0.818377092	12469.48333	13200.18014	13253.52929	14802.19873	16157.9845	17529.33799	15553.33462	14395.54644	14932.9251
1.20_173.0092m/z	173.0092182	1.202333333	neg	Aconitic acid	3300	Organic acids and derivatives	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives	**	C00417	55.3	77.6	M-H	C6H6O6	0.325908687	136714.1647	148603.7076	163321.8151	153632.319	137198.6801	142722.9323	135889.2277	160432.6271	155530.7287
3.85_193.0619m/z	193.0619091	3.84605	neg	aminohippuric acid	3927	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*	D06890	55.3	79.1	M-H	C9H10N2O3	0.223105331	7879.605902	8518.476183	8972.860622	9743.968247	9256.198595	8938.010846	9470.023681	10138.26208	10286.16661
3.85_179.0575m/z	179.0575348	3.84605	neg	Theophylline	1458	Organoheterocyclic compounds	Imidazopyrimidines	Purines and pyrimidines	***	C07130	55.1	83.8	M-H	C7H8N4O2	0.476254429	37968.79315	40431.53772	43248.93508	45501.61693	46444.48607	45868.25177	45864.43434	49028.21345	48796.13821
4.00_158.0823m/z	158.0823066	4.002233333	neg	Acetyl-DL-Valine	73550	Unclassified	Unclassified	Unclassified			55.1	77.7	M-H	C7H13NO3	0.249879672	13429.13336	14291.72598	15129.43165	17545.26393	16797.04205	16655.49944	17853.74972	19470.78368	18667.09039
7.47_528.2641m/z	528.2641439	7.46525	neg	Glycochenodeoxycholate-3-sulfate	HMDB0002497	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	***		55.1	84.3	M-H	C26H43NO8S	0.910740107	62031.67561	60857.95704	70116.04313	30358.71857	31124.48522	29591.54769	58415.22885	66032.61074	59982.30187
0.76_131.0463m/z	131.0462575	0.757316667	neg	L-Asparagine	14	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00152	55	78.6	M-H	C4H8N2O3	0.316560769	3039.754656	2818.375689	2944.7837	2669.396985	3973.07334	3946.41896	4097.654036	4321.946009	4393.177548
1.58_182.0459m/z	182.0459329	1.577833333	neg	4-Pyridoxic acid	HMDB0000017	Organoheterocyclic compounds	Pyridines and derivatives	Pyridinecarboxylic acids and derivatives	***	C00847	55	77.1	M-H	C8H9NO4	0.281810364	16567.11221	14056.41415	15198.66818	29983.24156	27379.10067	28988.40559	12387.33782	16612.91197	13968.70905
1.90_296.1002m/z	296.1001622	1.899016667	neg	2-Methylguanosine	58332	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	*		54.9	79.4	M-H	C11H15N5O5	0.403990779	16558.6101	17689.20476	15061.06441	18454.05186	19208.27157	17927.11515	16555.68912	16638.43005	16287.90098
5.70_431.1926m/z	431.1924916	5.701283333	neg	Corchorusoid C 6-glucoside	HMDB0029772	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		54.8	77.4	M+FA-H	C19H30O8	0.571760666	18278.9711	17969.74995	18062.85571	18040.59758	17590.0186	18615.54492	19213.83457	19656.1053	21926716518
6.48_200.1294m/z	200.1293813	6.477433333	neg	2,2,6,6-Tetramethyl-4-piperidinone	HMDB0031179	Organoheterocyclic compounds	Piperidinones	Piperidines	*		54.8	75.7	M+FA-H	C9H17NO	1.05913836	25031.64947	25904.75714	30729.5533	47455.53024	43594.81709	43430.87628	36450.75714	40297.37738	39197.98999
9.32_293.1761m/z	293.176076	9.321783333	neg	Furanofukinin	HMDB0036640	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		54.7	76.6	M+FA-H	C16H24O2	0.979573425	123548.8785	118417.4059	90341.85133	114693.4052	139498.9823	124164.5435	102670.1346	101025.5454	124791.6545
4.18_137.0244m/z	137.0244351	4.181333333	neg	p-Salicylic acid	3263	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	**	C00156	54.4	74.9	M-H	C7H6O3	0.126609109	7653.656046	6492.337561	6217.17795	4618.711867	4436.053052	5359.078174	7647.41548	5790.626146	6012.477203
4.41_179.0583n	178.0510155	4.41115	neg	Hippuric acid	1301	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	**	C01586	54.4	82.2	M-H, 2M-H	C9H9NO3	0.272509782	394708.7497	447411.8227	417240.3151	175356.5311	170266.6304	173008.5625	314542.8832	361681.1797	338761.5757
3.87_182.0581m/z	181.050758	3.868533333	neg	Hydroxyphenyllactic acid	34515	Phenylpropanoids and polyketides	Phenylpropanoic acids	Unclassified	*	C03672	54.3	74.1	M-H2O-H, M-H	C9H10O4	0.851488422	54828.01894	58647.34207	61367.98467	23091.83562	21979.60411	22540.13542	61556.39723	66244.65444	62454.52444
3.94_183.0300m/z	183.0299862	3.9351	neg	Ethyl acontitate	HMDB0040275	Organic acids and derivatives	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives			54.3	73.9	M-H2O-H	C8H10O6	0.441973222	10954.42023	11607.79973	12417.15675	10915.29934	10170.29317	10469.64399	8446.955098	9335.073331	9212.493043
4.75_202.1207n	201.1133927	4.747466667	neg	9,10-dihydroxy-2-decenoic acid	LMFA01050428	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			54.3	73.8	M-H, 2M-H	C10H18O4	0.792025519	227738.334	243708.1469	246582.114	217390.5351	214558.6137	209027.9182	211194.5861	233910.0021	232501.3791
4.09_153.0194m/z	153.019406	4.091783333	neg	2,3-Dihydroxybenzoic acid	3276	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*	C00196	54.2	73.6	M-H	C7H6O4	0.479110894	4153.430221	4013.63588	4160.061425	2486.367644	2231.739442	2409.337049	2973.629448	3012.588404	2905.818119
4.75_208.0616m/z	208.0616529	4.747466667	neg	3-Methyldioxyindole	HMDB0004186	Organoheterocyclic compounds	Indoles and derivatives	Indolines	**	C05834	53.9	71.1	M+FA-H	C9H9NO2	0.598634819	131521.9077	135502.8561	138175.5432	61243.54721	63137.36682	63153.37458	113118.08	131291.7169	121469.4627
4.88_173.0820m/z	173.0819524	4.880083333	neg	Suberic acid	4243	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*	C08278	53.9	71	M-H	C8H14O4	0.114229274	74095.94903	79153.31141	80759.75306	78765.24311	75831.94437	78047.96824	57282.17655	61930.73618	59694.3412
6.57_213.1134m/z	213.113397	6.570233333	neg	2,2'-(3-methylcyclohexane-1,1-diyl)diacetic acid	96295	Unclassified	Unclassified	Unclassified			53.9	72.9	M-H	C11H18O4	0.767727971	23084.75807	25230.54363	26697.35711	21589.77248	21428.5689	21196.40279	15225.6365	17618.62179	15909.06697
3.96_279.0987m/z	279.0987348	3.957583333	neg	Asp-Phe	64957	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			53.6	73	M-H	C13H16N2O5	0.319832325	3994.151568	4791.856291	4798.105546	5478.176138	5100.80732	5807.565536	4375.778704	4805.226978	4409.375703
4.16_175.0612m/z	175.0612271	4.15895	neg	2-Isopropylmalic acid	HMDB0000402	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	***	C02504	53.6	69.9	M-H	C7H12O5	0.170403061	10427.41717	10545.93524	10892.50821	15438.96226	11873.72054	12802.30454	13530.07961	10625.21068	10239.2395
5.30_423.2027m/z	423.20279	5.302883333	neg	18-Hydroxycortisol	LMST02030193	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	*		53.6	74.6	M-H-FA-H	C21H30O6	0.921446834	8614.354286	8063.726494	9140.62405	9356.660231	11388.39485	11507.54847	12186.19354	13946.51955	14925.70007
1.96_561.2040m/z	561.2039566	1.95955	neg	indoprofen	HMDB0253478	Unclassified	Unclassified	Unclassified			53.4	72.2	2M-H	C17H15NO3	1.505363482	25840.24389	24364.82044	20002.9153	206.1507667	0.001403199	96.6509771	21337.88107	21667.57476	19554.81778
0.76_146.0692n	145.0619439	0.757316667	neg	D-Glutamine	63630	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00819	53.3	72.9	M-H2O-H, M-H	C5H10N2O3	0.365811811	28488.04569	26836.55019	26041.88158	21194.14233	24995.80934	27542.44618	28474.96522	32851.70613	32601.1453
5.83_199.0977m/z	199.0977044	5.825	neg	Matsutakic acid A	HMDB0036715	Organic acids and derivatives	Hydroxy acids and derivatives	Medium-chain hydroxy acids and derivatives			53.2	68.1	M-H	C10H16O4	0.608928114	73973.98224	74424.52178	81590.52749	96979.4885	76761.91289	76706.18006	65127.31027	64309.798	62271.11868
6.21_203.1289m/z	203.128932	6.206233333	neg	Pelargonic acid	LMFA01010009	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*	C01601	53.2	69.1	M+FA-H	C9H18O2	0.31185941	3414.40651	3458.621648	3916.968264	5364.635338	4759.830036	5098.053256	2669.345705	2922.156056	3174.750976
1.16_151.0261m/z	151.0261847	1.160166667	neg	Xanthine	HMDB0000292	Organoheterocyclic compounds	Imidazopyrimidines	Purines and pyrimidines	***	C00385	53.1	71.9	M-H, 2M-H	C5H4N4O2	0.235174736	3371.71433	3666.428621	3915.04753	1598.248204	1283.10677	1411.814	1377.4694	9960.238554	1209.6328
5.06_164.0355m/z	164.035473	5.05975	neg	N-formylanthranilic acid	34537	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	**	C05653	53.1	72	M-H	C8H7NO3	0.947085273	3411.080989	3486.850998	3525.601463	5010.568553	4649.58683	5111.375369	4095.443555	4235.803733	5293.463472
1.20_180.0667m/z	180.0667375	1.202333333	neg	L-Tyrosine	34	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00082	53	68.3	M-H	C9H11NO3	0.666486829	8153.409991	8309.63602	8402.157393	11107.70907	10685.38542	10665.27209	9247.742009	9875.511231	10836.52294
2.71_131.0350m/z	131.0350158	2.709983333	neg	Glutaric acid	3254	Organic acids and derivatives	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives	**	C00489	53	67.6	M-H	C5H8O4	0.2538414	4746.094822	4580.176767	4779.538329	4941.93651	4614.837546	4949.756313	4654.711006	4248.960266	4502.928766
3.80_195.0532n	194.0459171	3.801716667	neg	L-Dopaquinone	HMDB0039119	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			53	75.4	M-H, M+FA-H	C9H9NO4	0.18314937	33333.37354	28706.40352	28958.11846	4468.129983	3865.340166	3339.982406	16462.58124	16793.95743	17303.96378
6.10_291.1734m/z	291.1134043	6.101316667	neg	2-hydroxy-2,6,6-trimethylcyclohexanone	HMDB0037023	Organic acids and derivatives	Organooxygen compounds	Carbonyl compounds	*		53	67.1	M-H	C9H16O2	1.099881626	52816.58961	61273.48821	63105.16815	70282.2155	75898.59569	71693.51326	81348.82193	83003.38432	84058
0.97_174.0408m/z	174.0408221	0.967616667	neg	N-acetylaspartate	3769	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C01042	52.9	68	M-H	C6H9NO5	0.149569313	7303.734794	7457.247106	7772.256635	9093.376785	8815.55256	8202.921639	7887.737011	8999.637041	8364.551914
3.69_145.0507m/z	145.0507092	3.685866667	neg	Adipic acid	115	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C06104	52.9	67.9	M-H	C6H10O4	0.525903502	5213.771106	4944.319215	5033.483912	7436.686392	7682.014395	5590.765095	5520.501509	5290.157375	5709.80256
4.86_401.1441m/z	401.1441182	4.858383333	neg	xi-3-Hydroxy-5-phenylpentanoic acid O-beta-D-Glucopyranoside	HMDB0031695	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		52.9	74.3	M+FA-H	C17H24O8	-3.376074141	57409.55663	59771.12496	62073.24997	81417.52548	77645.43448	78119.33506	70952.03245	77026.79613	75113.29539
7.65_269.1396m/z	269.1395695	7.65305	neg	3-Methyl-5-pentyl-2-furanpropanoic acid	HMDB0112084	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates			52.9	66.9	M+FA-H	C13H20O3	0.545065515	15862.9685	16854.48912	18611.46052	10233.86112	9319.22639	10030.4533	14469.42526	15113.9123	15950.8521
5.12_233.0946n	204.0667102	5.132916667	neg	2-hydroxyphenylpropionylglycine	HMDB0094723	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			52.7	65.9	M-H2O-H, M-H	C11H13NO4	0.418627781	33575.73573	37555.43459	38823.83101	52790.00269	51839.94259	50271.62157	48341.36966	51061.80614	50264.3056
8.07_405.2648m/z	405.2647973	8.074883333	neg	(23R)-3alpha,7alpha,17alpha,23-Tetrahydroxy-5beta-cholan-24-oic Acid	LMST04010421	Unclassified	Unclassified	Unclassified			52.7	68.7	M-H2O-H	C24H40O6	-0.352239726	232710.9359	263745.2709	240438.357	44439.56986	41457.64625	39951.96879	111989.3075	136297.0466	131916.7707
4.52_287.0233m/z	287.0233001	4.521733333	neg	4-Hydroxy-5-(dihydroxyphenyl)-valeric acid-O-sulphate	HMDB0059978	Benzenoids	Phenols	Benzenediols	*		52.6	67.9	M-H2O-H	C11H14O8S	0.66257282	80598.8187	83071.97727	97276.0216	60281.27941	57366.007	55604.54391	149348.1402	165986.8798	165970.9427
3.98_222.0773m/z	222.0773102	3.97985	neg	Acetyl-L-tyrosine	5827	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C01657	52.5	67.3	M-H	C11H13NO4	0.5768499	2588.693337	2544.729402	2821.758891	2988.883053	2761.932137	2366.339979	2919.072938	2966.928251	2799.849328
2.35_141.0194m/z	141.0193803	2.34905	neg	(2E,4Z)-2-hydroxy-6-oxohexa-2,4-dienoic acid	LMFA01030926	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			52.4	65.9	M-H	C6H6O4	0.33827902	3517.129496	3387.291115	3273.555509	1699.181336	1755.53451	1552.150474	1052.008508	1160.480782	1213.550078
8.68_567.3178m/z	567.3178705	8.68065	neg	Deoxycholic acid 3-glucuronide	LMST05010046	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	**	C03033	52.4	65.2	M-H	C30H48O10	0.702483295	18977.2091	21186.32925	21792.70427	29714.68257	27737.18245	25616.41574	98035.57399	102552.3008	107316.6989
3.94_125.0243m/z	125.0243332	3.9351	neg	4-HYDROXY-6-METHYLPYRAN-2-ONE	44653	Unclassified	Unclassified	Unclassified			52.2	66.3	M-H	C6H6O3	-0.670201253	1681.207329	1828.28364	1929.082415	838.2690928	736.5257261	730.0179336	1479.757184	1635.478997	1554.379517
7.04_271.1553m/z	271.1552843	7.044716667	neg	Riesling acetal	HMDB0037562	Organoheterocyclic compounds	Tetrahydrofurans	Unclassified	*		52.2	64.6	M+FA-H	C13H22O3	0.826385665	6991.08507	7361.528153	6773.807644	12025.88408	11795.98898	10737.47544	6477.273938	7046.356413	6027.747028
2.86_195.0524m/z	195.0524266	2.864816667	neg	1,3-Dimethyluric acid	2822	Organoheterocyclic compounds	Imidazopyrimidines	Purines and pyrimidines	*		52.1	69.8	M-H	C7H8N4O3	0.320714272	36151.70914	36374.74729	40510.58389	56204.74629	53604.75584	52793.74901	44183.22363	46660.30896	42426.37755
3.96_187.0613m/z	187.0612868	3.957583333	neg	3-acetyl-3-methylindrofuran-2(3H)-one	LMFA07040006	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters			51.9	61.9	M+FA-H	C7H10O3	0.631997569	3797.344968	4099.567406	4516.659758	7096.362666	6881.080278	7415.108252	4287.120186	4935.713612	4678.607465
6.43_405.1921m/z	405.192126	6.433933333	neg	Aldosterone	HMDB0030026	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	**	C01780	52.1	77	M+FA-H	C21H28O5	0.691641832	26794.56473	24629.58257	24270.61069	25350.1656	23187.48124	25260.06698	35041.69753	35444.66902	34539.69531
0.93_146.0216n	191.0198685	0.925866667	neg	Oxoglutaric acid	119	Organic acids and derivatives	Keto acids and derivatives	Gamma-keto acids and derivatives	**	C00026	52	61	M-H, M+FA-H	C5H6O5	0.418166227	389591.3497	484469.8807	564170.5733	910328.1777	929902.2747	847668.5402	496383.3445	612087.1789	614000.3543
1.38_225.0631m/z	225.0631212	1.380283333	neg	5-Acetylamino-6-formylamino-3-methyluracil	HMDB0011105	Organoheterocyclic compounds	Diazines	Pyrimidines and pyrimidine derivatives	***	C16365	52	70.3	M-H	C8H10N4O4	0.852741347	235906.2323	192594.8402	202662.9284	340187.4979	314699.459	289608.5594	310562.4338	300043.2402	289906.9995
3.80_245.1144m/z	245.1143778	3.801716667	neg	Aspartyl-Isoleucine	HMDB0028756	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		52	64.6	M-H	C10H18N2O5	0.335485475	1797.545942	1865.516952	1945.392155	2514.628067	2594.789348	2277.755907	1699.605725	1883.984728	2038.193549
9.75_239.1290m/z	239.1290439	9.75225	neg	Cucujolide IV	LMFA07040036	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters			51.9	63	M+FA-H	C12H18O2	0.830357353	27793.89759	24836.18669	23637.61877	24935.31547	24773.42692	28744.48042	28509.20962	26876.6283	26517.35847
0.88_244.0833m/z	243.0622965	0.884633333	neg	Uridine	HMDB0000296	Nucleosides, nucleotides, and analogues	Pyrimidine nucleosides	Unclassified	**	C00299	51.9	61.9	M-H	C9H12N2O6	0.150891894	197104.6924	191227.1145	194450.8088	174126.9907	166684.4432	181192.0634	193882.4161	177959.8683	187582.2008
5.38_244.1312n	243.123801	5.384216667	neg	Polyethylene, oxidized	HMDB0032472	Organic acids and derivatives	Keto acids and derivatives	Medium-chain keto acids and derivatives	*		51.9	63.2	M-H2O-H, M-H	C12H20O5	0.580198357	49524.04738	58484.68139	54570.70578	47577.2074	47591.66649	45980.87861	35762.71807	41818.56292	40038.0341
5.45_234.0773m/z	234.0773196	5.451166667	neg	Phensuximide	HMDB0014970	Organoheterocyclic compounds	Pyrrolidines	Phenylpyrrolidines		C07437	51.9	61.6	M+FA-H	C11H11NO2	0.730419645	13316.76256	13099.80932	13836.55935	4756.75228	4451.621802	4737.084522	12079.96618	9478.218372	9785.999962
1.16_191.0199m/z	191.0198602	1.160166667	neg	Citric acid	HMDB0000094	Organic acids and derivatives	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives	***	C00158	51.8	60.3	M-H	C6H8O7	0.698108218	715698.6009	784459.5944	1044995.386	110180176	1170032.927	1088361.696	954172.9242	988344.9313	1094971.387
4.57_423.2029m/z	422.2028883	4.5668	neg	Eremopetasitenin C1	HMDB0032775	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*		51.8	63.8	M+FA-H	C21H30O6	1.181169419	5711.384146	6137.499799	6700.136644	9786.144599	9187.782676	8442.89143	6826.924693	6902.029625	7194.020605
1.55_103.0401m/z	103.0401011	1.553483333	neg	4-Hydroxybutyric acid	HMDB0000710	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*	C01991	51.7	60.2	M-H	C4H8O3	0.321648482	1842.499953	1585.977343	1476.038858	2726.437844	2780.372779	2497.641585	1777.629186	2609.956959	2201.075334
5.16_215.0022m/z	215.0022253	5.155116667	neg	Hydroxytyrosol 3'-sulfate	HMDB0240530	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates			51.7	66.4	M-H2O-H	C8H10O6S	1.099618929	58892.68463	72321.5565	62403.57038	19556.817148	1682.766792	1682.259188	48676.69844	53640.17441	55892.34014
3.94_302.0640n	301.0566972	3.9351	neg	Pyrogallol-2-O-glucuronide	HMDB0060017	Organic compounds	Organooxygen compounds	Organooxygen compounds	*		51.6	60.5	M-H, 2M-H	C12H14O9	0.634343121	119205.7944	125814.8252	134400.7538	6444.97756	5937.848805	6566.436265	109930.7518	119228.2215	116168.2293
5.22_185.0820m/z	185.0820076	5.222166667	neg	5-(2-Methylpropyl)tetrahydro-2-oxo-3-furancarboxylic acid	HMDB0030988	Organoheterocyclic compounds	Lactones	Gamma butyrolactones			51.6	60.4	M-H	C9H14O4	0.403444583	15146.02347	15575.98431	15568.00878	17035.61354	15714.23385	16239.38115	12738.61715	11882.31395	13339.95975
0.80_209.0303m/z	209.0303238	0.800366667	neg	D-Glucarate	5343	Organic acids and derivatives	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C00818	51.5	59.3	M-H	C6H10O8	0.157090788	8537.124054	7303.214375	7270.863982	8004.047613	8537.142454	9423.167381	2948.009426	2949.37664	3061.966344
0.84_179.0561m/z	179.0561477	0.841733333	neg	myo-Inositol	144	Organic acids and derivatives	Organooxygen compounds	Alcohols and polyols	**	C00137	51.5	59.4	M-H	C6H12O6

3.85_227.1039m/z	227.1039364	3.84605	neg	gamma-Glutamylvaline	HMDB0011172	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		50.5	56.5	M-H2O-H	C10H18N2O5	0.836367785	4605.649543	5454.710621	5612.975448	5867.658231	5700.289706	5920.069828	4712.662217	5197.905651	4923.436495
5.24_199.0072m/z	199.0071767	5.244033333	neg	4-Vinylphenol sulfate	HMDB0062775	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		50.5	58.8	M-H	C8H8O4S	0.616744442	107580.4039	94348.52716	97694.84126	6723.94277	6939.157812	7113.531819	91538.63601	79435.85399	96598.35132
0.84_132.0302m/z	132.030245	0.841733333	neg	L-Aspartic acid	HMDB0000191	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00049	50.4	55.5	M-H	C4H7NO4	0.102964292	5698.459666	6367.306582	6655.142355	6408.777146	7171.233727	6759.930989	6142.831924	6926.108499	7031.555656
3.73_343.0673m/z	343.0672742	3.730516667	neg	Isovanillic acid glucuronide	HMDB0240538	Unclassified	Unclassified	Unclassified	*		50.4	54.4	M-H	C14H16O10	0.592683993	73866.00472	67620.14538	73292.58588	21749.33942	22180.47524	16740.32788	47339.08267	53101.45362	53427.89718
5.85_433.2081m/z	433.2080936	5.84575	neg	9,13-Dihydroxy-4-megastigmen-3-one 9-glucoside	HMDB0036318	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		50.4	53.6	M+FA-H	C19H32O8	0.445073667	444419.7061	482361.4146	496523.3796	396903.7542	400951.8953	401871.2899	607512.0878	565818.575	592007.6873
2.28_164.0717m/z	164.0717191	2.2828	neg	L-Phenylalanine	28	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00079	50.3	53.9	M-H	C9H11NO2	0.102749486	82004363	83691920631	7636.046187	12348.22016	11894.54052	12378.52517	10199.95764	11199.78388	10950.26846
7.92_465.2495m/z	465.2495276	7.91555	neg	Androsterone glucuronide	HMDB0002829	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	**	C11135	50.3	53.1	M-H	C25H38O8	0.291399507	401955.193	396258.5944	410100.2363	525221.6373	520812.4289	549603.2769	402272.8868	495106.831	462137.2615
4.14_261.0075m/z	261.0075018	4.136366667	neg	3-(3,5-dihydroxyphenyl)-1-propanoic acid sulphate	HMDB0061117	Benzenoids	Phenols	Benzenediols	*		50.2	56.2	M-H	C9H10O7S	0.20815897	13573.94282	13513.87579	14153.5679	31808.56298	26599.84009	29201.79838	15524.82518	13308.58703	13070.00924
6.39_213.1134m/z	213.1134455	6.386066667	neg	Aleprestic acid	LMFA01030188	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			50.2	53.4	M+FA-H	C10H16O2	1.266446841	13193.68308	14355.65872	15468.82437	22541.85691	22895.3008	23693.58159	14792.8456	14847.24592	14823.9879
6.91_227.1291m/z	227.1290927	6.9072	neg	Traumatic acid	HMDB0000933	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	***	C16308	50.2	56.5	M-H	C12H20O4	0.92077138	10655.31317	11174.45781	10488.4779	15166.09282	15319.44892	14981.94279	9271.121136	9984.440198	9748.669519
0.78_325.0945m/z	325.0944988	0.778533333	neg	6-O-(-coumaroyl)-D-glucose	HMDB0039169	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives			50.1	64.7	M-H	C15H18O8	4.93004813	23707.07588	22867.95562	27326.31157	8948.445922	14801.25167	11372.59467	22381.2879	31011.36841	39126.12904
1.16_111.0088m/z	111.0087811	1.160166667	neg	2-Hydroxyglutaric acid lactone	HMDB0059743	Organoheterocyclic compounds	Lactones	Gamma butyrolactones			50.1	52	M-H2O-H	C5H6O4	0.103953425	8400.751485	9724.54989	11944.08608	13235.9305	13126.88197	12983.67898	10524.6067	11625.85478	12979.63995
1.20_160.0616m/z	160.0616431	1.202333333	neg	Glucosamine	HMDB0001514	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C00329	50.1	53.4	M-H2O-H	C6H13NO5	0.62354222	10264.28208	10514.0331	11184.6715	13128.53994	12792.05604	14008.6264	10787.97863	12198.20235	12944.87095
6.22_218.0824m/z	218.0823752	6.215	neg	Salsoline-1-carboxylate	HMDB0013067	Organoheterocyclic compounds	Tetrahydroisoquinolines	Unclassified	*		50.1	54.4	M-H2O-H	C12H15NO4	0.456959489	9323.143781	2656.671859	3544.82604	1199.508732	1190.95251	1224.402676	3344.03145	3406.034639	3480.945556
0.74_104.0354m/z	104.0353629	0.7359	neg	L-Serine	30	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C00065	50	51.6	M-H	C3H7NO3	0.439937707	1366.171856	922.5363625	1308.425665	1137.615636	2460.224095	1920.508633	995.6570042	1836.225195	1991.374382
3.44_194.0459m/z	194.0459383	3.440016667	neg	3-Hydroxyhippuric acid	HMDB0006116	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*		50	51.8	M-H	C9H9NO4	0.138121075	119897.3707	138490.056	141535.6599	75191.84904	73125.97987	74809.90787	133252.6125	124871.8459	126518.4469
4.11_306.0411n	287.0232829	4.113883333	neg	4-hydroxy-5-[4-hydroxy-3-(sulfooxy)phenyl]pentanoic acid	HMDB0127746	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		50	54.8	M-H2O-H, M+FA-H	C11H14O8S	0.606570723	17889.79418	18045.73118	18334.70527	24101.92597	19427.8595	21441.51468	81008.10851	79279.21749	78340.49457
4.48_210.0774m/z	210.0773799	4.477166667	neg	4-Hydroxy-1-(3-pyridinyl)-1-butanone	HMDB0062402	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C19565	50	53.4	M+FA-H	C9H11NO2	1.202253872	2645.109966	2869.718482	2987.123647	654.4181163	774.031023	616.2900998	662.218227	696.857234	859.5126291
4.66_259.1188m/z	259.1187904	4.660483333	neg	alpha-Carboxy-delta-decalactone	HMDB0030985	Organoheterocyclic compounds	Lactones	Delta valerolactones	*		50	51	M+FA-H	C11H18O4	0.366646188	36370.8902	35227.01946	38377.44439	79043.11901	74513.80584	81498.52511	48040.44445	52902.24469	38750.46819
3.75_204.0303m/z	204.03029	3.747833333	neg	Xanthurenic acid	HMDB0000881	Organoheterocyclic compounds	Quinolines and derivatives	Quinoline carboxylic acids	***	C02470	49.9	51.6	M-H	C10H7NO4	0.286232944	5428.831194	4681.661416	4873.727613	10249.02333	9811.385954	6861.216815	5396.180445	6290.300109	6123.390078
3.82_123.0452m/z	123.0451987	3.82415	neg	4-Methylcatechol	64945	Benzenoids	Benzenoids	Phenols	**	C06730	49.9	52	M-H	C7H8O2	0.463418893	1370.988083	1438.775208	1447.307223	1340.020192	1271.60479	1088.176006	1131.142937	1265.920171	1213.480222
4.54_217.1083m/z	217.1082548	4.54425	neg	(3R,6S)-3-Hydroxy-1,7-dioxaspiro[5.5]undecane	LMPK09000005	Unclassified	Unclassified	Unclassified			49.9	53.7	M+FA-H	C9H16O3	0.624856739	6337.28196	7268.16224	7012.111959	7394.520238	7267.678246	7349.920251	5306.127106	5755.158203	6357.289207
4.95_445.0782m/z	445.0781732	4.94705	neg	Genistein 5-O-glucuronide	HMDB0041738	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavonoid O-glycosides	*		49.9	55.6	M-H	C21H18O11	1.206483317	347.4360035	246.3325995	366.5580062	19292.62244	17962.51835	18698.85734	65.46482111	44.50161153	0.001403199
5.49_194.0459m/z	194.0459339	5.489016667	neg	N-Acetyl-5-aminosalicylic acid	1146	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*		49.9	53.4	M-H	C9H9NO4	0.26936731	2177.763349	1471.545019	1500.802291	1653.52547	1629.778848	2094.132672	2251.748438	1728.706906	1742.615811
5.95_218.0823m/z	218.0823471	5.95155	neg	N-Deschlorobenzoyl indomethacin	HMDB0013988	Organoheterocyclic compounds	Indoles and derivatives	Indolyl carboxylic acids and derivatives	*		49.9	54.2	M-H	C12H13NO3	0.36851188	2854.611025	3079.289797	3158.30637	2877.663044	3172.608979	3683.985575	2555.784083	2894.646581	2780.068297
2.07_245.1143m/z	245.1143356	2.070366667	neg	(5)-3-Sulfolactate	HMDB0060176	Organic acids and derivatives	Hydroxy acids and derivatives	Alpha hydroxy acids and derivatives	**	C11499	49.8	53.4	M-H	C3H6O6S	0.156927206	20506.62171	23404.15355	24133.29258	27115.94696	25311.33098	22924.25645	23925.49369	24540.65431	24534.53431
3.89_261.0075m/z	261.0075174	3.8906	neg	Homovanillic acid sulfate	HMDB0111719	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		49.8	56.8	M-H	C9H10O7S	0.267746155	24409.0463	26321.43859	27877.88681	21689.82754	20257.98889	20569.68819	20476.11205	22513.49363	23275.58169
5.08_236.0930m/z	236.0929915	5.080566667	neg	(E)-5-(3,4,5,6-Tetrahydro-3-pyridylidenemethyl)-2-furanmethanol	HMDB0033560	Organoheterocyclic compounds	Pyridines and derivatives	Hydropyridines			49.8	51.2	M+FA-H	C11H13NO2	0.837015484	8964.218789	8961.453116	9012.141125	9589.872229	7343.793527	8305.544135	12449.74149	10385.23396	10416.52953
5.83_185.1184m/z	185.1183806	5.825	neg	2,6-Nonadien-1-ol	HMDB0031262	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		49.8	54.3	M+FA-H	C9H16O	0.446416789	2215.39646	2334.095027	2274.205443	3852.137436	2700.101734	2940.084216	2808.705514	2629.115235	2390.857184
5.85_423.0759m/z	423.0759033	5.84575	neg	Enterolactone 3'-sulfate	HMDB0240505	Unclassified	Unclassified	Unclassified			49.8	59.8	M+FA-H	C18H18O7S	0.995961915	21989.63157	24944.76824	25426.78545	4370.40361	3157.112065	3134.16178	593.1187018	467.4948605	516.6968925
7.24_357.0620m/z	357.0619962	7.237866667	neg	PSORBIC ACID	43642	Unclassified	Unclassified	Unclassified			49.8	51.6	M-H	C18H14O8	1.036221885	29157.96753	21152.06238	19221.97191	29233.31128	23390.20336	21416.83135	23178.75372	21131.02085	22685.92171
7.35_567.3181m/z	567.3180629	7.346316667	neg	(3alpha,5beta,7alpha)-23-Carboxy-7-hydroxy-24-norcholan-3-yl-beta-D-Glucopy	HMDB0243600	Unclassified	Unclassified	Unclassified			49.8	57.9	M-H	C30H48O10	1.040921993	64317.47988	68173.64555	64764.49662	10859.35585	10950.524	10707.13907	27543.4456	33502.08998	35831.92942
1.27_189.0406m/z	189.0406411	1.26875	neg	2-O-Methylascorbic acid	HMDB0240294	Organoheterocyclic compounds	Dihydrofurans	Furanones			49.7	50.5	M-H	C7H10O6	0.944640243	24811.83448	31724.13936	35803.98697	51104.38158	48450.95728	47906.94783	28188.21664	33867.21759	32142.05495
2.07_245.1143m/z	245.1143356	2.070366667	neg	Glutamylvaline	HMDB0028832	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		49.7	51.4	M-H	C10H18N2O5	0.163842702	14765.89409	16589.19567	16965.14357	29668.87776	33083.56689	32526.51984	22596.50165	21657.7789	22226.00069
5.53_339.1087m/z	339.1086909	5.525416667	neg	trans-isoeugenol-O-glucuronide	HMDB0060021	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		49.7	52.4	M-H	C16H20O8	0.440173133	392049.6106	331039.0363	335670.0957	116019.7858	151205.7504	127937.5492	279872.9775	287912.8451	342341.8626
2.07_245.1143m/z	245.1143356	1.3958	neg	3-Methyluridine	HMDB0001886	Organoheterocyclic compounds	Pyrimidine nucleosides	Imidazopyrimidines	**	C16357	49.6	51.7	M+FA-H	C10H14N2O6	1.036307941	6914.814439	5513.343357	6003.512418	13336.88384	11923.28643	10685.32526	10118.64975	9546.753261	9286.780657
4.16_269.0668m/z	269.0668427	4.15895	neg	Phenyl glucuronide	1825	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		49.6	51.3	M-H	C12H14O7	0.615794844	8575.477352	8526.911294	8741.51106	10921.78598	7498.758942	8906.922127	14724.72224	10730.04767	11203.00452
4.54_250.0723m/z	250.0722616	4.54425	neg	4-Hydroxy-3-methoxy-cinnamoylglycine	HMDB0059747	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		C02564	49.6	51.7	M-H	C12H13NO5	0.659250465	11238.2968	11552.96058	12515.51228	8826.726444	8478.750618	8155.089681	8489.983035	8529.660565	9984.627132
4.79_351.0957n	350.0884143	4.792316667	neg	Indole-3-acetic-acid-O-glucuronide	HMDB0060001	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		49.6	52.8	M-H, 2M-H	C16H17NO8	0.780925824	153191.7259	168458.3003	164084.6768	251882.5431	248890.0916	244770.1302	132049.5639	146328.5416	140893.4973
5.19_211.0614m/z	211.0614022	5.1031	neg	Eudesmol	4069	Benzenoids	Benzene and substituted derivatives	Benzenediols	*		49.6	52.2	M-H	C10H12O5	0.967209423	4782.974646	4591.583392	4815.616573	8325.130608	7772.108197	8599.81072	7338.991145	5607.795829	6231.360811
5.27_611.2690m/z	611.2690371	5.271716667	neg	Canescein	HMDB0029313	Organoheterocyclic compounds	Isobenzofurans	Unclassified	*		49.6	56.7	M+FA-H	C29H42O11	-3.316387417	34514.33445	24742.69372	26267.80721	20731.10172	22279.79604	21873.69358	30655.46515	23331.41981	29188.02042
6.11_211.0978m/z	211.0977732	6.113516667	neg	2-Hydroxy-p-mentha-1,8-dien-6-one	HMDB0037012	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		49.6	51.9	M+FA-H	C10H14O2	1.14753723	7835.891613	8838.040323	8873.533104	9614.62622	10396.85321	10252.01781	6407.795375	7214.924624	7304.308206
8.29_489.2709m/z	489.2709052	8.294766667	neg	12-O-D-Glucuronoside-13-hydroxyoctadec-9Z-enoate	HMDB0060119	Lipids and lipid-like molecules	Saccharolipids	Unclassified	*		49.6	51.3	M-H	C24H42O10	0.783376903	143839.9667	164449.9818	173067.1998	157562.7095	136231.6618	142721.2539	132665.69	153326.2862	149992.8539
5.01_461.0727m/z	461.0726996	5.014716667	neg	Kaempferol 3-glucuronide	LMPK12111843	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	*		49.5	52.7	M-H	C21H18O12	0.32463743	4958.840682	4942.929838	5238.018345	22421.7653	23544.92662	24924.92838	9289.659661	9102.632626	9777.456414
5.06_255.0825m/z	255.0825397	5.05975	neg	Tyrosyl glucuronide	HMDB0240563	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			49.5	51.6	M+FA-H	C15H19NO8	0.879104541	21265.09059	21363.47514	21737.61412	4514.199778	4413.039106	4753.658228	25725.59995	24575.82332	24500.01778
5.30_617.1487m/z	617.1486645	5.302883333	neg	Rhamnazin 3-[6''-(3-hydroxy-3-methylglutaryl)glucoside]	LMPK12112636	Lipids and lipid-like molecules	Polyketides	Flavonoids			49.4	56.7	M+2O-H	C29H32O16	-3.975806101	17144.27341	16062.18757	16997.62316	0.001403199	161.7381735	0.001403199	1670.059788	991.0997772	1710.467185
5.57_199.0977m/z	199.0977156	5.57225	neg	5,7-nonadienoic acid	LMFA01030450	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			49.4	49.5	M+FA-H	C9H14O2	0.863043765	20292.42078	17951.85807	18502.78861	24289.56987	27692.81126	28130.14625	19145.14182	17209.69264	17965.4149
15.05_165.0409m/z	165.0408561	15.05453333	neg	S-Propyl 1-propanesulfinothioate	HMDB0034394	Organic acids and derivatives	Thiosulfinic acid esters	Unclassified			49.3	55.7	M-H	C6H14OS2	-2.857982706	32919.32838	158369.9305	18586.42073	103660.9678	51079.8735	23296.07163	135230.7162	16759.14953	18439.37852
4.16_252.0878m/z	252.0878353	4.15895	neg	N-lactoyl-Tyrosine	HMDB0062177	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			49.3	49.8	M-H	C12H15NO5	0.352063189	6211.59683	6104.384533	6381.488164	6022.01131	4272.24666	4364.404557	9384.11241	7022.73761	6785.789966
4.99_213.1239m/z	213.1239224	4.99225	neg	9-hydroxy-palmitic acid	LMFA01060028	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			49.3	48.7	M-H	C16H32O3	0.718590738	25967.19195	25247.03518	25917.6419	21730.75891	21641.26654	22431.7315	26142.18938	22685.92373	21861.1804
7.35_401.0880m/z	401.0880017	7.353466667	neg	Dihydrohydroxy-O-methylstergimatocystin	HMDB0033659	Phenylpropanoids and polyketides	Sterigmatocystins	Unclassified			49.3	50.4	M+FA-H	C19H16O7	0.550406694	146522.3129	138084.6498	123400.4931	129718.5332	143945.5864	139235.4194	148882.5535	140822.6093	148197.8977
4.43_233.0126m/z	233.0125525	4.432683333	neg	o-Cresol sulfate	HMDB0240655	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates			49.2	48.3	M-H	C7H8O4S	0.105755244	52211.68345	57564.1746	57804.07223	10701.17046	9908.602133	9751.624701	46830.68837	54565.73757	51742.09921
4.79_209.0457m/z	209.0456757	4.792316667	neg	5-Hydroxyferulic acid	HMDB0035484	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	**	C05619	49.2	48.7	M-H	C10H10O5	0.612699398	90409.45052	86305.34597	85095.78388	90741.28399	98124.36781	100027.7923	107515.5967	93917.8733	94838.10348
4.88_163.0402m/z	163.0401989	4.880083333	neg	m-Coumaric acid	HMDB0001713	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	***	C12621	49.2	50.2	M-H	C9H8O3	0.799640437	2435.745882	2556.879018	2707.911482	965.3991184	903.2983746	1003.625565	1703.926381	1771.001986	1905.701101
5.72_203.1282m/z	203.1282936	5.727283333	neg	3,10-dihydroxydecanoic acid	LMFA01050429	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			49.2	48.8	M-H	C10H20O4	0.053261404	7208.37995	7693.054946	6457.270319	5233.767726	4790.054208	5078.653615	8312.744883	7551.759302	4604.067606	5250.66685	5731.876919
1.80_202.0723m/z	202.0722972	1.798266667	neg	N-Acetylproline	HMDB0094701	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			49.1	49	M+FA-H	C7H11NO3	1.280174662	5481.092695	5208.51339	5577.775119	5443.748521	5423.446702	6150.62695	5359.021262	6028.737625	5654.969429
5.89_138.0197m/z	138.019716	5.894166667	neg	4-Nitrophenol	4100	Benzenoids	Benzenoids	Nitrophenols	*	C00870	49.1	51	M-H	C6H5NO3	0.355529708	3710.479252	3230.668742	3508.065615	3148.381234	3874.524822	3604.376592	3920.886599	3822.793406	4251.525363
5.91_517.1355m/z	517.1354617	5.908066667	neg	Medicarpin 3-O-(6''-malonylglucoside)	HMDB0038776	Phenylpropanoids and polyketides	Isoflavonoids	Furanoisoflavonoids			49.1	48.9	M-H	C25H26O12	0.601914156	72705.22567	86448.46558	78156.5948	70297.94641	84553.46118	70920.11322	22345.38392	27090.89682	29164.73398
5.99_196.0253m/z	196.0252606	5.9916	neg	3-Hydroxy-2-methylpyridine-4,5-dicarboxylate	HMDB0006955	Organoheterocyclic compounds	Pyridines and derivatives	Pyridinecarboxylic acids and derivatives	**	C04604	49.1	49.5	M-H	C8H7NO5	0.581935985	8281.642657	2449.916802	4122.405554	803.5873279	1051.434516	4549.883523	1027.64032	1068.138013	4781.726302
5.44_429.0829m/z	429.0829237	5.44425	neg	Daidzein 4'-glucuronide	HMDB0041717	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		49	50.2	M+FA-H	C21H18O10	0.472898993	10476.45905	9772.748232	9421.445266	10876.49802	10416.65943	11041.70292	206.7174511	195.6644987	192.1196455
4.73_243.1350m/z	243.1350345	4.725416667	neg	Hydroxyprolyl-Leucine	HMDB0028867	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		49	54.9	M-H	C11H20N2O4	0.015468928	33009.68965	32710.08828	34895.4468	73305.36004	73673.82686	73166.07678	35410.53309	39096.534	38255.53727
5.36_255.1240m/z	255.1239718	5.361783333	neg	2-furan-octanoic acid	LMFA01150037	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			49	49.8	M+FA-H	C12H18O3	0.83021591	7136.553418	7605.510597	8436.319678	6553.061083	8312.744883	7551.759302	4604.067606	5250.66685	5731.876919
6.46_435.2243m/z	435.2242673	6.458366667	neg	(3S,5R,6S,7E,9x)-7-Megastigmene-3,6,9-triol 9-glucoside	HMDB0041176	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		49	49.1	M+FA-H	C19H34O8	1.784580559	16495.12038	14590.09054	16951.36484	18561.26141	15257.38949	16769.16714	19639.73183	20258.46369	19914.83155
6.69_267.1239m/z	267.1239432	6.69475	neg	3,4-dimethyl-5-carboxyethyl-2-furanpentanoic acid	LMFA01150055	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			49	50.1	M-H	C14H20O5	0.544248201	5132.177139	6063.456119	6107.867302	7135.577701	6801.002593	6892.502722	4925.222263	6066.059598	6328.953504
0.86_254.9816m/z	254.9816395	0.86335	neg	Ascorbic acid 2-sulfate	HMDB0240641	Organic oxygen compounds	Organooxygen compounds	Dihydrofurans	*		48.9	48.6	M-H	C6H8O9S	0.050992854	21288.6979	23998.3512	25811.4759	553953.4736	504464.9808	523868.1543	29166.7244	35878.64133	29846.4222
2.92_168.0303m/z	168.0302916	2.9156	neg	2-Furoylglycine	5428	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		48.9	47.1	M-H	C7H7NO4	0.356648469	29081.10344	29872.4391	32038.70456	21478.9165	20085.6907	21959.84151	20644.63308	21707.51133	20289.96443
3.48_378.1034m/z	378.1033598	3.484883333	neg	Hyaluronan biosynthesis, precursor 1	HMDB0060071	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		C04794	48.9	52.2	M-H	C14H21NO11	-2.174088528	17164.77403	21393.32552	21432.03262	27535.58374	23506.03747	24778.84578	22215.09817	22055.67371	21687.47634
3.91_214.1087m/z	214.1087043	3.912566667	neg	2-amino-8-oxo-9,10-epoxy-decanoic acid	LMFA01060176	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates		C12027	48.9	49.1	M-H	C10H17NO4	1.035248964	3797.35949	3876.262239	4319.295275	2828.860964	2351.164168	2617.947127	3447.597577	3650.584692	3675.620934
3.34_203.0927m/z	203.092621	3.344733333	neg	Mycinonic acid I	LMFA01020402	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			48.9	47.5	M+FA-H	C8H14O3	0.97977752	2040.828503	2343.359715	2415.882985	2931.387622	2398.504344	2462.446771	1733.040975	2297.327641	2087.032566
5.10_192.0688m/z	192.0687183	5.1031	neg	4-Methylquinic acid	64936	Benzenoids	Benzene and substituted derivatives	Benzenediols	*		48.9	51.1	M-H	C10H11NO3	1.043491322	1890.960255	1785.953249	1766.333887	2398.003195	2657.637116	2883.232099	3294.753362	2792.740834	3110.367486
6.03_353.0339m/z	353.0339325	6.028183333	neg	cis-Resveratrol 4'-sulfate	HMDB0041714	Phenylpropanoids and polyketides	Stilbenes	Unclassified	*		48.9	51.9	M+FA-H	C14H12O6S	0.878324178	20010.20029	20510.88257	22400.38764	0.001403199	0.001403199	0.001403199	1078.722658	1193.87655	1268.148284
8.61_489.2709m/z	489.2708905	8.606866667	neg	9-Hydroxy-10-O-D-glucuronoside-12Z-octadecenoate	HMDB0060121	Lipids and lipid-like molecules	Saccharolipids	Unclassified	*		48.9	47.8	M-H	C24H42O10	0.75344944	154281.9657	158003.2577	152794.0425	180843.9289	167270.8278	176538.9785	161615.9533	168029.9507	156612.9262
4.37_369.0287m/z	369.0286842	4.367166667	neg	Catechin 3'-sulfate	HMDB0240485	Phenylpropanoids and polyketides	Flavonoids	Flavans			48.8	50.7	M-H	C15H14O9S	0.290882731	37447.26474	39477.30977	42121.52652	26505.2851	20377.53559	21939.4901	24175.59177	31001.43924	28711.19263
4.50_157.0508m/z	157.0508441	4.49225	neg	Parasorbic acid	HMDB0031801	Unclassified	Unclassified	Unclassified			48.8	48.9	M+FA-H	C9H8O2	0.461647467	8813.63398	1013.532098	945.2765219	691.3752443	589.711037	741.8413768	2144.640216	2236.771019	2093.538026
4.86_379.1613m/z	379.1612673	4.858383333	neg	Prenyl arabinofuranosyl-(1->6)-glucoside	HMDB0041360	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids	**	C00164	48.6	48.6	M-H	C16H28O10	0.780375182	125159.0374	130439.6266	140318.8606	146529.9962	147958.431	148594.7331	150206.378	169549.9473	158787.44919
4.97_471.1852m/z	471.1852371	4.969683333	neg	11,13-Dihydrotaraxinic acid glucosyl ester	HMDB0035867	Lipids and lipid-like molecules	Saccharolipids	Unclassified	*		48.8	58.3	M+FA-H	C21H30O9	-4.571522953	8405.668114	8719.29363	8592.275911	7498.69011	7323.885375	7388.607514	11922.5095	10780.15262	10176.73699
6.66_255.1240m/z	255.1239524	6.663683333	neg	Sedanonic acid	HMDB0032871	Organic acids and derivatives	Keto acids and derivatives	Gamma-keto acids and derivatives			48.8	46.7	M+FA-H	C12H18O3	0.73845852	8970.312055	10213.57508	10233.11177	6063.582464	5850.431264	5388.214439	3411.701511	4153.645294	4270.030912
3.13_215.1038m/z	215.1038139	1.534483333	neg	Etiracetam	HMDB0252105	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		C07841	48.7	44.1	M+FA-H	C8H14N2O2	0.489713098	17618.44154	14709.26028	15515.00126	14524.70203	13432.93928	13841.11623	15146.88398	17965.48849	16252.28916
2.14_299.0636m/z	299.0635265	2.140766667	neg	beta

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1.25_206.0494m/z	206.0494358	1.246333333	neg	(2R,2'S)-Isobuteine	HMDB0030411	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		43.9	33.9	M-H	C7H13NO4S	0.885489524	6423.415602	7225.230486	7364.462417	4043.113891	4106.035122	3973.580248	4231.681904	4746.769715	4519.675073
6.10_433.2083m/z	433.2082724	6.101316667	neg	5a,6a-Epoxy-7E-megastigmene-3b,9e-diol 9-glucoside	HMDB0038306	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		43.9	22.3	M+FA-H	C19H32O8	0.905612439	50665.39506	59285.8212	59092.62485	44136.45004	51840.6083	45684.12358	49668.58552	55721.0564	59748.59579
6.18_295.1665m/z	295.1664596	6.181866667	neg	3-Hydroxylidocaine	HMDB0060655	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C16560	43.9	24.1	M+FA-H	C14H22N2O2	0.514894281	6025.511502	6321.552338	6753.640554	11106.62189	10829.54848	11965.57025	6084.822037	7493.93544	7891.542729
7.55_511.2915m/z	511.29146	7.547766667	neg	(S)-Nerolidol 3-O-[a-L-rhamnopyranosyl-(1->2)-b-D-glucopyranoside]	HMDB0040844	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		43.9	21.7	M-H2O-H	C27H46O10	0.38372878	131498.8523	140210.663	137402.8048	182695.0597	179032.7558	176210.1816	120599.97596	129419.6845	128421.6907
1.16_173.0568m/z	173.0567732	1.160166667	neg	Formiminoglutamic acid	HMDB0000854	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00439	43.8	22.8	M-H	C6H10N2O4	-0.04147438	8829.580644	9517.586744	9909.143944	12196.13005	12009.28171	11359.21343	10689.8863	11163.60356	11181.32411
1.49_133.0507m/z	133.0507102	1.492933333	neg	2,3-Dihydroxy-2-methylbutanoic acid	HMDB0029576	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		43.8	21.4	M-H	C5H10O4	0.580545007	4754.324036	4913.788779	5519.903912	3766.12204	3588.874925	3492.474607	4538.404342	4403.759094	4408.363775
1.80_143.0350m/z	143.0349764	1.798266667	neg	2(R)-Hydroxyadipic acid	HMDB0000368	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		43.8	22.7	M-H2O-H	C6H10O5	-0.03632602	2602.716527	2417.377494	2776.50851	2481.068821	2489.165186	2644.007582	2506.834432	2858.836058	2618.297395
2.11_137.0244m/z	137.0244264	2.114866667	neg	Salicylic acid	HMDB0001895	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	***	C00805	43.8	23.3	M-H	C7H6O3	0.063345876	3894.583517	4192.342972	4115.891671	4511.225736	4683.634672	5061.633986	4569.820046	4033.08078	4433.194358
4.19_325.0931m/z	325.093136	4.189783333	neg	1-O-p-Coumaroyl-beta-D-glucose	HMDB0036936	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives			43.8	24.6	M-H	C15H18O8	0.751020873	11519.89822	9244.436535	10019.54313	5990.557568	5490.820638	7547.094713	7761.325065	5994.683197	5923.403425
4.48_267.0866m/z	267.0866396	4.477166667	neg	2,3-Dihydro-3-hydroxy-6-methoxy-2,2-dimethyl-4H-1-benzopyran-4-one	HMDB0041379	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans			43.8	27.1	M+FA-H	C12H14O4	-3.476768014	3090.342159	3548.459003	3394.700241	2583.405336	2448.94761	2652.954742	3443.445008	3887.170019	3692.214146
4.75_213.0770m/z	213.0770411	4.747466667	neg	Epoxyscopolorone	HMDB0032252	Organoheterocyclic compounds	Oxepanes	Unclassified	*		43.8	22.5	M-H-H	C9H12O3	1.153912798	10834.12021	10771.38699	11331.01497	10628.69808	10480.94635	10183.41522	13011.03936	13294.55596	13598.33916
0.78_181.0719m/z	181.0718771	0.778533333	neg	Dulcitol	4179	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C01697	43.7	24.8	M-H	C6H14O6	0.633622757	8880.484329	7517.730855	8747.000213	5871.709008	6332.412137	5372.455185	5443.815019	7997.13462	7273.93387
0.88_145.0375n	144.0302629	0.884633333	neg	2-Keto-glutaramic acid	HMDB0001552	Organic acids and derivatives	Keto acids and derivatives	Short-chain keto acids and derivatives	**	C00940	43.7	29.4	M-H2O-H, M-H	C5H7NO4	0.179755286	11555.46309	12314.86263	12316.72079	12235.08333	11168.47234	12108.29579	12063.9015	11929.29122	11963.70913
2.42_144.0666m/z	144.0666663	2.415216667	neg	2-Amino-4-ethoxy-3-hydroxybutanoic acid	HMDB0032862	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			43.7	21.8	M-H2O-H	C6H13NO4	0.303355657	5999.521334	6229.384536	7051.60923	7942.272316	7247.128581	7087.258834	6906.85086	7947.944324	6918.953188
3.13_117.0557m/z	117.0557412	3.131933333	neg	5-Hydroxypentanoic acid	HMDB0061927	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates		C02804	43.7	21.1	M-H	C5H10O3	0.198980337	10025.30076	10358.32205	10521.52435	16234.04895	15296.82727	14865.76481	12531.72825	13416.74358	12725.68966
3.15_216.9812m/z	216.9812451	3.153616667	neg	4-hydroxybenzoic acid-4-O-sulphate	HMDB0059982	Organic oxygen compounds	Organic sulfuric acids and derivatives	Arylsulfates	*		43.7	31.6	M-H	C7H6O6S	0.057767544	14107.23095	14388.26567	15116.66545	11653.34805	10589.63121	10737.86771	13863.23568	15788.88432	14610.53072
4.11_217.1082m/z	217.1082361	4.113883333	neg	(3S,6S)-3-Hydroxy-1,7-dioxaspiro[5.5]undecane	LMPK09000006	Unclassified	Unclassified	Unclassified			43.7	21.8	M+FA-H	C9H16O3	0.516482733	7803.486935	8117.630458	8848.139477	6515.593089	6277.338371	6353.418025	7076.170454	7003.33201	6802.050552
4.57_302.1149m/z	302.1148729	4.5668	neg	Carmofur	HMDB0249685	Unclassified	Unclassified	Unclassified			43.7	26.5	M+FA-H	C11H16FN3O3	-3.498690106	7964.169059	8275.284503	8136.068422	16243.33328	15849.06387	14980.12736	8707.24065	9334.390386	8994.297592
4.97_449.2033m/z	449.2032893	4.969683333	neg	Pisumionoside	HMDB0039947	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		43.7	21.1	M+FA-H	C19H32O9	1.122752162	26172.10831	25940.56891	28852.39633	25401.79482	27026.43138	23334.32682	38272.04194	36339.27758	34618.07964
5.26_375.1663m/z	375.1663314	5.263033333	neg	6-Hydroxy-2-bornanone glucoside	HMDB0034558	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		43.7	25.8	M+FA-H	C16H26O7	0.833929232	17406.89809	16313.7785	16147.56424	21457.23562	20217.67151	20455.1492	16836.20079	14931.04115	18440.29215
6.59_469.2082m/z	469.2082169	6.592933333	neg	4-(5'-((E,3E,5E,9Z)-dodeca-1,3,6,9-tetraen-1-yl)-[3,3'-bi(1,2-dioxolan)]-5-yl)-4-(	LMFA04060002	Lipids and lipid-like molecules	Fatty Acyls	Docosanoids	*		43.7	21.6	M-H-H	C22H32O8	0.697920106	64353.29885	66883.89732	66408.34157	17278.93045	17836.65091	17007.76191	43258.40407	51836.14624	48927.3825
6.66_157.0870m/z	157.0870494	6.663683333	neg	trans-2-trans-4-Heptadien-1-ol	HMDB0032301	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		43.7	20	M+FA-H	C7H12O	0.281246149	9435.767095	9710.898141	9781.780724	14008.75896	13793.51373	11351.40831	11564.49646	12603.3359	12963.04978
6.68_198.1137m/z	198.11367	6.680966667	neg	psi-Pelletierine	HMDB0034580	Organoheterocyclic compounds	Piperidines	Piperidinones		C10865	43.7	21	M+FA-H	C9H15NO	0.67311386	2414.703969	3001.649179	2950.811227	6056.366102	6209.799266	5274.020849	2440.136467	2741.702493	2845.464059
4.54_230.0130m/z	230.0129955	4.54425	neg	Norepinephrine sulfate	HMDB0002062	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		43.6	28.7	M-H2O-H	C8H11NO6S	0.51608552	1914.710463	2183.890781	2311.715652	1978.18693	2003.934314	1939.183989	2291.942269	2594.597349	2465.297915
4.61_467.1836m/z	467.1835805	4.611883333	neg	4'-Hydroxycarvedilol	HMDB0013947	Organoheterocyclic compounds	Indoles and derivatives	Carbazoles			43.6	29.5	M+FA-H	C24H26N2O5	2.855778188	17875.82405	19106.66739	18840.33246	14615.56966	14584.92458	12902.05322	18919.18626	17586.06006	21630.887
4.68_327.0722m/z	327.0722314	4.682483333	neg	6-[3-(carboxymethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic acid	HMDB0125161	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		43.6	20.9	M-H	C14H16O9	0.505341911	9096.403031	10128.85071	11295.44063	6536.691317	5375.021964	6642.892212	12258.28337	12634.4477	11437.33527
5.04_203.1290m/z	203.1289685	5.037216667	neg	Isovaleric acid	LMFA01020181	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C08262	43.6	20.3	2M-H	C5H10O2	0.420199189	3413.456142	3621.010655	3512.229793	3762.042242	4001.622081	4416.186827	2910.92089	3293.655662	3239.267927
0.78_369.0845m/z	369.0845068	0.778533333	neg	Ferulic acid 4-O-glucuronide	HMDB0041733	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		43.5	30.5	M-H	C16H18O10	4.827045197	70045.41385	79092.94708	77765.30049	70161.52638	144212.2451	83529.37595	80043.70837	91700.72797	104232.0975
3.11_232.9762m/z	232.9762164	3.112733333	neg	2-hydroxy-3-(sulfooxy)benzoic acid	HMDB0134105	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		43.5	25.2	M-H	C7H6O7S	0.296333699	15277.281	16524.63772	17880.29536	2350.235168	2249.645331	2102.132596	9615.997219	11256.15096	11011.0929
4.02_285.0618m/z	285.061781	4.024283333	neg	Catechol glucuronide	HMDB0240490	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		43.5	21.8	M-H	C12H14O8	0.664354047	1383.03799	1715.135022	1505.190697	381.0668397	626.1934907	610.5720455	2229.79767	2520.64855	2484.019844
4.26_228.1241m/z	228.1241137	4.2568	neg	Methyprylon	HMDB0015239	Organoheterocyclic compounds	Piperidines	Piperidinones			43.5	20.7	M+FA-H	C10H17NO2	0.098301032	21060.22107	23271.93724	24107.71242	1535.345714	1464.388983	1191.937505	1945.567375	2243.307781	2078.520125
4.37_402.1164n	383.0985387	4.367166667	neg	4-Hydroxy-5-(3',4'-dihydroxyphenyl)-valeric acid-O-glucuronide	HMDB0059971	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		43.5	25.3	M-H2O-H, M-H	C17H22O11	0.418417142	17998.46433	17733.85437	20428.9433	7748.009734	6231.139157	6357.852154	21561.54838	25015.61152	23663.64887
5.18_485.1668m/z	485.1668176	5.1777	neg	(S)-Multifidol 2-[apiosyl-(1->6)-glucoside]	HMDB0039930	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			43.5	19.7	M-H2O-H	C22H32O13	0.72914138	86859.19093	101134.122	97198.85539	98303.59634	95398.3323	95111.24426	88699.67542	93831.21227	95876.27236
5.63_137.0244m/z	137.0244421	5.628083333	neg	Ascladiol	HMDB0029610	Organoheterocyclic compounds	Dihydrofurans	Furanones	*		43.5	22.2	M-H2O-H	C7H8O4	0.156772046	6525.926528	5614.68009	6331.520216	2894.577416	3191.656866	3116.644471	4139.403875	3478.949448	3758.607077
7.65_207.1392m/z	207.1391645	7.65305	neg	Hexylbenzene	HMDB0061815	Benzenoids	Benzene and substituted derivatives	Unclassified			43.5	20.3	M+FA-H	C12H18	0.68482069	4845.622765	5345.510878	5369.195458	2873.647632	2592.999638	2928.776421	4224.433248	4441.673147	4821.864489
0.76_118.0511m/z	118.0510711	0.757316667	neg	Hydroxyethyl glycine	HMDB0061148	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		43.4	20.2	M-H	C4H9NO3	0.876593994	1840.176029	808.6224215	439.8268575	914.7801085	446.1446918	1961.834741	519.1261661	1132.381835	279.994323
2.03_433.1231m/z	433.123095	2.025516667	neg	Sulfinpyrazone sulfide	HMDB0060943	Organosulfur compounds	Thioethers	Aryl thioethers	*		43.4	29.9	M+FA-H	C23H20N2O2S	0.884269391	11995.41765	13547.09633	13668.78395	23903.75904	22302.21334	22018.1962	16270.80402	19573.90045	15446.50236
2.14_165.0418m/z	165.0417952	2.140766667	neg	1-METHYLXANTHINE	44228	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	**	C16358	43.4	23.6	M-H	C6H6N4O2	-0.023213068	51273.24253	56680.14291	56378.56024	105240.2951	98814.04251	101463.6685	82717.5778	85830.03288	96280.85199
4.02_313.0569m/z	313.0568691	4.024283333	neg	Beta-D-Glucopyranuronic acid	HMDB0010314	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		43.4	22.4	M-H	C13H14O9	1.157434477	5489.922348	5989.442159	5593.081348	8305.5105748	667.1971869	596.8966549	959.5585935	1270.261435	995.6429831
4.16_371.0985m/z	371.0985268	4.1595	neg	Melilotoside	HMDB0035251	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides		C05158	43.4	21.5	M+FA-H	C15H18O8	0.479503861	10294.36133	10584.65005	10450.36424	15085.35451	9318.556377	10944.05927	9960.839865	7696.946414	7919.387984
4.23_341.0880m/z	341.0880324	4.234483333	neg	rhamnetin 3-rhamninoside	HMDB0304579	Lipids and lipid-like molecules	Polyketides	Flavonoids			43.4	22.2	M+FA-H	C14H16O7	0.765628886	13108.6023	13135.0936	13887.81741	5232.86263	3895.807945	4203.142491	7197.712013	7442.166445	7006.980066
4.39_371.0985m/z	371.0984531	4.3893	neg	cis-Melilotoside	HMDB0060077	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		C05839	43.4	19.9	M+FA-H	C15H18O8	0.253731961	29952.03792	29650.14659	29976.60138	39184.4293	35422.86258	35771.4333	27994.5305	32694.43652	30979.18366
4.84_373.1143m/z	373.1142725	4.836566667	neg	Ethylvanillin glucoside	HMDB0037682	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			43.4	21.4	M+FA-H	C15H20O8	0.76797363	28150.76574	28712.81898	29363.27329	38029.36112	37127.53479	37549.50987	42136.63605	47152.97892	46256.97807
5.08_445.1866m/z	445.1865898	5.080566667	neg	Estrone 3-glucuronide	43173	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	**	C11133	43.4	32.2	M-H	C24H30O8	-0.451959467	11065.50404	11524.9522	10976.20878	21792.16945	19280.85213	22529.35671	13067.83461	12091.16618	12900.53736
6.82_167.0705m/z	167.0705139	6.825	neg	5-Perhydrofuro-2-oxo-3-furancarboxylic acid	HMDB0030989	Organic oxygen compounds	Lactones	Gamma butyrolactones	*		43.4	20.6	M+FA-H	C10H16O4	0.508443598	24170.89848	24619.52972	25177.99508	2274.971322	1057.99608	2462.024483	4355.65057	5575.170995	5167.477841
6.92_374.2551m/z	374.2550693	6.915966667	neg	Undecanoylcamitine	LMFA07070110	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		43.4	27.7	M+FA-H	C18H35NO4	0.783142972	19808.44411	19915.58061	17148.19867	19128.96133	20266.36229	18163.25986	20654.70646	20558.32185	21392.06758
7.15_222.1137m/z	222.1137061	7.147366667	neg	2,3,6,7-Tetrahydro-6,7-dimethylcyclopent[b]azepin-8(1H)-one	HMDB0039667	Organoheterocyclic compounds	Azepines	Unclassified	*		43.4	18.9	M+FA-H	C11H15NO	0.785376023	27400.59579	30539.85932	29333.86851	46838.52195	50111.9762	44188.77651	30921.9169	38818.84294	36473.00671
2.65_230.0129m/z	230.0129497	2.651566667	neg	Paracetamol sulfate	HMDB0059911	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		43.3	26.9	M-H	C8H9NO5S	0.357962998	1758.008711	1862.103739	1568.357355	13338.96973	12181.99593	11992.56684	1580.213146	1845.331528	2017.541088
3.28_125.0243m/z	125.024325	3.280233333	neg	Hydroxyhydroquinone	506	Benzenoids	Phenols	Benzenediols and derivatives	**	C02814	43.3	19.3	M-H	C6H6O3	-0.734504503	32511.66545	34085.25674	33530.01502	6850.726892	6410.937877	6382.030993	27554.4884	30834.13889	30196.47889
3.89_282.9696m/z	282.9696	3.8906	neg	Ellagic acid	HMDB0002899	Phenylpropanoids and polyketides	Tannins	Hydrolyzable tannins	*	C10788	43.3	20.4	M-H2O-H	C14H6O8	3.761535793	6284.15044	6699.11656	7253.188814	6258.219111	6088.09055	5769.09578	5354.541909	6089.695032	6933.824817
4.92_150.0561m/z	150.0560748	4.92485	neg	Dopamine quinone	HMDB0012219	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C17755	43.3	19.8	M-H	C8H9NO2	0.150080519	3454.738279	3991.646515	3894.482268	483.3972946	524.3959369	394.1828136	703.4317862	834.8271216	874.3388482
6.07_387.1664m/z	387.1663848	6.07	neg	Jasmolone glucoside	HMDB0032870	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		43.3	20.7	M+FA-H	C17H26O7	0.960814137	79061.75547	88657.01106	87270.13834	66602.4001	69739.84113	60199.84959	80453.7123	81370.78071	81397.51738
7.55_579.2792m/z	579.279157	7.547766667	neg	Corchoroside A	HMDB0033846	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid lactones	*		43.3	24.9	M+FA-H	C29H42O9	-3.60998084	35382.39076	38262.85878	37889.1655	48501.58506	48737.67972	47457.55453	33179.28221	36467.90853	34859.16807
0.80_339.0739m/z	339.0738984	0.800366667	neg	Dihydrocaffeic acid 3-O-glucuronide	HMDB0041720	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		43.2	27.7	M-H2O-H	C15H18O10	4.866807701	155997.5797	159458.3169	149706.4678	120019.4989	156170.278	137180.4701	150542.1599	199145.3807	188932.3735
1.48_375.1296m/z	375.1296398	1.480083333	neg	Pseudomonine	HMDB0044138	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			43.2	24.8	M+FA-H	C16H18N4O4	1.235551044	43579.7426	35828.72204	36142.30331	47795.41464	47181.02819	48039.73995	37322.573	38244.59232	37604.79301
4.92_535.1467m/z	535.146682	4.92485	neg	Isoorientin 7,3',4'-trimethyl ether	LMPK12111058	Lipids and lipid-like molecules	Polyketides	Flavonoids			43.2	20.9	M+FA-H	C24H26O11	1.973769087	28821.11286	29748.16807	28286.84629	237.8718076	407.0859623	0.001403199	2384.380317	1862.794784	3106.028343
4.95_273.1346m/z	273.1345855	4.94705	neg	9,12-dioxo-dodecanoic acid	LMFA01060092	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			43.2	19.2	M+FA-H	C12H20O4	0.97959946	6655.676165	6859.187054	6793.679297	6962.69508	7072.293765	7023.32462	5285.106138	5139.837601	5038.110471
5.83_462.1774m/z	462.1773806	5.825	neg	Etodolac acyl glucuronide	HMDB0060916	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		43.2	20.4	M-H	C23H29NO9	0.918602819	12720.82959	14385.24646	13658.68398	46214.40028	38385.92616	38839.62014	39379.43154	39692.44277	42252.41364
0.88_176.0321m	351.0570953	0.884633333	neg	D-Glucurono-6,3-lactone	HMDB0006355	Organoheterocyclic compounds	Furofurans	Isosorbides	**	C02670	43.1	17.9	M-H, 2M-H	C6H8O6	-0.029206325	17198.62015	19527.29994	23357.51689	38347.52069	37661.49611	38376.71974	19460.73374	23346.89741	19742.97452
1.31_174.0073m/z	174.0772651	1.3134	neg	Vigabatrin	HMDB0015212	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		C07500	43.1	23.1	M-H	C6H11NO2	1.648217104	32614.70013	34220.38026	34715.55217	3196.598013	2898.788467	3038.605802	3110.643301	3241.15239	3143.387098
1.80_171.0664m/z	171.0664147	1.798266667	neg	3-(3-Ethyloxiranyl)-2-propenal	HMDB0034835	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds			43.1	19.6	M+FA-H	C7H10O2	1.049328559	9531.502434	9653.947549	9394.646349	3575.938603	3863.496825	3891.500124	4490.010496	4268.989525	4252.139194
4.28_483.9522m/z	483.9522285	4.278183333	neg	Gamitrinpe triphosphate	HMDB0060638	Organoheterocyclic compounds	Diazines	Pyrimidines and pyrimidine derivatives	*		43.1	20.3	M-H2O-H	C9H14F2N3O13P3	-1.360314692	46022.79301	44365.57492	44742.75271	2958.139847	2864.473639	2761.190945	40159.94225	42879.175	41655.58606
4.30_189.0769m/z	189.0769433	4.300033333	neg	5-aceto valeric acid	LMFA01060015	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			43.1	18.8	M+FA-H	C7H12O3	0.667661799	957.5796293	1135.423368	1179.741251	1561.410357	1394.866467	1414.546935	1235.216172	1201.659584	1170.209978
4.30_245.0126m/z	245.0126071	4.300033333	neg	3-[4-(sulfooxy)phenyl]propanoic acid	HMDB0125171	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		43.1	21.3	M-H	C9H10O6S	0.302987616	12168.31969	12196.59008	13532.84283	1973.361287	2136.973261	1476.824555	6154.28584	7235.97294	6673.728439
4.66_214.1299m/z	214.1298097	4.660483333	neg	trans-Menth-2-ene-1,4-diol	HMDB0037291	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		43.1	19.4	M+FA-H	C10H18O2	0.158611656	4224.813482	4013.917985	4794.628221	5699.445295	5366.466754	5911.304498	3797.472153	4015.867381	3930.659009
5.73_229.0177m/z	229.017694	5.727283333	neg	Polystyrene sulfonate	HMDB0015435	Benzenoids	Benzene and substituted derivatives	Benzenesulfonic acids and derivatives	*		43.1	22	M+FA-H	C8H8O3S	0.412920682	8956.847925	9990.317317	9599.31411	4965.2844	5422.727831	4821.210475	9029.767832	10788.94487	11079.05594
6.30_433.2082m/z	433.2082063	6.302033333	neg	Icariside B8	HMDB0036846	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		43.1	17.9	M+FA-H	C19H32O8	0.73517941	117005.4128	147837.1791	148711.5256	152153.8227	148592.3732	125597.3101	142826.3614	144658.5942	175856.4664
3.14_186.0772m/z	186.0772493	3.142483333	neg	N-(3-hydroxy-butanoyl)-homoserine lactone	LMFA08030029	Lipids and lipid-like molecules	Fatty Acyls	Fatty amides			43	19.9	M-H	C8H13NO4	0.362487089	5656.860788	5978.04405	6561.539023	3600.466996	3339.354399	3334.282193	5366.905154	5456.913846	5552.714306
6.07_165.0921m/z	165.0921088	6.07	neg	Isopropylbenzene	HMDB0034029	Benzenoids	Benzene and substituted derivatives	Cumenes		C14396	43	16.2	M+FA-H	C9H12	0.029400249	3351.541278	3842.956352	3722.0436	5937.924736	5903.152632	5293.921947	4226.674446	4411.678426	4358.498485
6.82_357.1167m/z	357.1194432	6.817666667	neg	Moringine	HMDB0031724	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		43	18.7	M+FA-H	C15H20O7	1.080914166	38160.9302	35322.0609	35340.0882	33900.5612	33992.9511	36857.56532	33249.31854	35486.86041	26219.61356
8.27_207.1028m/z	207.1027849	8.273616667	neg	Allixin	HMDB0040705	Organoheterocyclic compounds	Pyrans	Pyranones and derivatives			43	19.7	M-H2O-H	C12H18O4	0.517067754	6339.36441	6583.094235	6505.174218	6713.784133	6687.550189	6594.902599	7147.660349	6712.423936	6988.888472
1.45_160.0372n	319.0672734	1.4461	neg	3-oxo-adipic acid	LMFA01170096	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			42.9	21.5	M-H, 2M-H	C6H8O5	0.053989462	74521.13728	93153.49111	75079.63401	28384.241	23856.74659	25214.66094	32508.16352	23341.79248	27208.50009
2.36_329.0881m/z	329.0880766	2.36465	neg	Hydroxytyrosol 4'-glucuronide	HMDB0240531	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates			42.9	19.7	M-H	C14H18O9	0.820681101	10246.85623	10321.34319	10491.79219	0.001403199	0.001403199	49.13984489	8387.494213	9978.067517	10128.09443
2.62_232.9963m/z	232.9962466	2.622366667	neg	3,5-Dihydroxybenzoic acid sulfate	HMDB0240373	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates			42.9	22.5	M-H	C7H6O7S	0.425083964	10286.03324	10752.04185	12005.13772	1185.398863	1007.405069	982.1942811	5189.953974	5560.257201	5360.87231
4.26_239.9974m/z	239.997401	4.278183333	neg	2,8-Quinolinediol 8-sulfate	HMDB0240658	Organic oxygen compounds	Quinolines and derivatives	Quinolines and derivatives			42.9	24.4	M-H	C9H7NO5S	0.763973802	3881.582682	4392.290616	4132.419317	5579.796588	4980.134092	4724.145904	3578.004403	4025.19513	3598.340275
4.63_361.1144m/z	361.1144068	4.632666667	neg	Vanilloloside	HMDB0032013	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		42.9	18.6	M+FA-H	C14H20O8	1.2201642	7098.961585	7720.567015	6727.836093	13177.50648	13583.52637	11751.77854	11834.4416	9717.309105	11837.86504
5.29_373.1506m/z	373.1506488	5.28555	neg	Tetranor-PGEM	HMDB0253059	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates			42.9	20.6	M+FA-H	C16H24O7	0.740094437	25618.73523	23621.09537	22944.89204	25608.05567	30229.19887	32336.08135	27584.75115	22312.59578	27426.10618
5.43_144.1150n	125.0971868	5.428733333	neg	Valeraldehyde propyleneglycol acetal	HMDB0032551	Organoheterocyclic compounds	Dioxolanes	1,3-dioxolanes	*		42.9	16.2	M-H2O-H, M-H	C8H16O2	-0.012619355	3896.129583	4445.018

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8.07_677.2149m/z	677.2148646	8.074883333	neg	Rutagravine	89278	Organoheterocyclic compounds	Quinolines and derivatives	Benzoquinolines			38.5	0	2M-H	C19H17NO5	1.173302103	22410.97671	26602.27619	23375.76562	3862.83781	3529.961485	3597.684663	11280.37135	13938.06106	12836.90766
8.62_223.0285m/z	223.0284642	8.6174	neg	3,3'-Thiobispropanoic acid	87455	Organic acids and derivatives	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives	*		38.5	0	M+FA-H	C6H10O4S	1.581373799	1154.801536	951.7996716	961.1394407	823.522879	829.0669138	975.8231563	1243.877537	944.0704907	936.1769195
8.79_507.1074m/z	507.1073617	8.791166667	neg	5,7-Dihydroxyflavone	HMDB0036619	Phenylpropanoids and polyketides	Flavonoids	Flavones	***	C10028	38.5	0	2M-H	C15H10O4	-2.321247924	2504.563843	2618.593315	2606.33266	0.001403199	0.001403199	0.001403199	1857.810221	2092.748609	2474.220495
8.95_406.2720n	405.2647708	8.953233333	neg	3,7-Dihydroxy-12-oxochiolanoic acid	5389	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	*		38.5	0	M-H, M+FA-H	C24H38O5	0.302543695	12935.55725	13205.74182	16766.8906	1547.461816	1840.643985	1783.766944	6007.737745	6446.905543	7902.527812
9.02_297.1707m/z	297.1707286	9.01635	neg	6alpha-Carissanol	HMDB0035309	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.5	0	M+FA-H	C15H24O3	-0.075087257	671.6923158	775.4434697	498.865767	1144.384345	918.5762352	817.7656933	313.1661884	399.2528801	377.5578367
9.02_409.2868m/z	409.2867743	9.01635	neg	3-Ethylethanthinone	96613	Unclassified	Unclassified	Unclassified			38.5	0	2M-H	C13H19NO	1.760441125	8019.245933	10499.29141	10084.34441	629.2734001	674.1884482	654.4969314	3815.269987	4329.82991	4085.804807
9.08_441.1746m/z	441.1746266	9.077466667	neg	2'-Deoxyespintetrin	HMDB0000389	Organoheterocyclic compounds	Pteridines and derivatives	Pterins and derivatives	*		38.5	0	2M-H	C9H11N5O2	-1.461354412	8855.098809	7858.773203	8706.947829	5856.429457	5074.294992	5431.088958	4719.737337	4717.247655	5829.172355
9.66_211.0361m/z	211.0361432	9.662666667	neg	N-phosphocreatinate(2-)	HMDB0062567	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			38.5	0	M-H	C4H11N3O5P+	-1.001915684	911.8082753	811.7308762	737.8248455	853.9944949	1040.066083	827.7601839	1105.364224	886.5817566	951.5616053
0.67_307.1514m/z	307.1513881	0.6701	neg	Fructoselysine	71227	Unclassified	Unclassified	Unclassified			38.4	0	M-H	C12H24N2O7	1.017162284	1991.957348	1911.277614	1942.560484	3053.557954	2992.60959	3388.700505	1894.404819	1936.340032	2064.934376
0.76_298.1147m/z	298.1147112	0.757316667	neg	Penciclovir	HMDB0014444	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives		C07417	38.4	0	M+FA-H	C10H15N5O3	-3.87561606	600.7587819	216.3076255	0.001403199	656.637708	0.001403199	1225.386755	0.001403199	224.6443371	0.001403199
0.80_155.0020m/z	155.0019752	0.800366667	neg	METHYLMETHANE SULFONATE	44135	Unclassified	Unclassified	Unclassified			38.4	0	M+FA-H	C2H6O3S	0.06650584	1432.799857	1618.921395	1402.154014	227.7954096	93.8957605	0.001403199	0.001403199	0.001403199	0.001403199
0.82_331.0456m/z	331.0455734	0.819566667	neg	4-Hydroxyphenylglycoyl acetate	63853	Unclassified	Unclassified	Unclassified			38.4	0	2M-H	C8H6O4	-1.106880019	8816.186497	11060.5046	10796.59691	11768.60656	10321.21597	11977.64087	11320.31278	11772.21089	12303.08979
0.86_423.0814m/z	423.0813682	0.86335	neg	7-Methylguanosine 5'-phosphate	HMDB0059612	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		C03998	38.4	1.07	M+FA-H	C11H17N5O8P+	4.47296083	31047.44039	33867.70034	38137.9189	37352.36225	36955.33084	37007.2217	40662.11921	37352.39299	39077.92489
0.90_153.0306m/z	153.0306074	0.904683333	neg	2-Amino-4-nitrophenol	HMDB0244990	Unclassified	Unclassified	Unclassified			38.4	0	M-H	C6H6N2O3	0.271467111	4771.803008	4488.356133	5085.317218	4305.29668	4006.667349	4325.555828	4699.449984	4340.685197	4674.306632
0.90_154.9988m/z	154.998803	0.904683333	neg	trans-Aconitate	3771	Organic acids and derivatives	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives	**	C02341	38.4	0	M-H2O-H	C6H6O6	1.184774541	1216.928665	1679.463775	2052.658146	3261.469439	1497.787712	2681.947259	1696.070794	1700.540343	989.6247591
0.90_337.0778m/z	337.0777726	0.904683333	neg	3-O-beta-D-Galactopyranuronosyl-D-galactose	HMDB0039726	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			38.4	0	M-H2O-H	C12H20O12	0.386478172	3072.138654	2933.896811	2933.736873	504.0743119	0.001403199	519.074857	1247.837715	658.1547148	0.001403199
1.08_159.0664m/z	159.0663964	1.078266667	neg	4-Methyl-2-pentenoic acid	HMDB0031095	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.4	0	M+FA-H	C6H10O2	0.999549389	528.2472897	377.3652405	302.3356737	317.2735018	473.9116653	484.4490444	561.9716767	350.7311379	520.8960673
1.14_294.9936m/z	294.9936495	1.1382	neg	Dihydroxyfumarate	6460	Organic acids and derivatives	Keto acids and derivatives	Short-chain keto acids and derivatives	**	C00975	38.4	0	2M-H	C4H4O6	-2.195144878	677.5503303	833.4697131	751.2645972	631.1795202	833.8029135	922.7527938	634.0593746	1040.012819	1004.546735
1.34_215.0175m/z	215.0174865	1.335933333	neg	Sodium aliginate	HMDB0303715	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C01768	38.4	0	M-H	C6H9NaO7	0.768507621	1382.816571	1427.182926	1563.838976	1057.553514	1217.952531	1068.51397	974.3911782	1159.853945	1062.804956
1.62_188.9865m/z	188.9864721	1.615883333	neg	4-Sulfocatechol	66486	Unclassified	Unclassified	Unclassified			38.4	0	M-H	C6H6O5S	0.811732391	14370.0411	14410.78279	15483.2374	7440.071053	7112.850502	7239.379065	13221.86872	12821.86398	12972.28589
1.80_250.0756m/z	250.0756245	1.798266667	neg	N-Pivaloylmethionine	HMDB0094704	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			38.4	0	M+FA-H	C11H19NO3S	0.767127362	2021.188036	1923.336574	2035.595213	1735.97862	1905.477977	2006.384358	2041.699656	2128.727222	2017.971119
10.76_269.2123m/z	269.2123271	10.76333333	neg	(+/-)-Dihydrofarnesol	HMDB0032218	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.4	0	M+FA-H	C15H28O	0.48470864	2001.850067	2735.77721	1342.349602	1602.200884	1355.877003	1524.05973	1971.303061	1455.712502	1400.565698
10.99_269.2123m/z	269.2123275	10.98771667	neg	5,10-Pentadecadien-1-ol	HMDB0031111	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		38.4	0	M+FA-H	C15H28O	0.486571798	3198.776364	3402.600155	2986.720513	2825.005148	2846.21901	2743.913731	3115.30331	3462.821921	3384.922416
2.19_209.0569m/z	209.0568934	2.194566667	neg	5-aminosalicyluric acid	1147	Unclassified	Unclassified	Unclassified			38.4	0	M-H	C9H10N2O4	0.538092243	1480.40852	1341.397931	1645.060513	2648.511867	2313.932543	2552.25059	1412.145144	1592.311099	1538.305764
2.24_168.0303m/z	168.0303021	2.236416667	neg	Nicotinic acid	HMDB0001488	Organoheterocyclic compounds	Pyridines and derivatives	Pyridinecarboxylic acids and derivatives	***	C00253	38.4	0	M+FA-H	C6H5NO2	0.575374829	904.8276683	740.3430792	791.3202684	544.2793029	624.0751159	463.0586824	290.1632308	375.2059302	434.5892683
2.29_270.1098m/z	270.1097676	2.2828	neg	4-(Methylnitrosamino)-1-(3-pyridyl-N-oxide)-1-butanol	73258	Organoheterocyclic compounds	Pyridines and derivatives	Pyridinium derivatives	**	C19603	38.4	0	M+FA-H	C10H15N3O3	0.992502744	894.8119124	850.2056637	694.6246023	982.8302256	986.2041913	983.0829938	729.2225759	873.0971238	852.1784253
2.39_109.0293m/z	109.029318	2.390833333	neg	3-Hydroxy-4,5-dimethyl-2(5H)-furanone	HMDB0031306	Organoheterocyclic compounds	Dihydrofurans	Furanones	**		38.4	0	M-H2O-H	C6H8O3	-1.444739397	126.5964247	102.0100204	130.160183	24.2352165	34.77590991	55.83443331	238.4251141	328.0082296	250.596845
2.67_499.0710m/z	499.0710046	2.6698	neg	SAICAR	HMDB0000797	Nucleosides, nucleotides, and analogues	Imidazole ribonucleosides and ribonucleotides	1-ribosyl-imidazolecarboxamides	**	C04823	38.4	0	M+FA-H	C13H19N4O12P	-1.997440264	1431.725762	1512.371959	1656.456085	0.001403199	0.001403199	0.001403199	1254.486998	1541.136536	1150.247899
2.78_303.0725m/z	303.0724728	2.776216667	neg	Isosorbide-2-glucuronide	864	Unclassified	Unclassified	Unclassified			38.4	0	M-H2O-H	C12H18O10	0.984774746	4624.232628	4196.960615	4474.150436	2881.492859	2434.538082	2734.76362	2844.718561	3420.357723	2989.166137
3.44_150.0560m/z	150.0560461	3.440016667	neg	5-Hydroxydopamine	HMDB0004817	Benzenoids	Phenols	Benzenediols	*		38.4	0	M-H2O-H	C8H11NO3	-0.035504585	1549.984956	1932.935727	1947.610313	1125.690984	1056.267788	1040.845743	1906.838554	1969.302725	1721.894439
3.60_449.0681m/z	449.068106	3.601516667	neg	Dinitrobis	88528	Benzenoids	Benzene and substituted derivatives	Toluenes	*		38.4	0	2M-H	C8H7N2O5	0.906433692	914.7722522	1506.939862	1209.345959	915.0438604	990.3081153	1289.23616	914.155967	1322.432414	1054.800929
3.73_569.0118m/z	569.0117771	3.730516667	neg	trans-zeatin riboside triphosphate	HMDB0304509	Unclassified	Unclassified	Unclassified			38.4	0	M-H2O-H	C15H21N5O14P3-3	-0.284069626	5290.324817	4861.509274	5042.663159	1318.272894	1435.97579	1277.706594	3736.776595	3357.486306	4143.688627
3.75_333.0832m/z	333.0831601	3.747833333	neg	8-hydroxy Guanine	34520	Unclassified	Unclassified	Unclassified			38.4	0	2M-H	C5H5N5O2	5.350888917	283.4116611	285.6951776	246.7657575	1013.851646	909.9841252	476.7978709	425.7317199	494.1699982	525.2274323
3.75_448.1721n	895.3294761	3.747833333	neg	2,3,4,5,2',3',4',6'-Octamethoxychalcone	52155	Unclassified	Unclassified	Unclassified			38.4	0	M-H2O-H, 2M-H	C23H28O9	-2.720802617	8224.667178	7134.267282	8062.428026	12627.12547	12236.77886	7485.601702	6998.821323	9344.231846	7277.143787
3.82_349.0995m/z	349.0995376	3.82415	neg	Vicine	66974	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		C08437	38.4	0	M+FA-H	C10H16N4O7	-1.855216386	3043.169749	3666.390829	3385.698947	4586.87992	4578.67296	4496.786916	4007.084476	4372.909662	4646.506469
3.89_378.0343m/z	378.0342862	3.8906	neg	beta-nicotinate D-ribonucleotide	HMDB0304543	Nucleosides, nucleotides, and analogues	Pyridine nucleotides	Nicotinic acid nucleotides	**	C01185	38.4	0	M+FA-H	C11H12NO9P-2	3.350328663	1016.837426	823.508667	1160.458766	287.0525138	248.5860103	321.0995682	331.4327605	388.0892969	249.1942073
3.91_467.1196m/z	467.1196161	3.912566667	neg	Rumexoside	91540	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			38.4	0	M+FA-H	C20H22O10	0.27568301	1506.964665	1354.6429	1612.387022	0.001403199	0.001403199	186.4933298	2419.259989	2394.71576	2527.493439
4.02_467.1192m/z	467.1192498	4.024283333	neg	1,8-Naphthyridine-3-carboxylic acid, 1-ethyl-1,4-dihydro-7-hydroxy-4-oxo-	1413	Unclassified	Unclassified	Unclassified			38.4	0	2M-H	C11H10N2O4	-3.390853273	585.1324972	637.4656124	340.747485	74.34347339	0.001403199	0.001403199	911.9314496	1033.856094	800.7362035
4.07_125.0608m/z	125.0607644	4.069216667	neg	Toluene-cis-dihydrodiol	66219	Unclassified	Unclassified	Unclassified			38.4	0	M-H	C7H10O2	-0.306970798	187.4706571	153.7514859	175.8598815	56.29800423	57.89939425	96.61143001	124.3814889	171.9505813	128.3763207
4.11_343.1036m/z	343.1036439	4.113883333	neg	Thalianoside	65686	Unclassified	Unclassified	Unclassified			38.4	0	M-H	C8H19N4O6P	4.092729013	1024.38661	793.4452052	1061.072418	1804.851042	1636.468249	1678.079128	1165.331746	1308.753541	
4.11_407.2191m/z	407.2190723	4.113883333	neg	Triethylenemelamine	HMDB0259195	Organoheterocyclic compounds	Triazines	1,3,5-triazines		C08737	38.4	0	2M-H	C9H12N6	4.066269904	890.1829072	1433.639362	1464.683173	1112.285097	1128.295164	890.4198361	969.0409204	1094.36491	1296.937201
4.19_123.0087m/z	123.0086906	4.189783333	neg	Cis,trans-muconate	HMDB0062661	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.4	0	M-H2O-H	C6H6O4	-0.542040522	298.8313763	291.1610609	290.7595019	128.8580924	116.1132297	132.3268455	365.422171	310.8515544	295.2646617
4.19_127.0765m/z	127.0764572	4.189783333	neg	4-Pentenyl acetate	88478	Organic acids and derivatives	Carboxylic acids and derivatives	Carboxylic acid derivatives	*		38.4	0	M-H	C7H12O2	0.03091581	198.9681023	171.8831251	202.8722025	184.1651087	196.245262	289.5395066	250.3602011	203.9085713	193.2398934
4.21_344.0789m/z	344.0789476	4.212111667	neg	Avenanthramide 1c	86155	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	*		38.4	0	M+FA-H	C16H13NO5	4.588011477	84.03424968	321.1600993	420.4805646	653.4627642	767.0500054	873.8164604	542.9445224	441.7721192	537.7924821
4.34_507.0661m/z	507.0660521	4.344733333	neg	Sulfuramid	HMDB0258587	Unclassified	Unclassified	Unclassified			38.4	0	M+FA-H	C10H8F17NO2S	2.114015392	1304.87753	1236.222617	1182.402016	1755.20649	1493.158196	1488.924861	1290.139003	1424.305199	1400.066783
4.41_435.1412m/z	435.1412344	4.41115	neg	1-Hydroxypyrene	64943	Benzenoids	Pyrenes	Unclassified	*	C14519	38.4	0	2M-H	C16H10O	5.000482448	374.8885375	566.9868061	0.001403199	903.5318675	462.0199567	1215.908771	370.8237764	659.3944663	297.6463688
4.43_441.1039m/z	441.1039257	4.432683333	neg	L-Histidinol phosphate	3355	Unclassified	Unclassified	Unclassified			38.4	0	2M-H	C6H12N3O4P	-4.258788561	3501.395311	4067.34705	3540.842242	311.2379141	562.4099924	385.0316878	0.001403199	267.2463303	222.0749909
4.48_241.0699m/z	241.0698532	4.477166667	neg	Glutamyl-Asparagine	85728	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.4	0	M-H2O-H	C9H14N3O6-	-2.175464083	400.5168818	224.2028444	187.666699	236.3807143	0.001403199	260.7006388	406.7501078	448.0169535	458.3141604
4.52_292.1303m/z	292.1302631	4.521733333	neg	Glutaminylphenylalanine	HMDB0028804	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.4	0	M-H	C14H19N3O4	-0.056489919	469.8947408	429.6962505	401.2906132	425.5745741	487.2610379	442.2985349	548.6068874	704.9518427	804.3866878
4.63_309.0982m/z	309.0982408	4.632666667	neg	1''-Acetylvitexin rhamnoside	HMDB0036544	Benzenoids	Phenols	Phenol esters			38.4	0	M+FA-H	C14H16O5	1.000950656	1114.865193	1064.88778	1072.723445	1497.001753	1254.695454	1282.635979	1629.840456	1469.525574	1291.72645
4.63_327.1089m/z	327.108873	4.632666667	neg	Flutrimazole	HMDB0252420	Unclassified	Unclassified	Unclassified			38.4	0	M-H2O-H	C22H16F2N2	-4.162883734	1833.852259	1853.787212	1851.188704	1130.236844	1204.141645	1194.114107	1840.040833	2333.436795	2125.711324
4.66_485.0631m/z	485.0631142	4.660483333	neg	2-(Methylthio)-3H-phenoxazin-3-one	HMDB0035996	Organoheterocyclic compounds	Benzoxazines	Phenoxazines			38.4	0	2M-H	C13H9NO2S	-0.840181942	3038.092002	3066.814492	3256.288475	7573.115156	6493.230188	7761.725127	4481.544663	5031.34776	3084.967146
4.68_123.0451m/z	123.0451241	4.682483333	neg	Guaiacol	HMDB0001398	Benzenoids	Phenols	Methoxyphenols	*	C15572	38.4	0	M-H	C7H8O2	-0.233156911	115.3179631	82.7283272	119.8663131	41.77721078	26.70613026	0.001403199	48.73872453	42.23167278	24.60904658
4.68_499.0864m/z	499.0863574	4.682483333	neg	2-Hydroxy-6-oxo-6-(2-hydroxyphenoxy)-hexa-2,4-dienoate	66735	Unclassified	Unclassified	Unclassified			38.4	0	2M-H	C12H10O6	-3.683839598	1708.675443	1905.846677	1678.951239	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199
4.73_227.0696m/z	227.0696629	4.725416667	neg	Ethionamide sulfoxide	2594	Organic oxygen compounds	Organooxygen compounds	Pyridines and derivatives	*		38.4	0	M+FA-H	C8H10N2OS	0.417645619	339.0979373	449.5066878	392.3313665	835.0957769	849.5708555	728.7925252	956.4268667	1006.540151	1006.943707
4.79_524.1178m/z	524.1177687	4.792316667	neg	Pulchellidin 3-glucoside	LMPK12010413	Unclassified	Unclassified	Unclassified			38.4	0	M+FA-H	C22H23O12+	1.282963991	442.8093053	167.5268558	284.0649834	1030.348545	640.6789644	629.9967554	213.086518	657.08969	0.001403199
4.88_472.2373m/z	472.2372509	4.880083333	neg	20-hydroxy N-Arachidonoyl Taurine	45183	Unclassified	Unclassified	Unclassified			38.4	0	M+FA-H	C22H37NO5S	-0.459310542	5131.614692	5321.657531	5425.308327	4093.354664	4432.411724	4646.096411	5922.167057	6295.569647	4732.389216
4.92_443.1560m/z	443.1560017	4.92485	neg	Methyl 3,4-dihydroxy-5-prenylbenzoate 3-glucoside	HMDB0040121	Phenylpropanoids and polyketides	Tannins	Hydrolyzable tannins			38.4	0	M+FA-H	C19H26O9	0.292338501	5194.75213	6257.276185	5772.251974	8293.558604	8264.821092	8624.933898	6776.395569	7843.594868	6663.801084
5.04_441.1776m/z	441.1776303	5.037216667	neg	2-Deoxysepiapterin	5378	Unclassified	Unclassified	Unclassified			38.4	0	2M-H	C9H11N5O2	5.331505799	1199.986952	753.2091365	1182.46848	369.2591807	541.978785	477.2649153	528.2020312	1145.452214	685.3519411
5.08_515.1061m/z	515.1060667	5.080566667	neg	4,11,13,15-Tetrahydrojoenoridin B	HMDB0036150	Lipids and lipid-like molecules	Prenol lipids	Prenol lipids	*		38.4	0	M+FA-H	C15H24O4	1.345592859	9648.153407	10711.94148	10364.01472	11656.57011	11480.37823	12424.02292	9049.783867	7835.799075	8657.137584
5.08_411.2027m/z	411.2026905	5.080566667	neg	12-oxo-20-dihydrox-leukotriene B4	LMFA03020048	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids	*		38.4	0	M+FA-H	C20H30O6	0.679769557	2153.930921	2357.397461	2196.903604	1499.894704	1219.515148	1566.986705	2837.427226	2587.476685	2432.195382
5.08_535.1461m/z	535.1461477	5.080566667	neg	7-Hydroxy-2',4',5'-trimethoxyisoflavone 7-O-glucoside	LMPK12050064	Unclassified	Unclassified	Unclassified			38.4	0	M+FA-H	C24H26O11	0.88386913	12960.03032	13062.37198	13147.27964	851.1156634	734.7610743	628.2462622	4920.993745	4981.44133	5180.145367
5.18_577.1819m/z	577.18192	5.1777	neg	Acronycidine	68446	Unclassified	Unclassified	Unclassified			38.4	0	2M-H	C15H15NO5	-1.46790935	9478.692472	9556.35176	9945.22116	6184.392596	5181.79264	5130.877021	10116.90377	9879.552414	9182.534738
5.24_353.0882m/z	353.0882071	5.244033333	neg	Allamandin	67925	Unclassified	Unclassified	Unclassified			38.4	0	M+FA-H	C15H16O7	1.302644869	4055.099289	4206.570028	3857.848523	2402.652384	1969.496925	2180.23505	3957.96959	3469.491638	3746.762936
5.26_279.1704m/z	279.1344398	5.263033333	neg	(-)-11-epi-Dihydrojasmonyl-9,10-dihydrojasmonic acid	45942	Lipids and lipid-like molecules	Fatty Acyls	Octadecanoids	*		38.4	0	M+FA-H	C18H30O4	0.340855286	1116.853054	827.2928221	878.8710214	1134.702967	942.3734844	1117.306035	696.6671698	668.0560401	726.2196204
5.30_263.0902m/z	263.0901549	5.302883333	neg	CAY10574	45317	Unclassified	Unclassified	Unclassified			38.4	0	M+FA-H	C9H10N6O	1.57313781	2661.144853	2680.428668	2529.213763	4823.38626	5535.668262	5863.188593	3226.322046	3074.895293	3624.556697
5.34_224.1294m/z	224.1293994	5.3394	neg	3,4-Dimethyl-2-(1-pyrrolidinyl)-2-cyclopenten-1-one	94232	Organoheterocyclic compounds	Pyrrolidines	Unclassified	*		38.4	0	M+FA-H	C11H17NO	1.017910804	530.6569112	674.7932602	605.376416	740.0784336	965.3170966	845.7452927	836.6174047	828.8903776	997.0817505
5.38_347.2077m/z	347.2077014	5.384216667	neg	xi-7-Hydroxyhexadecanedioic acid	HMDB0037830	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.4	0	M+FA-H	C16H30O5	0.57718996	9816.855832	8687.463987	8635.138469	5325.177954	5397.172572	5436.938257	7873.887369	7063.442888	7887.40273
5.43_537.2344m/z	537.2344172	5.428733333	neg	4-Hydroxyretinoic acid glucuronide	HMDB0061688	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		38.4	0	M+FA-H	C26H36O9	0.572068729	736.97758	996.3864811	1688.928724	1439.972029	730.4879335	1307.006586	901.5237578	1000.958992	1340.422402
5.45_355.1038m/z	355.1037662	5.451166667	neg	(3E)-1-O-Cinnamoyl-beta-D-glucose	86865	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Cinnamic acids and esters	*		38.4	0	M+FA-H	C15H18O7	1.001019403	3309.031681	2830.027211	2994.388738	1222.629345	1186.134251	1287.086348	3558.302463	2490.452342	2402.553545
5.53_163.0764m/z	163.076405	5.525416667	neg	Benzenebutanoic acid	5528	Benzenoids	Benzene and substituted derivatives	Unclassified	*		38.4	0	M-H	C10H12O2	-0.293424127	633.6779253	524.3529196	523.3587443	166.6519155	216.4880168	180.3669631	504.7402012	500.4510313	490.2157925
5.53_289.1659m/z	289.1658917	5.525416667	neg	2-methyl-dodecanedioic acid	LMFA01170010	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			38.4	0	M-H	C13H24O4	0.940435381	4263.676521	3802.174958	4083.563125	3043.870727	3336.113994	3328.804101	3731.216601	3777.867952	3822.669676
5.53_383.1713m/z	383.1712704	5.525416667	neg	Oxoamide	HMDB0001004	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		38.4	0	2M-H	C10H12N2O2	-3.145473299	10013.40664	8163.303984	8532.16077	4928.587704	6663.734887	5468.062292	8438.03403	8247.070127	7599.040785
5.32_473.2579m/z	579.1493589	5.525416667	neg	Epicatechin	HMDB0001871	Phenylpropanoids and polyketides	Flavonoids	Flavans	***	C09727	38.4	0	2M-H	C15H14O6	-2.483836248	851.8081394	859.2269572	779.9984929	1529.605038	1288.354104	1270.131541	907.8068486	862.0604973	1141.638988
5.61_433.0553m/z	433.0553111	5.610733333	neg	5-Hydroxyhiabendazole	HMDB0247680	Unclassified	Unclassified	Unclassified			38.4	0	2M-H	C10H7N3OS	1.432662333	805.1208071	877.1812762	1140.278828	1259.338028	934.9100946	1032.262519	919.1396698	812.6881457	1057.586889
5.65_611.2693m/z	611.2692717	5.650833333	neg	O-Isopentenylhalfordinol	86879	Organoheterocyclic compounds	Azoles	Oxazoles	*		38.4	0	2M-H	C19H18N2O2	4.724242392	3770.245529	3365.401636	5020.9043	4392.693692	4186.071881	4142.993028	4299.470709	2456.303481	4151.862173
5.70_479.1901m/z	479.1901439	5.701283333	neg	Melledonol	HMDB0035884	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.4	2.66	M+FA-H	C23H30O8	-4.89848227	15010.52868	13411.42166	12962.59872	6937.160891	8523.100843	9145.745436	13711.42224	14335.28141	18664.61328
5.81_422.1799m/z	422.1799495	5.806016667	neg	Deaminohydroxyblasticidin S	66067	Unclassified	Unclassified	Unclassified			38.4	0	M-H	C17H25N7O6	1.404523469	4063.085339	4729.075448	5247.744825	13843.11414	12882.40845	11383.59295	8211.167614	7682.677764	7523.098019
5.83_536.1646m/z	536.1646045	5.825	neg	Fluorescein glucuronide	HMDB0060607	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		38.4	0	M+FA-H	C26H26F3NO7	0.545843375	3900.51384	3518.286021	2988.847811	1588.928724	1439.972029	1671.66329	9735.833267	9285.829131	9392.360573
5.97_533.1666m/z	533.1666448	5.965483333	neg	Egonol glucoside	HMDB0034280	Phenylpropanoids and polyketides	2-arylbenzofuran flavonoids	Unclassified	*		38.4	0	M+FA-H	C25H28O10	0.399048066	3811.024853	4068.838868	4894.494866	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199
6.02_242.1520n	287.1502367	6.01945	neg	2-Carboxy-4-dodecanolide	HMDB0030987	Organoheterocyclic compounds	Lactones	Gamma butyrolactones	*		38.4	0	M-H, M+FA-H	C13H22O4	0.942795154	2922.853732	2647.290792	3051.448217	4331.242206	4282.853342	4540.84321	2538.532624	2480.967712	2402.951278
6.09_427.1973m/z	427.1972814	6.087383333	neg	Cinncassiol A	HMDB0035164	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*		38.4	0	M+FA-H	C20H30O7	-0.19565902	13941.64707

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0.82_344.0756m/z	344.0756155	0.819566667	neg	D-4'-Phosphopantothenate	3427	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C03492	37.4	0	M+FA-H	C9H18NO8P	1.36899491	1595.921845	1031.782853	1348.012322	1178.280313	326.5276053	1111.414551	553.8023109	836.1574927	695.9872438
0.88_175.0612m/z	175.0612001	0.884633333	neg	Sequoyitol	87689	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols	*	C03365	37.4	0	M-H2O-H	C7H14O6	0.01592202	1939.388507	2075.352146	2173.664872	703.1599022	497.0608247	525.0947223	1641.964239	1633.617674	1628.967143
0.93_321.0828m/z	321.0827733	0.925866667	neg	Ranunculin	67033	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C11H16O8	0.19191639	115.6780744	262.5258909	158.4010486	171.6535752	208.217057	0.001403199	257.3940226	0.001403199	202.1254788
0.97_191.0129m/z	191.0128815	0.967616667	neg	ZAPA	69642	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C4H6N2O2S	-2.190284312	209.6886922	17.24794584	105.2094609	152.0958086	479.7514934	465.9811876	91.5112601	142.170783	0.001403199
1.16_243.0988m/z	243.0988321	1.160166667	neg	gamma-Glutamylproline	HMDB0029157	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		37.4	0	M-H	C10H16N2O5	0.765737457	116.1370836	306.8973349	223.7322384	193.6087814	202.8436781	198.5990884	250.4968062	153.1174297	222.7799388
1.20_347.0598m/z	347.0597839	1.202333333	neg	5-Fluorocyclohexadiene-cis,cis-1,2-diol-1-carboxylate	71220	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C7H7FO4	3.983333439	221.8158946	419.1246778	194.9868483	283.2004726	139.8832252	283.0658115	103.2035089	240.4109571	253.6680839
1.49_188.0024m/z	188.0023924	1.492933333	neg	Lanthionine ketimine	7085	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		37.4	0	M-H	C6H7NO4S	0.476920915	575.8972887	747.0832101	691.3294977	145.4176865	153.295771	120.0211703	298.8453614	239.473392	296.2858948
1.49_346.0580m/z	346.0579649	1.492933333	neg	Adenosine 2'-phosphate	62385	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C00946	37.4	0	M-H	C10H14N5O7P	6.214570501	1035.429434	1005.41895	784.4884152	1088.479399	961.9280405	1081.569638	648.2483283	764.8106732	895.9798767
1.62_491.0278m/z	491.0277767	1.615883333	neg	(5'-[but-3-en-1-yn-1-yl]-[2,2'-bithiophen]-5-yl)methanol	LMFA12000361	Lipids and lipid-like molecules	Fatty Acyls	Oxygenated hydrocarbons			37.4	0	2M-H	C13H10O2S2	0.892713558	697.742715	908.3518214	901.9514857	1102.113686	1120.481872	1388.949714	1074.548715	1097.07049	1045.363528
1.63_303.0101m/z	303.0101118	1.631516667	neg	D-Gluconо-1,5-lactone 6-phosphate	3388	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C01236	37.4	0	M+FA-H	C6H11O9P	-8.346212698	2022.939343	2293.817861	2631.497128	2534.194022	2555.526	2528.555465	3418.540518	2740.430635	2577.745069
1.68_240.0186m/z	240.0185752	1.68365	neg	Carbodithiazine sulfoxide	1527	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C5H9NO3S	1.173969284	0.001403199	46.52421378	83.39754583	139.3228328	137.9096409	67.82733988	29.20481829	37.68671799	68.71229738
1.98_327.0852m/z	327.085165	1.980516667	neg	Phenylpyruvic acid	HMDB0000205	Benzenoids	Benzene and substituted derivatives	Phenylpyruvic acid derivatives	***	C00166	37.4	0	2M-H	C9H8O3	-6.848050195	2056.249577	2784.758415	2670.217946	2542.998571	3130.777403	4372.648236	2670.20282	2183.231395	1843.328682
10.46_585.2297m/z	585.2297233	10.45966667	neg	Desethylenenorfloxacin	1604	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C14H16FN3O3	3.173597807	14041.1393	15959.87232	19286.3372	16621.79598	18335.76288	15280.17398	15025.42977	18453.16851	17153.83952
12.32_379.1563m/z	379.1563006	12.31543333	neg	9-Fluoro-16alpha-hydroxyandrost-4-ene-3,11,17-trione	70598	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C19H23FO4	0.180539479	11471.42475	7651.931951	7827.770369	6350.220937	6073.732479	6462.574186	8966.27532	16002.84376	7549.109534
13.42_269.1312m/z	269.1312017	13.42113333	neg	2'-Aminocacetophenone	88578	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		37.4	0	2M-H	C8H9NO	6.108998065	1566.065913	1301.634846	1291.752099	1571.612146	1551.702947	1240.85919	1900.671695	2074.767214	1308.898492
14.66_351.2518m/z	351.251782	14.6619	neg	5,8,11-eicosatrienoic acid	34827	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		37.4	0	M+FA-H	C20H34O2	-7.514079156	71935.30716	62757.61335	67240.54177	47565.04356	58792.3698	55655.67928	64126.16304	57746.67707	59946.89703
15.09_141.0208m/z	141.0207672	15.08646667	neg	2-Formylglutarate	63877	Unclassified	Unclassified	Unclassified			37.4	0	M-H2O-H	C6H8O5	8.966491059	196.3827625	175.3239103	208.9960283	152.2390938	128.2652492	102.0299308	166.6291283	150.1164902	212.9883608
2.00_216.1071m/z	216.1070926	2.004766667	neg	2,5-Dihydro-4,5-dimethyl-2-(2-methylpropyl)thiazole	HMDB0037159	Organoheterocyclic compounds	Azolines	Thiazolines			37.4	0	M+FA-H	C9H17NS	4.202896155	13698.13811	12614.7905	13749.16329	8744.705704	7755.471886	7848.493601	8981.800627	11103.99013	9508.687684
2.00_361.0343m/z	361.0343341	2.004766667	neg	CAY10562	45271	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C8H7NO2S	5.832504608	5342.245921	4496.414032	4687.877732	2483.663473	2191.829026	2300.681441	2561.808571	3344.198944	2873.78068
2.07_222.9920m/z	222.9919567	2.070366667	neg	Alliinlin	HMDB0031154	Organosulfur compounds	Organic trisulfides	Unclassified	*		37.4	6.51	M+FA-H	C6H10S3	-3.986151455	7674.336537	9259.940219	9808.067469	2599.555947	2849.098546	2379.42334	7930.832756	7943.637556	7896.513119
2.07_392.0555m/z	392.0554703	2.070366667	neg	5'-Hydroxypioroxicam	HMDB0014096	Organoheterocyclic compounds	Benzothiazines	Unclassified	*		37.4	0	M+FA-H	C15H13N3O5S	-0.933806728	13311.79634	14836.90392	14159.46426	13995.94488	15720.78584	14178.33245	16510.45033	14665.04649	14282.93508
2.30_547.0847m/z	547.0846914	2.303733333	neg	Athyriol	68096	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C14H10O6	-6.400804875	1214.516854	1096.447491	1380.809665	1990.297281	2571.253802	2339.353349	1265.084076	1899.782367	1661.309018
2.36_456.9933m/z	456.9932838	2.36465	neg	DIMETHOATE	44564	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C5H12NO3PS2	2.874322364	7518.617379	7498.233907	7323.441721	13042.02585	13651.65998	14015.62527	10230.75514	11892.57914	10918.44879
2.68_365.0186m/z	365.0186341	2.680233333	neg	ACEPHATE	44455	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C4H10NO3PS	5.761756754	2020.408475	1983.672979	2120.377467	298.2753641	368.7995046	240.7480561	911.6744179	1230.458299	954.8207266
2.86_263.0399m/z	263.0398956	2.864816667	neg	3-methyl sulfolene	96259	Organoheterocyclic compounds	Dihydrothiophenes	Unclassified			37.4	0	2M-H	C5H8O2S	-6.926670685	10324.85496	10433.05314	11592.235	16911.21022	15731.30157	16082.31538	13071.57322	13617.75879	12497.04763
3.44_411.0812m/z	411.0812435	3.440316667	neg	Homosiocin 3	3341	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C17H11O7	7.800736805	2395.804704	2841.728037	3349.542775	729.2979477	437.229018	653.9222099	1856.738021	2328.352727	1985.370171
3.69_180.0289m/z	180.0289028	3.685866667	neg	2-Methyl-3-hydroxy-5-formylpyridine-4-carboxylate	58601	Organoheterocyclic compounds	Pyridines and derivatives	Pyridinecarboxylic acids and derivatives	**	C06050	37.4	0	M-H	C8H7NO4	-7.338258421	1427.566599	1628.519154	1630.917232	2719.230545	2495.121178	1799.379994	1848.759628	2247.325406	2119.986921
3.87_385.0910m/z	385.0910433	3.868533333	neg	Vulgaxanthin-II	67072	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C08569	37.4	0	M+FA-H	C14H16N2O8	6.395320113	614.6490481	245.3216652	592.4265439	0.001403199	18.87577667	78.35066733	1179.909811	1265.502161	1137.893813
3.89_357.0262m/z	357.0262335	3.8906	neg	Distemonanthin	51801	Lipids and lipid-like molecules	Polyketides	Flavonoids			37.4	0	M-H	C17H10O9	2.871419881	522.7440495	588.8881485	650.5905046	134.863871	72.56584863	260.3457139	418.8524821	683.3319721	498.1740499
3.96_277.0308m/z	277.0308057	3.957583333	neg	D-Ribitol 5-phosphate	63137	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C5H13O8P	-9.486313294	4504.213954	4791.827335	5042.154648	8539.748186	9056.404035	8921.102998	4977.804805	5554.667145	5576.930366
3.96_480.9934m/z	480.9933833	3.957583333	neg	Fosthiazate	72750	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C9H14N2O3PS2	0.937782263	1743.667367	1496.398679	1743.570602	3222.741204	4093.318997	3393.057327	1869.477828	1871.026481	1742.670508
4.00_563.1022m/z	563.10223	4.002233333	neg	5,6,7-Trihydroxyflavone 7-(6''-malonylglucoside)	LMPK12111089	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C24H22O13	-3.886606889	5238.374907	5186.963906	5795.154168	4695.580747	3741.736561	4196.994706	5804.382181	5757.670217	5113.72578
4.09_280.0810m/z	280.0809929	4.091783333	neg	7-Methylxanthosine	HMDB0301918	Unclassified	Unclassified	Unclassified			37.4	0	M-H2O-H	C11H15N4O6+	-1.08727011	1206.224745	1173.649738	1354.289247	1021.018728	974.5834285	1154.160702	1171.968277	1347.817993	1076.809493
4.14_643.0924m/z	643.0924194	4.136366667	neg	7,7'-Dihydroxy-6,8'-bicoumarin	89369	Phenylpropanoids and polyketides	Coumarins and derivatives	Hydroxycoumarins			37.4	0	2M-H	C18H10O6	6.551378052	205.5433914	453.5789056	373.0628218	3865.734742	2863.675867	2859.053281	0.001403199	0.001403199	0.001403199
4.16_321.1194m/z	321.1193999	4.15895	neg	3'-Hydroxytrimethoprim	2961	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C13H16N4O3	-3.778627979	859.9696692	915.5963085	890.3725709	1335.210048	1302.237732	1246.633272	1313.856919	858.9767675	848.0508079
4.18_543.1223m/z	543.1222876	4.181333333	neg	5-Carboxy-2'-deoxyuridine	HMDB0060774	Unclassified	Nucleosides, nucleotides, and analogues	Pyrimidine nucleosides	*		37.4	0	M+FA-H	C10H12N2O7	1.217579858	1103.560294	810.2368215	884.5158454	470.2296198	540.4210372	629.702552	882.5100743	644.4987356	772.0104365
4.30_457.1151m/z	457.1150679	4.300033333	neg	N-Tris[hydroxymethyl]methyl-2-aminoethanesulfonic acid [TES]	44793	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C6H15NO6S	-3.649860794	3539.886209	2942.901667	2816.797357	3734.209355	3128.768751	3367.572063	2816.37262	3684.070015	2840.186818
4.32_380.0789m/z	380.0788564	4.3224	ves	4-Hydroxy-6-methylpretetramide	63774	Unclassified	Unclassified	Unclassified			37.4	0	M-H	C20H15NO7	3.361433188	1224.735145	1173.369153	1380.042364	1248.838346	870.9867128	1321.396726	1164.339078	1581.39275	1042.734357
4.34_392.0722n	391.0649537	4.344733333	ves	5,7,3',4',5'-Pentahydroxy-3,6,8-trimethoxyflavone	51769	Unclassified	Unclassified	Unclassified			37.4	0	M-H, M+FA-H	C18H16O10	-5.398350386	16379.90531	17068.20945	17211.53006	6398.746131	5347.094175	5566.352038	13564.09284	14513.0285	14769.08673
4.39_384.0905m/z	384.0904589	4.3893	ves	9-Hydroxy-4-methoxypsoralen 9-glucoside	93653	Phenylpropanoids and polyketides	Coumarins and derivatives	Coumarin glycosides			37.4	0	M+FA-H, M+FA-H	C18H18O10	-5.738333162	5265.760786	4916.598093	4628.995328	8261.803975	8397.713207	6934.973363	3416.667899	4290.722035	4547.94447
4.41_263.0287m/z	263.028706	4.41115	neg	Oxalureate	63388	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C3H4N2O4	6.700818884	31590.98474	36407.16676	35856.5987	16280.84971	14937.87342	15658.68672	28649.25634	29491.2565	29115.54474
4.41_375.0813m/z	375.0813331	4.41115	neg	SOTS-1	64678	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C16H14N2O6	-6.228452633	10006.31177	9982.047707	8294.450567	7028.098287	4985.629269	6968.972734	9881.409021	10991.40762	10458.49019
4.43_287.1251m/z	287.1251071	4.432683333	neg	N-Hydroxypentobarbital	1765	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C11H18N2O4	1.020798118	2219.990029	2708.458799	2287.457313	3131.416259	3214.59801	3921.24626	2078.779066	2544.085104	2349.494088
4.45_465.1013m/z	465.101325	4.454616667	neg	benfotiamine	HMDB0248951	Unclassified	Unclassified	Unclassified			37.4	0	M-H	C19H23N4O6PS	2.165472494	257.3515081	273.0530338	251.3571221	735.9299923	247.7759647	492.0796659	902.3215951	1290.908652	1154.815983
4.50_343.1259m/z	343.1254509	4.49925	neg	1-(1,2,3,4,5-Pentahydroxypent-1-yl)-1,2,3,4-tetrahydro-beta-carboline-3-carboxylic acid	HMDB0012492	Alkaloids and derivatives	Alkaloids and derivatives	Harmala alkaloids			37.4	0	M-H2O-H	C17H22N2O7	1.614041176	1603.203259	620.7139156	479.7963915	734.7389839	525.4498545	462.5755021	709.6534966	725.6437019	734.2709303
4.52_363.1181m/z	363.1181333	4.521733333	neg	16-iodo-hexadecanoic acid	LMFA01090039	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			37.4	0	M-H2O-H	C16H31IO2	-2.365177459	1217.728221	1571.236332	1516.375634	1085.67522	865.0469913	914.5684794	820.0740311	935.9213848	838.8239585
4.52_405.2134m/z	405.2134179	4.521733333	neg	Kiwiinoside	93346	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		37.4	0	M-H	C19H34O9	1.013477634	1309.225606	1125.884995	1322.861894	65.22519688	77.78831771	0.001403199	798.1477498	1056.185592	768.6920891
4.54_497.0705m/z	497.0704783	4.54425	neg	5-Carboxypyranocyanidin 3-O-beta-glucopyranoside	47199	Unclassified	Unclassified	Unclassified			37.4	0	M-H2O-H	C24H20O13	-4.013342329	1016.613685	980.7170805	1001.209189	3904.097188	3259.56219	3377.494218	34.77190363	112.1238602	102.1867951
4.57_242.0171n	287.0155368	4.5668	ves	Inositol cyclic phosphate	6020	Organic acids and derivatives	Organic phosphoric acids and derivatives	Unclassified	*	C04299	37.4	0	M-H, M+FA-H	C6H11O8P	-8.576921295	4041.044011	5138.089622	4728.730111	918.9781702	1250.923886	1177.239457	778.8651417	551.3961331	565.4927709
4.61_399.1961m/z	399.1961248	4.611883333	neg	Fluorodone 17-acetate	70218	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C24H31FO5	-3.793301335	1373.334825	1373.37564	6513.424773	49085.18273	4947.06297	42055.96318	64778.29871	59270.22313	72870.49099
4.61_403.1977m/z	403.1977119	4.611883333	neg	1-Octen-3-yl primeveroside	88859	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		37.4	0	M+H2O-H	C19H34O10	0.842638505	1834.50673	2134.197211	1642.187325	721.0736987	656.302454	640.2712969	1793.535409	1556.174175	1994.472973
4.63_531.1360m/z	531.1360408	4.632666667	neg	Carbamazepine-o-quinone	71260	Organoheterocyclic compounds	Benzazepines	Dibenzazepines	**	C16606	37.4	0	2M-H	C15H10N2O3	9.457863231	1310.339122	1006.078794	1005.131082	377.6574596	606.5650674	511.2046749	1184.99355	1045.130334	788.9740922
4.75_293.1008m/z	293.1008169	4.747466667	neg	Deoxyanisatin	69293	Unclassified	Unclassified	Unclassified			37.4	0	M-H2O-H	C15H20O7	-7.192533355	1174.024945	879.3203954	797.8126354	825.1531094	810.7558927	691.9422561	437.5715191	568.335044	250.3245665
4.75_493.2034m/z	493.2034052	4.747466667	neg	Fluociconide	2747	Lipids and lipid-like molecules	Steroids and steroid derivatives	Pregnane steroids		C07007	37.4	0	M-H	C26H32F2O7	-1.878104103	5013.781123	5991.256114	6915.851553	4660.58542	4053.816884	3627.71848	4644.566769	5609.88805	5152.88454
4.79_313.1659m/z	313.165984	4.792316667	neg	Bisacurone epoxide	93181	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		37.4	0	M+FA-H	C15H24O4	1.200283855	1419.99786	1663.463766	2146.411223	2378.933284	2165.511768	2177.196712	1636.524689	1959.162834	2150.926564
4.79_352.0938m/z	352.093774	4.792316667	neg	CI Pigment Red 3	73076	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C17H13N3O3	-0.391382716	3128.649275	3181.129022	3732.538036	5960.780439	5765.143382	5676.909386	2722.86142	3066.796467	3009.323451
4.79_413.0845m/z	413.084518	4.792316667	neg	Vitexin	LMPK12110194	Lipids and lipid-like molecules	Polyketides	Flavonoids	***		37.4	0	M-H2O-H	C21H20O10	-7.608551005	377.58206	631.2109744	581.4311934	1193.846826	1053.88643	1089.009709	500.382422	567.2133408	553.6684388
4.88_335.1350m/z	335.1349914	4.880083333	neg	Benomyl	HMDB0031767	Organoheterocyclic compounds	Benzimidazoles	2-benzimidazolylcarbamic acid esters	*	C10896	37.4	0	M+FA-H	C14H18N4O3	-3.798007675	1960.10272	2082.776131	1988.189287	3041.017512	2793.268662	2973.288407	2201.251204	2407.319899	2094.074854
4.88_527.0875m/z	527.0875394	4.880083333	neg	alpha-D-Galactopyranuronosyl-(1->4)-alpha-D-galactopyranuronosyl-(1->4)-D-g	HMDB0039751	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			37.4	0	M-H2O-H	C18H26O19	-2.651637688	2951.476275	3600.195565	3511.652529	5678.739961	5063.023798	4185.554832	4740.910159	5183.262044	3738.246148
4.95_771.1094m/z	771.1084184	4.94705	neg	Lithol-Rubine	HMDB0041567	Benzenoids	Benzenoids	Naphthalenecarboxylic acids and derivatives			37.4	0	2M-H	C18H14N2O6S	1.528833033	2301.139625	1840.480564	1477.332177	0.001403199	0.001403199	0.001403199	726.7642479	0.001403199	0.001403199	726.7642479	442.9584557
4.97_332.1637m/z	332.1636713	4.969683333	neg	Zolmitriptan	44026	Organoheterocyclic compounds	Indoles and derivatives	Tryptamines and derivatives		C07218	37.4	0	M+FA-H	C16H21N3O2	7.283389319	6280.036405	6013.548526	6539.244185	4158.457409	3831.448051	4064.321185	6002.410672	5655.862474	5054.026603
5.01_453.1391m/z	453.1390659	5.014716667	neg	Ginkgolide A	41244	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		37.4	0	M-H	C20H24O9	-2.864920119	531.1486383	1319.164197	1228.129742	1902.308144	1706.474672	1806.502792	968.2209345	1228.842854	810.6967125
5.06_551.0490m/z	551.0490138	5.05975	neg	5-(4-Acetoxybut-1-ynyl)-2,2'-bithiophene	66192	Organoheterocyclic compounds	Bi- and oligothiophenes	Unclassified		C04485	37.4	0	2M-H	C14H12O2S2	0.990802089	3524.133591	3249.781849	3429.014658	6066.722921	6053.936987	6218.972424	4840.546215	4841.887747	5342.848926
5.10_499.2189m/z	499.218754	5.1031	neg	6S,9R-Dihydroxy-4,7E-megastigmadien-3-one 9-[apiosyl-(1->6)-glucoside]	HMDB0029773	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		37.4	0	M-H2O-H	C24H38O12	0.752261332	1130.795898	982.2094091	851.3538428	1110.184011	1474.178846	1766.982343	1071.889825	1015.802508	1049.473946
5.16_323.0777m/z	323.0776891	5.155116667	neg	Glucosinolic acid	HMDB0034313	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			37.4	0	M-H	C11H19O9	1.309661398	1193.03818	1848.600988	1673.890717	703.8907127	1103.783734	774.1913488	1603.331577	1563.843853	1707.401215
5.16_515.0811m/z	515.0811313	5.155116667	neg	4',5-Dihydroxy-3,3'-dimethoxy-6,7-methylenedioxyflavone 4'-glucuronide	92577	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	*		37.4	0	M-H2O-H	C24H22O14	-3.712727023	3989.883056	5586.27193	4662.61173	2540.634174	2446.384862	2220.865548	3838.070034	4412.613056	3967.95392
5.20_209.0822m/z	209.0822233	5.20005	neg	3-Hydroxy-4-phenylbutan-2-one	HMDB0032336	Benzenoids	Benzene and substituted derivatives	Unclassified	*		37.4	0	M+FA-H	C10H12O2	1.772308041	405.8506349	390.3962293	366.4586146	247.8080958	210.3834322	281.4154046	421.5374993	236.0703432	430.4982561
5.22_533.1666m/z	533.1666387	5.222166667	neg	PD 98059	64632	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C16H13NO3	-9.681082087	1213.940057	1764.590139	1215.744879	3473.853423	3165.677719	3441.938273	1099.60821	1032.271475	1156.415487
5.22_570.0661m/z	570.0660885	5.222166667	neg	Guanosine diphosphofucose	4187	Nucleosides, nucleotides, and analogues	Purine nucleotides	Purine nucleotide sugars	**	C00325	37.4	0	M-H2O-H	C16H25N5O15P2	2.87091311	744.8994646	780.6604566	903.8348145	970.3616143	592.6076344	1251.031926	1162.139903	1669.544356	1376.170095
5.30_383.1536m/z	383.153577	5.302833333	neg	Dehydrogeissoschizine	71922	Unclassified	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	*		37.4	0	2M-H	C11H12O3	9.28002833	7637.534895	6614.435043	6402.081274	10074.043	13085.25861	12703.51435	10379.19343	7511.433048	10685.466
5.30_535.2163m/z	535.2162982	5.302883333	neg	EUGENYL BENZOATE	44605	Phenylpropanoids and polyketides	Depsides and depsidones	Unclassified	*		37.4	0	2M-H	C17H16O3	6.873767113	1900.481249	1348.01366	1446.522602	1660.30796	2115.259259	2697.719205	1752.746968	1558.863174	1785.703561
5.32_345.1203m/z	345.1202958	5.320233333	neg	Diaziquone	HMDB0251150	Unclassified	Unclassified	Unclassified			37.4	0	M-H2O-H	C16H20N4O6	-0.404841707	1159.646846	1185.197619	1232.344399	1165.076408	1736.106749	1588.508483	1489.816029	1299.672399	1964.797226
5.34_477.2140m/z	477.2139689	5.3394	ves	Mellecilide B	HMDB0038787	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		37.4	0	M+FA-H	C24H32O7	2.227247439	1703.90621	2133.929526	1973.70716	2916.252107	2801.32268	2316.440406	1767.529244	2245.57052	2728.140439
5.41_337.1383m/z	337.1383254	5.406433333	neg	Norepinephrine (noradrenaline)	63	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C8H11NO3	-6.460428137	7156.23356	8184.25666	7415.72144	146909.0846	112587.5384	89006.24615	105367.9693	116.7643545	89006.24615
5.43_494.2738m/z	494.2737677	5.428733333	neg	Clondrine	67106	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C25H39NO6	-4.837075234	1599.496344	1128.056857	1599.356282	2702.011845	2213.567838	1858.415749	1165.318256	2217.996846	1414.737186
5.53_611.0583m/z	611.0582925	5.525416667	neg	UDP-alpha-D-galacto-1,4-furanose	66033	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C15H24N2O17P2	8.954980799	28867.62264	25368.16944	23993.73686	9491.220046	11958.89987	9436.268931	20304.85786	20285.22805	26801.20294
5.56_599.2247m/z	599.2247344	5.56185	neg	23-Hydroxyphysalolactone	HMDB0031388	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid lactones	*		37.4	0	M+FA-H	C28H39ClO10	-3.119584299	18104.89307	15153.63636	15402.39422	22307.68665	26193.42493	23665.20664	15041.54045	17889.15498	14466.29584
5.60_323.0646m/z	323.0646065	5.602	neg	2-Oxo-5-methylthiopentanoic acid	64490	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C6H10O3S	5.407967361	668.9324811	639.5145832	895.609612	1681.42593	1822.450275	1600.47826	542.8391478	748.208839	635.0536309
5.70_725.1243m/z	725.1243892	5.701283333	neg	Flufenacet	HMDB0252330	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C14H13F4N3O2S	1.728958814	1000.405225	1031.080514	833.9180988	717.8088818	428.7364001	1417.728293	1796.515677	1796.515677	1796.515677
5.71_263.0926m/z	263.0926048	5.709933333	neg	Dihydroneopurin	67164	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C13H14O3	0.493638934	872.1355554	955.59829	722.8666186	611.6578242	984.7639927	966.7608865	846.0194407	957.4219742	1593.809828
5.74_313.1660m/z	313.1659679	5.744566667	neg	Deoxydihydro-artemisinin	HMDB0060570	Organoheterocyclic compounds	Dioxolopyrans	Unclassified	*		37.4	0	M+FA-H	C15H24O4	1.140446258	709.7269901	825.7011556	690.2155541	535.1899117	575.7590619	630.6479154	438.6545874	441.6762261	601.6581544
5.81_553.1026m/z	553.1025571	5.806016667	neg	Fluorescein monoglucuronide	2756	Unclassified	Unclassified	Unclassified			37.4	0	M+FA-H	C26H20O11	7.464571882	33358.40639	34673.12826	35613.34234	56636.10559	44673.46449	47018.23617	5417.407661	5334.605726	5388.229599
5.83_279.0382m/z	279.0382307	5.825	neg	Uracil 5-carbaldehyde	71607	Unclassified	Unclassified	Unclassified			37.4

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6.14_193.0905m/z	193.0904913	6.143466667	neg	Burimamide	66645	Unclassified	Unclassified	Unclassified			36.3		0	M-H2O-H	C9H16N4S	-5.823029972	624.5979608	807.955922	624.7899298	652.3721157	731.8868927	779.0278415	751.0927265	691.6565023	725.0308281
6.15_533.0894m/z	533.0894003	6.154666667	neg	Bilobetin	87220	Phenylpropanoids and polyketides	Flavonoids	Biflavonoids and polyflavonoids	*		36.3		0	M-H2O-H	C31H20O10	2.888125286	15126.66165	16384.35551	15993.47603	9307.050554	10451.07844	11643.84976	9596.885927	10869.72899	11964.13913
6.17_261.1167m/z	261.1167308	6.171316667	neg	N-HISTIDYL-2-AMINONAPHTHALENE (BNA)	44316	Unclassified	Unclassified	Unclassified			36.3		0	M-H2O-H	C16H16N4O	7.713489772	404.7173176	396.8079826	464.5094065	191.1720158	326.2894998	382.6041875	421.5701799	413.1280327	477.810766
6.32_497.1260m/z	497.1259722	6.320716667	neg	7-Hydroxybutylidenephthalide 7-(6-malonylglucoside)	90179	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			36.3		0	M+FA-H	C21H24O11	-9.051075455	8392.362427	9573.352066	10460.80088	12657.00855	12752.91052	11145.26456	7232.570072	7745.57952	9369.591189
6.35_323.1481m/z	323.1480581	6.348783333	neg	Diisobutyl phthalate	70692	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*	C15205	36.3		0	M+FA-H	C16H22O4	-7.024601405	1293.830809	1549.900345	1355.091821	2359.315245	2363.569201	2348.54398	1169.560883	1083.054338	1355.097955
6.37_356.0755m/z	356.0755037	6.373833333	neg	Furoparadine	95520	Organoheterocyclic compounds	Quinolines and derivatives	Benzoquinolines			36.3		0	M+FA-H	C17H13NO5	-6.659647088	1472.647963	1670.329461	2001.890917	1962.569046	2849.272337	2535.492	2871.6405	3311.920504	3105.958037
6.43_450.1162m/z	450.1162386	6.433933333	neg	Buclarosine	HMDB0249421	Unclassified	Unclassified	Unclassified			36.3		0	M-H2O-H	C18H24N5O8P	-4.624760898	2020.96471	1709.199349	1473.079845	3182.46296	2719.491027	2892.284219	2026.281027	2192.689244	1939.276195
6.51_320.1298n	365.1229824	6.509966667	neg	Enoxacin	HMDB0014610	Organoheterocyclic compounds	Diazines	Pyrimidines and pyrimidine derivatives		C06979	36.3		0	M-H, M+FA-H	C15H17FN4O3	4.012391609	3792.497681	3052.288739	3955.904603	4510.418432	4686.613159	4742.430001	4009.387789	4501.811874	4577.15124
6.58_477.0994m/z	477.0993664	6.582416667	neg	Naphthofluorescein	45440	Unclassified	Unclassified	Unclassified			36.3		0	M+FA-H	C28H16O5	3.216558124	5625.575672	5928.696007	5497.000179	11594.37912	12136.68486	11508.82356	6669.971762	8496.236987	7749.979585
6.62_467.1149m/z	467.1148811	6.61635	neg	MDL 73492 sulfate	2370	Unclassified	Unclassified	Unclassified			36.3		0	M+FA-H	C19H22N2O7S	4.515753531	5390.59093	5185.629686	4931.814474	10147.16176	10024.40831	10368.93186	8186.98095	9734.172687	9732.315686
6.86_479.1151m/z	479.1151357	6.86835	neg	3'-O-Methyl-(-)-epicatechin 7-O-glucuronide	96020	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	*		36.3		0	M-H	C22H24O12	-9.089326735	58890.78749	60323.18088	53762.4862	63215.58195	65437.78532	60891.42962	53884.4856	57473.26358	53278.96272
6.93_511.1458m/z	511.145838	6.926366667	neg	3-(4-Hydroxy-3-methoxyphenyl)-1,2-propanediol 2-O-(galloyl-glucoside)	91519	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives			36.3		0	M-H	C23H28O13	0.241027074	7033.21478	445.8779104	23427.32172	1076.998201	1185.618892	786.3950701	863.2720896	707.7776375	3776.992632
6.99_420.1078m/z	420.1077906	6.993516667	neg	3-Hydroxymethyltriazolopthalazinone glucuronide	3168	Unclassified	Unclassified	Unclassified			36.3		0	M+FA-H	C17H17N3O7	7.8319746	930.9727713	884.0226608	856.9138702	1711.947663	1552.856351	1749.350151	1298.182756	1309.280786	1100.284843
7.07_155.0715m/z	155.07148	7.0658	neg	(E,Z)-2,4-Heptadienal	HMDB0061891	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds			36.3		0	M+FA-H	C7H10O	1.019032632	983.6246442	1061.155	1087.074727	1032.226449	982.1994735	821.4991708	983.2405146	914.7678563	988.3522036
7.16_378.1511m/z	378.1511236	7.1647	neg	Tiaprost	96518	Unclassified	Unclassified	Unclassified			36.3		0	M-H2O-H	C20H29O6S	1.208718333	1711.334693	1829.735101	1604.437592	2246.030287	1731.820928	1780.36679	1510.689134	2002.191174	1394.884277
7.18_452.1362m/z	452.1362142	7.178516667	neg	8-Carboxymethyldihydrocherilerythrine	HMDB0029832	Alkaloids and derivatives	Benzophenanthridine alkaloids	Dihydrobenzophenanthridine alkaloids	*		36.3		0	M+FA-H	C23H21NO6	2.760548838	4169.251764	4891.010653	4540.502669	5251.265703	5350.3627	5956.14309	3571.921674	4972.749392	3666.337034
7.20_533.2267m/z	533.2267417	7.201166667	neg	Acarbose (M7)	762	Unclassified	Unclassified	Unclassified			36.3		0	M-H2O-H	C24H40O14	5.028266667	2886.987204	2687.222671	2720.925371	1602.152214	1854.299092	1782.51992	1536.425093	1734.106041	1369.013686
7.44_651.3006m/z	651.3005645	7.440866667	neg	(+)-Galeon	87743	Phenylpropanoids and polyketides	Diarylheptanoids	Cyclic diarylheptanoids	*		36.3		0	2M-H	C20H22O4	6.473367759	122495.0576	116630.4159	143468.1302	24248.26204	23372.2706	20929.44156	58941.19249	68395.98312	59467.77337
7.92_805.1871m/z	805.1871242	7.91555	neg	4-Methylpentyl glucosinolate	HMDB0038420	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			36.3		0	2M-H	C13H25NO9S2	0.314876882	12989.11859	13042.39098	14085.12818	17356.47012	17019.23227	17520.93202	12761.53565	17348.92098	15318.62791
8.07_813.1897m/z	813.1897374	8.074883333	neg	S-Succinylglutathione	65921	Unclassified	Unclassified	Unclassified			36.3		0	2M-H	C14H21N3O9S	-3.299855414	9541.603452	10279.66706	9506.236858	1276.799843	721.3501869	149.5764989	3984.616201	4671.486609	4714.787203
8.55_388.2342m/z	388.2342215	8.55215	neg	Geranylgeranylcysteine	62417	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	*		36.3		0	M-H2O-H	C23H37NO3S	6.501206886	1545.097994	1277.437028	1130.496772	1273.969041	1438.952566	1679.43669	1315.388617	1174.096831	1191.237865
9.02_443.2573m/z	443.2572543	9.01635	neg	1-(11Z,14Z-eicosadienoyl)-glycero-3-phosphate	HMDB0062303	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphates	*		36.3		0	M-H2O-H	C23H43O7P	0.984437831	18786.35599	24973.58971	24477.54967	1520.54901	1239.831583	1520.882993	9236.819578	10096.56466	9361.884458
0.54_759.5182m/z	759.5181869	0.535283333	neg	PG(13:0/22:2(13Z,16Z))	LMGP04010090	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols			36.2		0	M-H	C41H77O10P	0.036913488	1243.480772	776.983049	1717.847597	0.001403199	0.001403199	0.001403199	1085.80816	0.001403199	307.0178196
0.67_222.9850m/z	222.9849558	0.6701	neg	2,3-Diketo-5-methylthio-1-phosphopentane	5947	Organic acids and derivatives	Organic phosphoric acids and derivatives	Phosphate esters	**	C15650	36.2		0	M-H2O-H	C6H11O6PS	5.790081159	929.1195523	905.959424	716.6777631	1035.900274	546.1459959	932.7205593	924.3477421	636.1822448	605.4467263
0.71_867.2912m/z	867.2911739	0.714216667	neg	Epimedin C	LMPK12112015	Lipids and lipid-like molecules	Polyketides	Flavonoids			36.2		0	M+FA-H	C39H50O19	-2.016785548	4852.303238	4497.821189	4798.141093	1977.908559	7881.032592	5300.588727	3837.749326	1120.031067	4445.72407
0.74_977.2583m/z	977.2583145	0.7359	neg	Pelargonidin 3-O-[2-O-(6-O-(E)-feruloyl-beta-D-glucopyranosyl)-beta-D-glucopyranoside]	46838	Unclassified	Unclassified	Unclassified			36.2		0	M+FA-H	C43H48O23	1.580856212	5814.222422	6108.693504	6450.39841	1570.879696	5647.837726	3435.175125	3640.715434	2297.65033	3071.652917
0.78_217.0484m/z	217.0483651	0.778533333	neg	Dillapional	87076	Organoheterocyclic compounds	Benzodioxoles	Unclassified	*		36.2		0	M-H2O-H	C12H12O5	-9.60437849	67100.02656	72357.38927	91100.41716	33285.01722	44480.09552	34280.25016	51750.45483	70709.8388	64639.40283
0.82_353.0532m/z	353.0532489	0.819566667	neg	2-Caffeoylisocitrate	65864	Unclassified	Unclassified	Unclassified			36.2		0	M-H	C15H14O10	5.165019711	2147.055394	2562.786426	2068.89633	1473.399311	1102.519654	953.8296566	1268.200808	1846.251228	895.2079358
0.82_410.0728m/z	409.0654975	0.819566667	neg	Zeanic acid	88862	Organoheterocyclic compounds	Quinolines and derivatives	Quinoline carboxylic acids			36.2		0	M-H, M+FA-H	C20H14N2O8	-5.46603209	27260.5869	28274.85379	27279.3153	45012.33766	41798.90031	40745.18589	35301.05448	32997.36126	31054.72052
0.88_194.0274m/z	194.0273825	0.884633333	neg	2-Methylbenzothiazole	88895	Organoheterocyclic compounds	Benzothiazoles	Unclassified			36.2		0	M+FA-H	C8H7NS	-4.96931224	0.001403199	204.0744442	206.5894716	177.7650496	327.5443055	226.6110696	0.001403199	112.660723	68.82521557
0.90_287.9778m/z	286.9705278	0.904683333	neg	2,6-Naphthalenedisulfonic acid	71139	Unclassified	Unclassified	Unclassified			36.2		0	M-H, 2M-H	C10H8O6S2	3.466745732	156070.1323	164323.6808	167915.0548	163926.6605	176191.6107	177056.3275	147927.0477	183356.6152	
0.93_188.9997m/z	188.9997236	0.925866667	neg	1-Naphthalenesulfonic acid	71143	Unclassified	Unclassified	Unclassified			36.2		0	M-H2O-H	C10H8O3S	-8.895291161	91.1170697	132.1684445	240.0178687	0.001403199	0.001403199	0.001403199	0.001403199	78.88114144	1.02653693
0.97_219.0118m/z	219.0118355	0.967616667	neg	Phenylmethanesulfonyl fluoride	66517	Unclassified	Unclassified	Unclassified			36.2		0	M+FA-H	C7H7FO2S	-8.309767079	0.001403199	901.7731491	1472.137914	8584.247791	4915.206541	7681.867905	1393.893777	4127.691623	3151.813726
1.16_286.9705m/z	286.9704733	1.160166667	neg	1,6-Naphthalenedisulfonic acid	71138	Unclassified	Unclassified	Unclassified			36.2		0	M-H	C10H8O6S2	5.277428706	87325.02269	128107.3554	114826.5274	13207S.301	10341S.881	105292.2674	122058.0393	92166.25652	102962.14
1.68_331.0785m/z	331.0785244	1.68365	neg	Ethyl phenothiazine-2-carbamate	1352	Unclassified	Unclassified	Unclassified			36.2		0	M+FA-H	C15H14N2O2S	9.517827914	621.524724	693.7492065	701.0762459	837.4273905	791.2861401	706.8103962	683.068648	779.4647865	728.49913S7
1.76_446.1421m/z	446.1420945	1.7577	neg	14-Deoxycalystegine sulfate	2214	Unclassified	Unclassified	Unclassified			36.2		0	M-H	C18H29NO9S2	-0.909550861	1444.128922	1481.885001	1530.361751	1283.220665	1389.151648	1536.457138	1005.078965	1552.214139	1144.385368
1.79_215.0539m/z	215.0538994	1.7861	neg	1-Isopropyl citrate	88461	Organic acids and derivatives	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives			36.2		0	M-H2O-H	C9H14O7	-9.451239024	708.5693684	700.2056757	709.6487262	710.3205663	524.131308	829.8875647	782.0907321	652.8963885	634.9515472
10.43_701.5128m/z	701.5127622	10.42685	neg	PA(20:1(11Z)/16:0)	LMGP10010532	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphates	*		36.2		0	M-H	C39H75O8P	0.11758458	14427.87737	12466.03835	11061.21464	15256.90423	16659.86121	15843.10691	13282.98409	15464.26958	15410.76078
11.05_481.0389m/z	481.0389302	11.05113333	neg	C.I. Food Red 1	HMDB0033383	Benzenoids	Naphthalenes	Naphthalene sulfonic acids and derivatives			36.2		0	M-H2O-H	C18H16N2O7S2	1.913811727	6291.375176	7534.241455	6604.606498	6440.119483	8202.629774	8213.509998	7963.824232	8095.45637	7600.385697
2.00_300.0813m/z	300.0813847	2.004766667	neg	Ro 19-4603	69655	Unclassified	Unclassified	Unclassified			36.2		0	M-H2O-H	C15H17NO3S	0.512080768	4353.283584	4223.983816	4138.118316	2847.845988	3222.226101	2860.265974	2494.983544	2875.449409	2540.806624
2.00_409.0370m/z	409.0370002	2.004766667	neg	XMP	3505	Nucleosides, nucleotides, and analogues	Purine nucleotides	Purine ribonucleotides	**	C00655	36.2		0	M+FA-H	C10H13N4O9P	-8.837730873	2835.8111	2689.178856	2585.658812	1733.544265	1627.581555	1698.284292	1718.019474	2218.85504	2017.903628
2.28_300.0468m/z	300.0467522	2.2828	neg	N-Acetyl-D-mannosamine 6-phosphate	63213	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C04257	36.2		0	M-H	C8H16NO9P	-7.437391842	7467.312651	7036.540046	6537.641977	11944.89804	11106.18703	11167.714	10072.6481	10486.73642	9524.738531
2.28_368.0343m/z	368.0342665	2.2828	neg	EPN	70057	Unclassified	Unclassified	Unclassified			36.2		0	M+FA-H	C14H14NO4PS	-6.351897285	9723.3553	9987.206563	9385.519272	15638.01745	13818.89696	14514.58161	12150.81418	12948.9396	12744.07557
3.06_354.0785m/z	354.0784798	3.05735	neg	Deacetylcephalosporin C	64542	Unclassified	Unclassified	Unclassified			36.2		0	M-H2O-H	C14H19N3O7S	5.226363186	7999.806246	7916.155094	8934.016716	18902.72625	19935.64818	17836.64644	13882.13182	13684.32674	12777.48522
3.29_227.0709m/z	227.0708792	3.293883333	neg	Ammonium peroxydisulfate	92479	Unclassified	Unclassified	Unclassified			36.2		0	M+FA-H	H8N2O8S2	-7.153977265	1167.2062	1344.934984	356107971	25028.22213	24435.93266	25050.20931	10701.83445	11765.3062	11111.1111
3.35_450.0882m/z	450.0882458	3.350266667	neg	4'-Desmethylpapaverine sulfate	1707	Unclassified	Unclassified	Unclassified			36.2		0	M+FA-H	C19H19NO7S	4.492732492	11506.76628	13891.35242	11781.89458	16488.32267	15732.68565	15934.6715	12569.54663	15165.1478	12579.51399
3.66_248.9962m/z	248.9962188	3.6635	neg	4-Hydroxyrilluzole	2323	Unclassified	Unclassified	Unclassified			36.2		0	M-H	C8H5F3N2O2S	4.448578582	145.8562212	121.0800773	341.5635321	0.001403199	0.001403199	0.001403199	98.33276461	107.8632431	128.405294
3.66_329.0865m/z	329.0864813	3.6635	neg	Musca-aurin-VII	67066	Unclassified	Unclassified	Unclassified			36.2		0	M-H2O-H	C15H16N4O6	-7.64657666	2486.94325	2555.123271	2951.944505	4060.40768	4259.439129	3268.799866	2569.342625	2711.437849	2937.29134
3.69_198.0602m/z	198.0602289	3.685866667	neg	1,3,7-Trimethyluric Acid - 13C4, 15N3 (2,4,5,6-13C4, 1,3,9-15N3)	103469	Unclassified	Unclassified	Unclassified			36.2		0	M-H2O-H	C[13]4C[12]4H10N[15]3N[14]O3	-8.034378481	32.90167972	0.001403199	0.001403199	55.55196139	57.40044798	56.46736448	33.39540072	28.71578121	0.001403199
3.95_355.0627m/z	355.0627215	3.94605	neg	Neodioxynin	86326	Benzenoids	Naphthalenes	Naphthoquinones	*		36.2		0	M-H2O-H	C22H14O6	4.075113228	501.9617248	521.9485607	673.9072444	721.7013473	513.7164758	758.2974005	496.3693819	525.2773408	493.693767
3.89_265.0136m/z	265.0135758	3.8906	neg	Cassic acid	LMPK13040015	Benzenoids	Anthracenes	Anthracenecarboxylic acids and derivatives		C10401	36.2		0	M-H2O-H	C15H8O6	-2.362661645	39.3087015	0.001403199	45.83021693	87.99344664	89.84216615	64.08006499	61.22222215	68.97674488	143.9362048
3.91_374.1574m/z	374.1573926	3.912566667	neg	AM2201 6-hydroxyindole metabolite	96610	Unclassified	Unclassified	Unclassified			36.2		0	M-H	C24H22FNO2	3.230354145	556.4639121	653.0461969	499.5893314	608.4767543	680.3907769	617.5385092	465.7132246	523.4375256	534.979306
3.91_450.9826m/z	450.9826463	3.912566667	neg	2,2'-Dithenyl sulfide	HMDB0032982	Organoheterocyclic compounds	Heteroaromatic compounds	Unclassified			36.2		0	2M-H	C10H10S3	2.203845979	4812.841301	4740.852333	5168.599355	6567.370288	5920.328066	5469.318042	5655.772324	5886.135093	6072.073738
4.02_214.0335m/z	214.0335326	4.024283333	neg	Brassicanal B	93257	Organoheterocyclic compounds	Indoles and derivatives	Indoles			36.2		0	M-H2O-H	C12H11NO2S	1.390673239	173.9492105	233.2502625	233.7426077	454.0653693	564.8525644	441.557808	357.5235934	412.4619232	418.229798
4.05_414.9966m/z	414.9965378	4.046666667	neg	Sanguisorbic acid dilactone	3408	Unclassified	Phenylpropanoids and polyketides	Tannins			36.2		0	M-H2O-H	C21H10O12	4.337223935	2627.528568	2792.899418	3003.532587	4824.757104	4366.544075	4294.224124	3133.799667	3857.391321	3584.109556
4.07_385.1139m/z	385.1139182	4.069216667	neg	4-O-beta-D-Glucosyl-sinapate	65860	Unclassified	Unclassified	Unclassified			36.2		0	M-H	C17H22O10	-0.264848078	152.4525431	384.6150232	385.1822025	125.9702625	1.163223778	58.5885272	808.5048321	922.396463	687.0451691
4.11_451.0714m/z	451.0714023	4.113883333	neg	(Z)-Resveratrol 3-(6"-sulfoglucopyranoside)	HMDB0037077	Phenylpropanoids and polyketides	Stilbenes	Stilbene glycosides			36.2		0	M-H2O-H	C20H22O11S	2.044085867	1133.973809	1284.570036	1346.65889	1791.263189	1384.451343	1550.449117	1586.499881	1438.248287	1514.107768
4.14_285.0958m/z	285.0957606	4.136366667	neg	Isosalicin	89665	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			36.2		0	M-H	C13H18O7	-7.744932595	3182.100049	3359.438542	3715.323951	2901.11393	2507.266028	2549.781423	2730.547699	2710.111407	2503.543974
4.16_181.0494m/z	181.0492578	4.15895	neg	2-Phenoxyethanethiol	88580	Benzenoids	Benzene and substituted derivatives	Unclassified	*		36.2		0	M-H	C8H10OS	3.314390816	69.15536669	91.05632032	90.9936853	83.93115506	74.1942176	170.1683412	77.4278491	76.41029813	83.93115835
4.21_452.0587m/z	452.0587351	4.212116667	neg	o-O-sulfate rosiglitazone	HMDB0060858	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		36.2		0	M-H	C18H19N3O7S2	-0.949982322	552.7367631	583.6257468	496.0787846	860.1728555	760.3623086	1000.640763	675.6449098	851.6037771	678.6289968
4.52_240.0863m/z	240.0863424	4.521733333	neg	Proacacipetalin	66917	Unclassified	Unclassified	Unclassified			36.2		0	M-H2O-H	C11H17NO6	-5.417716932	1065.07237	731.9695448	407.743788	475.8344047	665.6911389	753.4822887	931.4561497	927.0759505	983.1829
4.70_328.0417m/z	328.0417379	4.703166667	neg	N2-Acetyl-L-aminoadipyl-δ-phosphate	63445	Unclassified	Unclassified	Unclassified			36.2		0	M+FA-H	C8H14NO8P	-7.659685739	1182.494555	1055.262484	1265.328725	275.4014007	347.196718	348.3249011	1304.53959	1334.187127	1544.940594
4.81_481.1319m/z	481.131942	4.814166667	neg	Arthromerin B	47243	Lipids and lipid-like molecules	Polyketides	Flavonoids			36.2		0	M-H2O-H	C21H24O10	-7.355096077	7699.513676	8058.870979	7753.983872	5791.286849	5299.826381	5663.431701	8062.0529	8889.948625	8047.138714
4.86_474.2527m/z	474.2527463	4.880083333	neg	Mebeverine	1078	Unclassified	Unclassified	Unclassified			36.2		0	M+FA-H	C25H35NO5	7.035975444	2727.27	2965.945899	2490.539693	2506.283983	2570.097048	2307.763041	2097.486053	2513.545421	2373.005183
4.90_615.1035m/z	615.1035293	4.902316667	neg	Delphinidin 3-(2"-galloylgalactoside)	47032	Unclassified	Unclassified	Unclassified			36.2		0	M-H	C28H24O16	7.094705204	14565.01548	15175.74487	16513.51658	14697.28468	13655.23566	14708.66084	14623.24462	14702.93123	10982.65769
4.95_425.0920m/z	425.0919629	4.94705	neg	Formononetin 7-O-glucuronide	96093	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavonoid O-glycosides	*		36.2		0	M-H2O-H	C22H20O10	9.360878138	8868.717679	9568.411648	9534.558657	2742.895212	2735.33001	2702.739073	1752.528872	1405.28836	1464.551572
4.97_410.1800m/z	410.1799584	4.969683333	neg	Abiraterone sulfate	HMDB0060584	Lipids and lipid-like molecules	Steroids and steroid derivatives	Sulfated steroids	*		36.2		0	M-H2O-H	C24H31NO4S	0.978632108	1674.641833	2788.667289	3054.215249	1492.421589	1899.69018	1275.505419	1843.358482	1482.039217	1951.099986
4.99_252.0855m/z	252.0855086	4.99225	neg	Deidaclin	66908	Unclassified	Unclassified	Unclassified			36.2		0	M-H2O-H	C12H14O6	-8.253290862	795.1656397	875.5141266	907.2637401	229.1737602	205.132162	308.5367798	1070.948905	853.7327181	786.8357309
4.99_341.1063m/z	341.023389	4.99225	neg	Glucoasiaticoside	HMDB0301840	Unclassified	Unclassified	Unclassified			36.2		0	M-H2O-H	C15H18O9S2	-2.96638151	973.1274141	1294.744414	1150.816187	1028.15638	1259.244614	1215.337685	951.7927228	853.0293104	551.6193722
4.99_343.0844m/z	343.0843929	4.99225	neg	8-Demethylsideroxylin	49445	Phenylpropanoids and polyketides	Flavonoids	O-methylated flavonoids	*		36.2		0	M+FA-H	C17H14O5	6.932490896	834.9301954	801.8053547	805.359416	759.6015457	1098.570224	967.1462432	1314.489332	1023.244879	1039.390422
5.01_471.0976m/z	471.0975767	5.014716667	neg	Cyanidin 3-(6-acetylgalactoside)	46876	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	*		36.2		0	M-H2O-H	C23H22O12	8.756563738	820.3123391	730.3913519	1035.53197	2124.195359	2399.739427	2279.045649	433.99643	849.0960524	565.6913253
5.08_347.1715m/z	347.1715065	5.080566667	neg	(1S,2S,4R)-p-Menth-8-ene-1,2,10-triol 2-glucoside	94041	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		36.2		0	M-H	C16H28O8	1.048516684	762.3629356	853.2236716	881.4491107	734.1248969	589.2226286	911.4376201	827.8399321	1089.022644	775.8364962
5.18_217.0483m/z	217.0483541	5.1777	neg	Methoxsalen Metabolite	1209	Unclassified	Unclassified	Unclassified			36.2		0	M-H2O-H	C12H10O5	-9.650675217	5864.381873	6701.177924	5504.160962	1183.06851	1239.710127	1027.386407	699.3914698	721.0453918	835.7074286
5.18_247.0824m/z	247.082383	5.1777	neg	3-Deacetonosine	HMDB0245849	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	*	C01736	36.2		0	M-H2O-H	C11H14N4O4	-4.906196193	205.7218713	478.3866273	247.0895521	0.001403199	0.001403199	0.001403199	155.3516709	46.34148216	368.7483087
5.24_297.1322m/z	297.1321821	5.244033333	neg	Sesamex	72887	Unclassified	Unclassified	Unclassified			36.2		0	M-H	C15H22O6	-7.311624763	1565.013214	1508.928654	1418.45795	2335.687304	2247.390055	2130.266916	1200.859391	1217.346617	1516.71496
5.29_365.0858m/z	365.0857697	5.28555	neg	4-p-Coumaroyl-1,5-quinolactone	86164	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	*		36.2		0	M-H	C16H16O7	-6.360664635	0.001403199	132.4677974	127.0342625	1430.74057	1674.594703	1807.06386	2971.505757	2458.869674	2865.725571
5.47_267.0851m/z	267.0851446	5.471616667	neg	Methylarbutin	71805	Unclassified	Unclassified	Unclassified			36.2		0	M-H2O-H	C13H18O7	-7.924208634	1619.360411	1628.664171	1745.788986	1543.052608	1341.250156	1738.602857	1588.763008	1435.762076	1196.144283
5.56_735.1997m/z	735.1997218	5.56185	neg	Penicillic acid V	1740	Unclassified	Unclassified	Unclassified			36.2		0	M-H	C36H32O16S	-1.924083422	6021.074979	5572.742409	4838.742662	8816.386822	10662.28951	9201.127507	5066.588905	6670.235522	5647.596786
5.56_803.1871m/z	803.1870719	5.56185	neg	Pelargonidin 3-arabinoside	46856	Unclassified	Unclassified	Unclassified			36.2		0	2M-H	C20H18O9	5.202720492	4746.775056	4467.660515	3921.504027	5758.236828	7176.65531	5832.712963	3474.727583	3695.673371	2505.63828
5.92_377.0804m/z	377.0804396	5.9168	neg	N-Acetylisatin	63543	Unclassified	Unclassified	Unclassified			36.2		0	2M-H	C10H7NO3	6.691154022	280.4385148	123.0505472	49.11959182	333.5597722	242.7947143	298.3344954	131.4473721	288.516721	194.072784
6.03_259.0589m/z	259.0588722	6.028183333	neg	(S)-ACPA	69626	Unclassified	Unclassified	Unclassified			36.2		0	M+FA-H	C8H10N2O5	7.931747545	373.4784102	518.3461788	455.1312534	1114.473035	1024.435372	858.4265005	516.0495513	643.0894222	599.6853858
6.17_320.1531m/z	320.1530941	6.171316667	neg	4,5-Dihydropiperlonguminine	95874	Organoheterocyclic compounds	Benzodioxoles	Unclassified	*		36.2		0	M+FA-H	C16H21NO3	9.986000123	144.105643	47.08749231	76.17916177	998.25915	1079.22455	1195.624681	213.0591604	286.8272407	229.8209798
6.20_527.2677m/z	527.2676882	6.195716667	neg	ent-6R,8S,9R,10R,17-Trihydroxy-7-oxo-6,7-seco-19,6-kauranolide 6-O-glucoside	HMDB0038546	Lipids and lipid-like molecules	Terpene glycosides	Diterpenoid glycosides	*		36.2		0	M-H	C26H40O11	3.970536038	1545.097994	2563.334537	3606.128948	2803.562838	2275.33268	2988.971783	3190.094663	1951.166231	
6.

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0.56_476.8308m/z	476.8308219	0.557883333	neg
0.56_488.8041m/z	488.8041335	0.557883333	neg
0.56_503.7884m/z	503.7884101	0.557883333	neg
0.56_515.8159m/z	515.8158598	0.557883333	neg
0.56_520.8373m/z	520.8373249	0.557883333	neg
0.56_529.8698m/z	529.8697512	0.557883333	neg
0.56_530.7927m/z	530.792746	0.557883333	neg
0.56_538.8256m/z	538.8256143	0.557883333	neg
0.56_598.7802m/z	598.7802029	0.557883333	neg
0.56_606.8134m/z	606.8133529	0.557883333	neg
0.56_666.7682m/z	666.7681567	0.557883333	neg
0.56_734.7564m/z	734.7564229	0.557883333	neg
0.56_803.8188m/z	803.8188463	0.557883333	neg
0.56_812.7723m/z	812.7722827	0.557883333	neg
0.58_102.9487m/z	102.9487493	0.58075	neg
0.58_103.9203m/z	103.9203034	0.58075	neg
0.58_104.9539m/z	104.9538778	0.58075	neg
0.58_119.9470m/z	119.9470278	0.58075	neg
0.58_140.9807m/z	140.9806598	0.58075	neg
0.58_146.9660m/z	146.965986	0.58075	neg
0.58_152.8951m/z	152.8951488	0.58075	neg
0.58_156.8949m/z	156.8949297	0.58075	neg
0.58_158.8933m/z	158.8932565	0.58075	neg
0.58_163.9290m/z	163.9289561	0.58075	neg
0.58_164.8956m/z	164.8955504	0.58075	neg
0.58_177.9208m/z	177.9207918	0.58075	neg
0.58_178.8155m/z	178.8154944	0.58075	neg
0.58_179.9365m/z	179.9364516	0.58075	neg
0.58_187.9290m/z	187.9290378	0.58075	neg
0.58_188.9130m/z	188.9129526	0.58075	neg
0.58_188.9333m/z	188.933288	0.58075	neg
0.58_190.9286m/z	190.9286158	0.58075	neg
0.58_196.8850m/z	196.88504	0.58075	neg
0.58_198.9365m/z	198.9365124	0.58075	neg
0.58_205.9157m/z	205.9157089	0.58075	neg
0.58_207.9313m/z	207.9313427	0.58075	neg
0.58_213.9185m/z	213.9185126	0.58075	neg
0.58_221.8007m/z	221.8007196	0.58075	neg
0.58_223.8819m/z	223.8819275	0.58075	neg
0.58_225.7962m/z	225.7961992	0.58075	neg
0.58_232.9057n	464.802768	0.58075	neg
0.58_247.9239m/z	247.9238962	0.58075	neg
0.58_250.8839m/z	250.8839491	0.58075	neg
0.58_256.9208m/z	256.920808	0.58075	neg
0.58_258.9159m/z	258.9159447	0.58075	neg
0.58_261.8511m/z	261.8511167	0.58075	neg
0.58_262.8584m/z	262.8584338	0.58075	neg
0.58_264.8725m/z	264.8725238	0.58075	neg
0.58_273.9034m/z	273.9033749	0.58075	neg
0.58_296.8905m/z	296.8904849	0.58075	neg
0.58_297.8275m/z	297.8274753	0.58075	neg
0.58_297.9008m/z	297.9008423	0.58075	neg
0.58_307.8562m/z	307.8562467	0.58075	neg
0.58_323.9104m/z	323.910368	0.58075	neg
0.58_326.9036m/z	326.9035845	0.58075	neg
0.58_332.8602m/z	332.8602039	0.58075	neg
0.58_341.8906m/z	341.8905753	0.58075	neg
0.58_355.8596m/z	355.8596414	0.58075	neg
0.58_365.8883m/z	365.8882973	0.58075	neg
0.58_371.9012m/z	371.9011592	0.58075	neg
0.58_373.8281m/z	373.8281213	0.58075	neg
0.58_375.8436m/z	375.8435837	0.58075	neg
0.58_376.8516m/z	376.8515835	0.58075	neg
0.58_392.8959m/z	392.8958614	0.58075	neg
0.58_393.8513n	374.8334265	0.58075	neg
0.58_400.8473m/z	400.8472846	0.58075	neg
0.58_404.8460m/z	404.8459618	0.58075	neg
0.58_409.8776m/z	409.8776199	0.58075	neg
0.58_411.8814m/z	411.8814018	0.58075	neg
0.58_418.8260m/z	418.8260282	0.58075	neg
0.58_423.8473m/z	423.8472526	0.58075	neg
0.58_433.8023m/z	433.8022984	0.58075	neg
0.58_433.8758m/z	433.8757998	0.58075	neg
0.58_441.8156m/z	441.8156337	0.58075	neg
0.58_443.8312m/z	443.8311647	0.58075	neg
0.58_444.8378m/z	444.837771	0.58075	neg
0.58_447.8282m/z	447.8282022	0.58075	neg
0.58_460.8832m/z	460.8832326	0.58075	neg
0.58_462.8055m/z	462.8054568	0.58075	neg
0.58_462.8787m/z	462.8786888	0.58075	neg
0.58_468.8348m/z	468.8348174	0.58075	neg
0.58_470.8378m/z	470.8378022	0.58075	neg
0.58_472.8340m/z	472.8339852	0.58075	neg
0.58_476.7760m/z	476.7760454	0.58075	neg
0.58_479.8688m/z	479.8687867	0.58075	neg
0.58_486.8135m/z	486.8134734	0.58075	neg
0.58_488.8289m/z	488.8288641	0.58075	neg
0.58_501.7899m/z	501.7899435	0.58075	neg
0.58_501.8634m/z	501.8634134	0.58075	neg
0.58_509.8033m/z	509.8033165	0.58075	neg
0.58_511.8190m/z	511.8189705	0.58075	neg
0.58_519.7590m/z	519.7589877	0.58075	neg
0.58_521.7741m/z	521.7741226	0.58075	neg
0.58_536.8250m/z	536.8249722	0.58075	neg
0.58_540.8216m/z	540.8216102	0.58075	neg
0.58_545.8535m/z	545.8534806	0.58075	neg
0.58_554.7999m/z	554.7999088	0.58075	neg
0.58_569.7777m/z	569.777678	0.58075	neg
0.58_570.8582n	615.8394531	0.58075	neg
0.58_577.7909m/z	577.7909361	0.58075	neg
0.58_579.8071m/z	579.8070935	0.58075	neg
0.58_587.7471m/z	587.7471126	0.58075	neg
0.58_608.8094m/z	608.8093825	0.58075	neg
0.58_612.7527m/z	612.7526579	0.58075	neg
0.58_622.7868m/z	622.7867809	0.58075	neg
0.58_645.7776m/z	645.7775984	0.58075	neg
0.58_647.7947m/z	647.7946822	0.58075	neg
0.58_663.8416m/z	663.8415574	0.58075	neg
0.58_676.7969m/z	676.7968523	0.58075	neg
0.58_683.8308m/z	683.8307832	0.58075	neg

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1724.726847	1592.597904	1602.952544	1716.759896	1835.507892	1628.220794	1441.010832	1487.786134	1643.352192	
817.2579763	738.62794	807.284211	606.2141925	572.1397399	685.1445296	671.6001851	265.414701	888.4184937	
4632.918803	3785.392026	3207.225134	2556.179109	7756.024922	5605.673541	2971.852779	3239.379928	4413.936415	
6688.315959	6363.622679	6150.577322	4489.273061	5123.052221	5230.943181	6589.157114	4303.565492	5120.503721	
693.1825552	738.6450038	463.5859046	691.7894109	635.5703277	968.0485161	809.8379202	301.3197021	567.9520446	
6452.842482	4836.495691	3859.832107	3365.023261	3307.422776	3025.380114	4517.048091	2996.642754	3198.876884	
5696.174471	4085.597382	3900.008578	2700.288033	3209.452554	3040.778475	4287.064148	2729.922379	4000.678844	
5529.684979	4743.9275	5560.458727	3309.455284	2885.26512	3296.466816	4605.604986	2747.857006	2804.504174	
4681.113495	4205.432786	3486.397265	2633.134858	2141.83768	1976.096958	4051.834217	2221.436442	3023.509101	
2947.315852	2912.493462	2992.074634	1825.782907	1867.916444	2320.709899	2732.994049	1584.333365	1772.196266	
1849.041944	2184.530781	1605.305615	1536.934334	1428.292734	1551.803409	2221.222161	859.4424438	1387.036655	
375.7282892	706.4916641	462.163243	545.1108096	356.086681	596.8305426	541.7566969	162.5031959	202.8160642	
6509.218484	5674.117014	4798.837456	3539.433046	5307.764747	4677.689312	5603.736611	2475.109494	3277.060298	
945.4376954	731.8192023	684.0077513	780.8534599	693.4359965	865.8631323	828.5995781	635.3326891	604.6121986	
566.8261446	558.7562859	606.7009244	531.2224742	511.2969526	597.5763092	601.3749851	587.7170893	518.7195714	
371.896961	418.7002355	345.3580482	281.2505169	260.2346764	292.3652887	415.0376913	322.8347397	266.4191655	
265.7709445	265.3424733	257.4420936	216.3276586	192.254277	217.6938661	316.6764592	250.2016799	211.9063397	
254.9038874	283.9428607	240.2146615	237.4273571	247.1162109	257.5195774	296.7976073	269.1712914	242.7170804	
2971.983125	3066.418652	3621.687032	3203.002584	3412.794791	3219.405008	3480.646226	3014.538949	3200.011173	
1133.675633	1119.487325	1174.779242	1143.250925	1087.73957	1078.220348	951.8609254	933.1368841	1074.308727	
1356.280022	1244.457717	1244.949094	1258.609081	1353.291167	1273.120873	1422.676667	1238.646397	1337.250076	
835.0768561	777.6636841	913.0301386	769.0693986	870.3380886	912.0295169	847.6770823	849.9342681	851.1787656	
3868.020467	4699.704719	3847.565123	3432.31915	3507.858472	3724.38866	4568.908853	3872.17675	4476.49585	
793.6783449	874.5815611	975.5268282	865.1369426	940.170719	911.175544	962.5147383	925.2447104	945.443936	
422.0567384	348.9380877	267.9451968	387.2241748	270.671694	251.6115109	391.1662707	263.1889763	226.7231668	
348.0918043	324.1782645	226.9276001	277.1426646	65.97337661	157.6621251	345.2015498	184.1669502	89.45221721	
4498.790302	4303.487345	4847.352123	4128.886393	4202.343456	4199.087134	4489.739786	4122.192955	4668.194048	
694.4546626	674.8584089	591.9731546	591.7285887	870.8731342	814.4102394	548.712476	601.3427012	818.4980722	
720.7445435	684.5290125	587.3465184	753.6789715	665.4575137	654.5739152	698.9838957	601.3676688	708.9859881	
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88605.45229	75488.27944	75770.04382	68785.67774	73113.0286	80562.6682	76641.64422	62724.83161	67999.57835	
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5989.186021	5880.437669	6642.936853	5638.737237	6458.466039	5834.844428	6171.662188	5913.944253	6526.957863	
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685.3618354	729.5386526	716.8577233	543.2768814	610.4695005	590.8293312	523.4900304	528.2337689	587.3246661	
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862.527727	622.2834502	497.458698	600.3915603	540.7870527	640.6432581	638.8257801	505.1599426	454.1025909	
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933.7891373	1067.784986	1037.889758	942.2393553	700.1067521	1130.196083	1056.628811	1171.025439	949.9336604	
1099.520179	1203.430715	820.6709837	751.9291162	464.4329761	692.0537497	1341.651607	908.8415293	588.153876	
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10319.13314	8365.236654	7020.790745	7674.829036	6396.972744	6887.962273	7572.385622	6581.417202	6362.225002	
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97838.62544	83277.93723	85513.15932	72775.24644	78635.72561	82388.15014	85538.74405	69142.1939	74528.2202	
6569.75858	5215.398144	4905.404416	4900.837144	4405.542954	4861.631305	4514.948375	3629.365669	3966.620851	
2708.691451	2909.486418	3352.452055	2633.711633	3255.45246	2567.030487	2828.898045	2610.110517	2879.622229	
1734.821715	1810.098887	1609.035681	1328.878681	1159.415492	1392.60583	1758.345977	1426.522875	1131.37485	
12138.48778	12923.61653	14730.97677	11724.89241	13886.19006	12184.83767	13145.56118	11410.79506	14380.37127	
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5046.949163	4575.347642	4473.649669	3445.302489	4176.47387	4202.548264	3789.053606	3466.520225	3635.141551	
9104.759211	7258.90746	6535.234437	6669.991865	5471.678042	6711.192696	7365.951077	5915.436473	5172.879153	
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5338.959191	5059.107578	4785.706767	4376.760272	5091.396869	5303.671586	4931.976199	4147.388516	5505.620327	
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4400.562379	4334.637492	5015.712137	3618.920709	5232.129741	4515.063848	4508.327443	3908.84019	4166.461212	
5663.064378	3973.764138	3739.294239	3965.352788	3440.630598	3901.576274	3930.575366	3274.637223	2947.068837	
4160.922076	4380.845009	3829.490457	3684.004759	2900.611621	4105.358809	3983.486654	3809.944309	3254.055141	
27657.45447	25429.55455	27866.30673	26768.7039	29630.84175	29287.43313	29172.25154	27763.76859	29599.04773	
1092.454913	856.6993794	684.4650891	931.9669833	646.5540956	857.6836916	881.6680504	837.5775852	723.6884832	
1123.277279	1416.737266	1657.64373	1148.90117	1530.529533	1137.142715	1332.42083	1162.083697	1330.658612	
2941.326951	2866.445191	3559.261516	1949.676208	2727.43703	2097.662859	2445.18869	2424.528273	2524.818246	
8256.007458	8759.876382	9955.213401	7298.597602	12124.39606	10664.57154	9624.795634	9303.451913	13641.007	
6464.83314	5614.266834	5842.372824	4362.428427	5420.594888	4990.09654	4757.440243	4483.168991	5146.240491	
16208.8155	13595.59033	13343.96141	11309.93668	12241.07325	11867.97112	11812.72733	10212.33658	11194.33291	
5517.209004	4083.847205	5230.978579	3497.27545	5606.223019	4314.219599	4118.578552	3699.289277	5459.144834	
1048.250498	941.547379	1343.94695	734.2670431	1048.496444	1477.270146	939.9078926	932.3118838	1095.22061	
2009.270914	1679.117126	2068.497442	1322.826589	2430.312325	1994.090462	1869.395683	1572.802468	2241.397756	
5997.641378	4952.088046	2720.231695	3534.828427	2431.281218	2881.848554	4317.193137	3676.202499	2991.266267	
73764.05275	64586.97536	66561.55633	54403.37359	57244.90796	61309.27927	68137.90396	54202.96918	58964.12542	
2574.583347	2513.023349	2976.880755	2280.817669	2769.397543	2624.792814	2595.899181	2248.974653	2652.387152	
5862.57113	4283.317758	4449.453032	3837.78199	3409.741944	3886.824016	3746.622126	3364.553815	4537.144508	
34686.42458	25753.63998	25179.54808	22459.71171	22103.78335	24736.04044	24579.62908	18058.33417	19914.31582	
5615.455067	3196.111605	3154.50569	2888.218325	2817.61941	3654.509235	2956.563085	3123.522646	1945.018478	
6717.520824	6848.407514	6887.062085	6098.042429	6803.277544	6113.693578	7185.062612	6190.344129	6426.316702	
1461.589315	1693.05992	1972.112014	1356.070394	1672.180777	1891.549027	1717.674365	1330.500565	1327.980798	
540.785756	643.429113	670.3662726	481.7836911	498.741652	285.2270027	391.1846251	192.7565498	529.8069812	
1214.323017	971.3308561	1337.875769	900.3001777	1087.193179	966.4904178	1134.122489	1095.763454	894.1591322	
5071.746851	4966.986973	5515.663259	4231.672654	5446.901728	5170.711414	4965.238751	4171.270409	5460.368491	
6022.279161	5211.266118	5605.449699	4359.49437	5431.376083	4724.063494	5176.576074	5044.612102	5484.234574	
10203.00559	8942.2337	9682.898857	7446.673488	9574.206068	7775.053778	9668.869477	7673.793335	9453.229461	
981.9944253	533.5474222	437.5797539	490.1523666	293.5667495	451.3986274	436.9621713	308.5975216	336.0989195	
10486.03878	7940.800799	6029.162895	5253.822233	6094.672851	5609.821311	7125.681729	4824.666803	4709.895251	
3109.669645	4870.22875	3253.529618	2917.828595	2633.556795	3396.795542	3883.999263	3501.072296	3931.424126	
20944.03384	15402.46848	16965.70393	12086.7683	15595.97185	15416.35069	14310.63557	11259.28859	13693.06445	
1897.13827	2582.827919	2426.455783	2122.544235	1856.11667	2301.556165	2201.574252	2023.557251	2007.238423	
1566.538992	1581.890054	853.9384324	1082.086001	838.7292306	1125.812902	1283.396445	734.3326797	956.3923008	
1063.934137	1156.717889	1286.613593	950.3537929	917.6626913	873.0431026	1012.997206	760.9958458	732.1605127	
6635.382404	7359.30478	6090.724111	6425.332834	7320.906072	7263.785242	6843.350382	6675.899574	6075.930501	
5833.970261	5362.143045	5246.217797	3702.946628	4470.54341	4376.388353	4610.288315	4216.293799	4260.4657	
10796.85253	8979.233962	9135.459894	7057.199198	8424.647329	7388.666997	8843.778174	7141.411847	8663.27469	
1220.070369	808.2447344	557.3867007	451.1552078	450.5204414	679.3258908	1223.916902	760.9300919	550.9643592	
20113.1463	15902.8195	16177.525	12128.95715	15804.42802	15034.58941	15171.66728	9850.158023	12531.84615	
1838.806667	743.1637294	574.8282112	793.7228752	206.0404449	0.001403199	363.7645469	523.8854271	515.1899277	
1376.496872	1373.195358	1504.695079	710.8837182	739.2343383	1480.872864	526.755287	801.469925	1068.576409	
4245.308214	3566.968514	4492.503233	3731.811994	4133.116589	4265.498558	4510.581358	3925.285298	3509.882804	
7715.484573	7091.4873	7253.559075	5393.757786	4908.206573	5295.760543	6100.475996	5364.352515	6070.912197	
542.5366482	458.5149201	372.7966786	950.752404	1153.218455	339.5414303	1185.780974	806.6098874	810.1496024	
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0.58_713.7645m/z	713.7645078	0.58075	neg																		
0.58_715.7816m/z	715.7816149	0.58075	neg																		
0.58_744.7846m/z	744.784552	0.58075	neg																		
0.60_105.9359m/z	105.9359283	0.6034	neg																		
0.60_142.9963m/z	142.9962606	0.6034	neg																		
0.60_187.9419m/z	187.9419393	0.6034	neg																		
0.60_190.8886m/z	190.8886119	0.6034	neg																		
0.60_239.9033m/z	239.9033147	0.6034	neg																		
0.60_447.9198m/z	447.9197707	0.6034	neg																		
0.60_528.8693m/z	528.869319	0.6034	neg																		
0.60_567.8375n	612.8296931	0.6034	neg																		
0.60_593.8499m/z	593.8499006	0.6034	neg																		
0.60_596.8561m/z	596.8561344	0.6034	neg																		
0.60_623.7844m/z	623.7843758	0.6034	neg																		
0.60_625.8007m/z	625.8006547	0.6034	neg																		
0.60_664.8428m/z	664.8428261	0.6034	neg																		
0.60_674.8006m/z	674.8006357	0.6034	neg																		
0.60_693.7875m/z	693.7874685	0.6034	neg																		
0.60_728.8114m/z	728.8113996	0.6034	neg																		
0.63_114.9887m/z	114.9886631	0.62565	neg																		
0.63_118.9663m/z	118.9663052	0.62565	neg																		
0.63_120.9549m/z	120.9549102	0.62565	neg																		
0.63_122.8943m/z	122.8942694	0.62565	neg																		
0.63_123.9021m/z	123.9020551	0.62565	neg																		
0.63_127.8703m/z	127.8703499	0.62565	neg																		
0.63_130.9837m/z	130.9836927	0.62565	neg																		
0.63_146.9614m/z	146.9613531	0.62565	neg																		
0.63_148.9498m/z	148.9498021	0.62565	neg																		
0.63_150.9470m/z	150.9470166	0.62565	neg																		
0.63_152.9445m/z	152.9445025	0.62565	neg																		
0.63_158.9786m/z	158.97864	0.62565	neg																		
0.63_160.9828m/z	160.9827772	0.62565	neg																		
0.63_164.9350m/z	164.934979	0.62565	neg																		
0.63_164.9487n	145.9308274	0.62565	neg																		
0.63_168.8364m/z	168.8364499	0.62565	neg																		
0.63_175.9688m/z	175.9687967	0.62565	neg																		
0.63_180.9127m/z	180.9127076	0.62565	neg																		
0.63_189.8708m/z	189.8707905	0.62565	neg																		
0.63_193.974n	174.9561836	0.62565	neg																		
0.63_197.9025m/z	197.9025394	0.62565	neg																		
0.63_199.8996m/z	199.8996385	0.62565	neg																		
0.63_207.8369m/z	207.8368873	0.62565	neg																		
0.63_215.8687m/z	215.868655	0.62565	neg																		
0.63_216.9373m/z	216.9373081	0.62565	neg																		
0.63_216.9692m/z	216.9691952	0.62565	neg																		
0.63_217.8656m/z	217.8656298	0.62565	neg																		
0.63_225.8976m/z	225.8975528	0.62565	neg																		
0.63_226.9662m/z	226.9661985	0.62565	neg																		
0.63_228.9701m/z	228.9701211	0.62565	neg																		
0.63_231.9162n	276.9140597	0.62565	neg																		
0.63_232.9229m/z	232.9229271	0.62565	neg																		
0.63_234.9353m/z	234.9353157	0.62565	neg																		
0.63_236.9319m/z	236.931924	0.62565	neg																		
0.63_238.9642m/z	238.9642048	0.62565	neg																		
0.63_244.9510n	289.9492292	0.62565	neg																		
0.63_244.9641m/z	244.9640893	0.62565	neg																		
0.63_261.9543m/z	261.9543368	0.62565	neg																		
0.63_262.9304m/z	262.9303504	0.62565	neg																		
0.63_265.9350n	530.866128	0.62565	neg																		
0.63_266.8854m/z	266.8853677	0.62565	neg																		
0.63_268.8824m/z	268.8824395	0.62565	neg																		
0.63_272.9592m/z	272.9592073	0.62565	neg																		
0.63_275.9063m/z	275.9062596	0.62565	neg																		
0.63_278.9085m/z	278.908482	0.62565	neg																		
0.63_283.8754m/z	283.8754266	0.62565	neg																		
0.63_284.9249m/z	284.9249467	0.62565	neg																		
0.63_291.8840m/z	291.8839835	0.62565	neg																		
0.63_293.9045m/z	293.9044604	0.62565	neg																		
0.63_293.9369n	274.9190675	0.62565	neg																		
0.63_294.8801m/z	294.8800561	0.62565	neg																		
0.63_294.9536m/z	294.9535723	0.62565	neg																		
0.63_296.8772m/z	296.8772076	0.62565	neg																		
0.63_300.8225m/z	300.832523	0.62565	neg																		
0.63_301.9201n	300.9102186	0.62565	neg																		
0.63_302.9140m/z	302.9139639	0.62565	neg																		
0.63_304.9087m/z	304.9086871	0.62565	neg																		
0.63_305.9266m/z	305.9266093	0.62565	neg																		
0.63_306.9391m/z	306.9391215	0.62565	neg																		
0.63_307.9545n	288.9366914	0.62565	neg																		
0.63_312.9520m/z	312.9520197	0.62565	neg																		
0.63_318.8909m/z	318.8909436	0.62565	neg																		
0.63_319.8964m/z	319.8964104	0.62565	neg																		
0.63_320.8870m/z	320.88702	0.62565	neg																		
0.63_323.8971m/z	323.8970652	0.62565	neg																		
0.63_330.9177m/z	330.9176666	0.62565	neg																		
0.63_335.9423n	380.9391492	0.62565	neg																		
0.63_338.8888m/z	338.8888353	0.62565	neg																		
0.63_341.9590n	340.9466772	0.62565	neg																		
0.63_343.8940m/z	343.8940155	0.62565	neg																		
0.63_344.9019m/z	344.9018925	0.62565	neg																		
0.63_346.8951m/z	346.8950613	0.62565	neg																		
0.63_356.9243m/z	356.9242953	0.62565	neg																		
0.63_358.9450m/z	358.9450102	0.62565	neg																		
0.63_373.9057n	418.8932265	0.62565	neg																		
0.63_374.9261m/z	374.9260953	0.62565	neg																		
0.63_398.9043m/z	398.9042915	0.62565	neg																		
0.63_403.9244n	402.9171321	0.62565	neg																		
0.63_408.9342m/z	408.9341632	0.62565	neg																		
0.63_424.9119m/z	424.9118821	0.62565	neg																		
0.63_426.9317m/z	426.9317254	0.62565	neg																		
0.63_435.7994m/z	435.7993647	0.62565	neg																		
0.63_435.8745n	434.8672015	0.62565	neg																		
0.63_440.8846m/z	440.8845866	0.62565	neg																		
0.63_442.9099m/z	442.909916	0.62565	neg																		
0.63_444.8267m/z	444.8266982	0.62565	neg																		
0.63_455.9282m/z	455.9281736	0.62565	neg																		
0.63_457.8754m/z	457.8753875	0.62565	neg																		
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0.63_471.9121n	470.9048728	0.62565	neg																		

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2499.213071	1920.116629	2837.315878	1497.897748	1574.077342	1950.832029	1690.3137	1764.356147	2252.477421													
4398.778866	4299.942565	3818.027727	2270.91868	2683.547737	4097.541823	2781.053924	3188.059895	2795.697929													
9185.116867	8414.314219	8019.624878	6433.688856	6055.257783	7866.178178	8488.114887	4467.442933	6014.53613													
152.1129565	153.3552576	158.8807784	162.09326	107.4302896	161.3865352	165.2496652	170.1406985	150.0197622													
227.2086362	247.8955079	286.5325098	270.5626958	207.47388	303.2753343	311.1597365	231.2214279	232.1666379													
472.0709367	501.9458076	323.0992377	374.8240289	266.542107	242.0514443	387.9549484	229.8949566	104.0231447													
421.3862841	426.5335682	434.0996243	511.789771	325.8837269	379.264796	551.509395	424.6381607	438.564087													
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1122.158209	867.4225432	1080.915357	887.5617084	886.4912044	398.3230709	1815.232719	255.1326447	703.1545213													
3292.743008	3882.343498	4743.633925	3902.49049	4065.770784	4306.452278	4378.097754	3590.375447	3838.831769													
3787.724519	3807.29747	3035.129153	1920.217215	2905.74274	2454.259083	4632.483801	3432.976872	2600.640601													
1300.293409	1411.582908	1513.459258	806.0522038	1608.306295	150.9068188	1667.77469	1588.12945	758.3807973													
3639.871459	3035.808318	4556.105387	2766.863477	3737.018585	3302.039538	4542.744407	2856.489475	5069.008874													
2056.94303	1872.210861	1665.956102	1610.671722	2109.163102	1749.096077	2121.891934	2094.075408	1346.995543													
2564.428154	2171.024362	1516.276404	1804.091861	2253.777923	1837.418264	1892.024118	972.2287827	920.792493													
1254.878536	2106.344734	1859.689477	1177.557693	1332.130688	543.5412573	1056.666323	1645.111088	1195.229387													
2961.3001	2101.497785	1185.487851	1611.818136	2012.134085	1066.434573	1733.374358	2567.072656	2216.822292													
2157.717159	2223.351622	933.3744873	1470.41197	1455.275598	1513.967831	1640.059239	1402.25901	781.4680825													
3004.345344	2944.303389	2880.908697	1291.975127	1967.220785	1284.881426	3333.348553	1379.594894	2219.385229													
924.0473192	913.7378092	1187.161233	1328.555101	1734.001368	1364.856364	1414.288233	1788.861293	2051.566041													
292.5874973	403.4679447	306.7543752	263.4544707	246.5543109	367.6984057	413.8440602	377.7885662	417.3197873													
321.2558071	358.0385185	371.9015479	402.4779794	370.2276771	441.5963509	419.1800706	365.0125705	368.2305197													
768.2813748	868.6502794	771.8433618	831.5335569	721.7834299	821.9258292	1082.819285	897.711999	828.7461528													
726.6245859	719.3555923	689.9323293	792.9558178	571.8264095	691.6152206	786.2405704	756.6549038	551.8900282													
411.0938724	515.7683286	574.2207026	546.9411339	373.4044233	598.0692127	688.8200818	615.3599027	407.5213568													
5925.507004	6567.063123	6864.791172	8176.911355	8583.329511	8590.870119	8990.044944	9098.088377	9457.470099													
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59.85270518	76.50885958	142.0709542	64.58726452	75.70706159	79.567622	69.24854509	179.088595	134.8238599													
67462.70795	72897.0504	76999.13992	91202.85981	94687.74378	92571.14317	100901.1814	105918.6267	107209.3802													
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2696.107635	2753.111972	2608.30622	2561.023172	2273.175243	2732.712797	2889.762434	2642.791949	2278.538996													
186.5168566	202.432429	241.3293442	155.4569801	207.4424792	135.5893542	148.2865555	251.7556789	236.3248088													
3888.778298	4059.427606	4487.220936	4886.791845	5152.462752	5353.510727	5827.937549	5580.759913	5302.644499													
394.3349926	647.0180016	438.6656854	300.8940766	312.1164846	415.4054173	596.8579508	478.9601418	406.4034242													
1229.901363	1528.47697	1773.026757	1572.50072	1824.667448	1638.631735	1922.377121	2103.93283	1890.057602													
68719.24777	96178.53856	76620.10832	82566.2938	87747.42059	88639.36563	106182.362	110650.0608	123105.4421													
6770.425088	7968.146011	8598.743679	7900.430568	8613.513022	7707.494661	9140.830669	9479.441307	9739.162235													
2068.528006	2550.520673	2375.933323	2543.930263	2447.112921	2566.956444	2844.247229	3023.254361	2764.495692													
683.7008109	930.0323637	1161.750948	1053.04664	680.479707	1089.127147	1313.928012	1316.974777	692.6522814													
5035.227503	6476.131144	7417.010144	5244.48126	6983.584861	5835.030467	8054.822532	6770.233947	7226.986637													
1992.550284	1896.531145	2290.953971	2465.574488	2663.080707	2231.031655	3075.075189	2378.216564	2614.181821													
100.9132121	70.6903442	106.0589791	227.4077898	125.2913955	361.7321848	208.3820456	350.7195601	175.138107													
3826.607384	5252.747874	5636.221357	4165.788809	5646.027446	4492.993137	6422.610872	5608.729463	6138.286261													
5361.378475	6736.470859	6548.446471	5948.695857	6540.086592	6189.734813	7624.531679	7163.74373	7521.265491													
42666.69693	43842.00465	49302.94018	52686.95466	57306.87524	54409.21064	60200.76541	58609.07066	59404.66879													
476.9139155	625.51623	504.5766498	379.6701089	633.9907786	343.6025897	592.7934174	514.7149641	648.1568761													
20453.90541	19301.59911	18143.91303	22080.12617	23770.56023	23245.06069	22728.96218	23815.50514	23276.53439													
1606.791983	1593.017111	1752.665357	2137.644656	1897.80716	2132.79265	1893.654971	1936.249699	1869.371628													
588.0592238	787.8273621	964.9426207	1422.688133	1549.422583	1294.587416	1361.957359	1838.636404	1647.745403													
607.372836	624.2068521	669.2765103	841.2093313	1030.517699	1014.835419	764.8556972	1310.244617	1018.645822													
2221.507829	1515.534776	2184.630794	2091.263582	1678.699021	2767.187052	2307.469585	2358.733795	2399.549678													
9391.274719	12839.73188	13785.51575	23007.00879	21133.01986	22232.01514	22947.00875	27164.72834	24018.33481													
12731.16565	15282.69114	15547.22254	23861.9967	23569.36611	23041.37809	24958.82574	31058.84757	28612.6673													
1413.376894	1496.075477	1950.508821	2829.875586	2985.467738	3096.872956	3106.149859	3323.398857	3390.336922													
3111.231174	4625.036669	4126.838161	6745.428061	6261.141242	6472.349743	7463.882	8110.23416	8114.258196													
77888.51882	76077.01087	72880.46982	58264.20956	66362.40956	67065.15458	79520.10122	76706.77972	76136.09098													
4273.032034	4322.000879	4075.926217	5465.533941	5881.528407	5346.537641	5394.187822	5416.68293	5198.783272													
1911.915648	1750.254703	1717.578878	2096.129	2190.464663	2229.011979	2185.983389	2105.134349	2368.842862													
72773.67752	89899.598	91073.00463	136154.4778	137718.2779	138502.6094	144311.1458	176724.97	166122.4306													
7583.828795	6955.858153	6898.287915	7796.325893	7317.52979	8162.222615	8187.932145	8508.523995	7940.61884													
2365.384692	4217.134837	3133.745599	3206.176666	3328.449738	2937.770731	4287.968401	3657.344429	4220.446606													
445.9203827	388.0375916	353.5305929	529.4482314	209.33804	340.696934	459.5027833	530.656847	265.5218855													
2541.052319	2022.118041	2887.781575	2850.34952	3188.027645	2626.805826	3559.215032	2598.026286	2684.023439													
2613.394586	3272.455546	2184.787194	2166.292884	1798.898423	2335.357354	2446.074618	2876.002577	2931.19115													
1848.055094	1745.739691	1611.168101	2436.187425	2837.159273	2361.782544	2167.390299	2005.416131	2398.157064													
2985.256095	3672.558535	2899.360626	3806.944041	2904.761295	3442.139671	4265.57265	3538.25018	3973.126758													
8507.220179	8764.329924	7786.698878	10640.4446	10281.93005	10492.96061	10171.0546	10946.83454	10585.41843													
39863.20436	40924.44722	45739.53533	45699.36209	49917.17143	47096.13263	54016.0994	48108.6863	52389.70475													
3501.33294	3607.717053	3743.696535	5008.880189	5232.88436	4774.880403	4724.901114	4966.292827	4935.751248													
994.133683	729.8242263	601.6103325	761.2235291	237.9569656	642.0885988	639.2432855	558.2176135	206.9161461													
772.8245411	869.4318541	791.4799102	712.9990049	932.8416269	953.1392526	1274.943732	644.9850748	938.8608012													
3701.212983	3149.674766	2907.111773	3338.593044	3472.246272	3020.475895	3686.909096	3745.074884	3915.875564													
37754.00946	33277.46594	32333.48971	42625.67675	44115.16432	43085.61625	41159.71695	42744.81572	40007.19873													
2582.367349	5055.851927	3722.968678	3948.688694	2559.652732	4248.8952	5785.425031	5372.052628	4571.016705													
383.8838852	572.1160275	492.6849441	1036.201942	1128.832528	1353.040085	973.6930842	1335.166333	873.2463652													
53745.52213	85278.02037	63127.51504	73417.62772	70640.18833	75584.31641	96523.45872	103366.6596	112400.3724													
2877.913125	3553.595244	3954.604306	5517.210504	6136.014861	5661.11032	5739.327592	6896.13185	6280.868518													
1042.974225	1381.428994	816.4690521	768.5060698	1047.534585	950.1134828	1059.088545	949.8891593	1108.28474													
585.4575319	785.3997027	565.2023782	674.076531	722.9891496	785.5581741	796.2741703	366.2168694	727.9475701													
20341.46369	25247.10824	17722.65425	16449.00126	17640.61377	19593.06967	21820.15907	19169.6371	21711.88677													
452.5313152	293.2519895	156.2432557	389.8310862	282.1310601	336.6154084	372.0924784	627.0248642	282.4921086													
673.9427064	607.469676	1404.917016	1520.973527	1426.83204	1653.651228	1542.26244	1631.495845	1896.167631													
5876.407692	5524.050729	8375.785003	9238.53644	11502.05293	9308.628407	10163.292	11461.0314	10914.1806													
757.3922054	248.0012284	477.2945393	519.0156431	331.4118911	589.7026222	497.4402434	492.9274961	407.6862542													
14999.99627	16749.31657	20487.09314	27289.03096	28990.98765	26760.5927	27273.01528	29170.20551	31877.9932													
8484.359916	7013.546185	7757.008166	8145.773299	8172.026389	8044.173064	8503.493115	7326.059943	7955.083894													
5940.740932	5257.934972	5416.798729	5953.26335	6543.671142	6795.06024	6822.904989	5918.873515	6259.176165													
1929.850164	2002.815598	1741.546817	1555.808747	1618.167278	1487.346067	2233.491624	2106.235279	2389.186208													
26187.78576	39851.79301	30439.99849	33415.77712	34865.16633	35427.91325	44446.71752	45838.5949	49806.76464													
747.826633	971.4336242	1026.578292	1512.976053	2356.042264	2338.628381	2244.781495	3786.89739	2349.004418													
27412.68451	39988.47097	26405.04695	32030.21292	33870.21153	33830.62521	39356.84212	39743.93797	45618.14937													
647.2752622	289.4846793	556.0202689	1251.629035	805.3443746	1717.439941	1103.101641	1024.579704	855.5480625													
831.3445955	986.860798	1663.973457	1044.405591	2349.624309	1736.691978	1809.795185	1878.49132	2006.171012													
17035.95484	30900.64993	24413.01446	35207.89481	35912.02138	35690.93823	45870.90198	52515.74088	57136.92394													
24172.39694	24318.87639	31998.21487	35469.52191	42986.5898	38574.88807	41468.12622	44707.72605	41803.94928													
22183.43878	33062.77953	28280.5869	26453.00201	29263.82743	28992.0679	34443.84084	35109.04526	40121.03026													
4801.107428	5891.120744	6657.498234	13198.58416	13274.91206	13174.6359	12356.84131	17102.48446	14348.13617													
798.6998099	838.9946691	130.3985219	402.1237129	235.8386746	282.8470256	370.819463	0.001403199	229.9338773													
13778.01725	18222.75118	12473.94714	15484.56123	13682.05409	15786.43666	18815.52003	18445.27355	18997.32543													
32634.92684	34924.46739	32042.0456	30156.75847	34767.8525	33791.99031	36575.28766	31913.95423	33308.76277													
3087.395327	4785.397255	4374.372248	6067.883225	4959.427993	5982.99344	5860.719988	8264.4524	8072.749114													
11317.88379	8461.994213	5924.978321	7047.251855	7258.561483	7448.550879	7695.708039	5505.896324	4450.017202													
994.8576356	1259.985603	1220.015574	3377.441881	2622.388066	2859.250413	2290.39095	3950.584394	3536.236987													
5041.292713	7739.643613	7024.958582	8413.323366	9163.031971	8387.548684	9671.136345	9658.056408	11088.28117													
543.5431839	886.5481863	1189.040962	1035.704225	1679.811004	643.1324631	1414.305888	1204.295407	1423.766893													
19360.50751	30532.41704	23101.30345	34508.68232	33157.03837	34354.02731	42587.63888	49515.19931	51358.78168													

0.63_472.9252m/z	472.9251817	0.62565	neg	
0.63_474.8607m/z	474.8607186	0.62565	neg	
0.63_477.8633n	522.8519796	0.62565	neg	
0.63_489.8243m/z	489.8242806	0.62565	neg	
0.63_492.8259m/z	492.825944	0.62565	neg	
0.63_495.9394n	476.9215698	0.62565	neg	
0.63_501.9213m/z	501.9212577	0.62565	neg	
0.63_505.8999n	486.8820897	0.62565	neg	
0.63_506.8749m/z	506.8749293	0.62565	neg	
0.63_511.9171n	492.8992988	0.62565	neg	
0.63_518.8321m/z	518.8320672	0.62565	neg	
0.63_521.8732n	502.8553549	0.62565	neg	
0.63_523.9159m/z	523.9158786	0.62565	neg	
0.63_525.8633m/z	525.8632829	0.62565	neg	
0.63_533.8758m/z	533.8758277	0.62565	neg	
0.63_539.8937m/z	539.8936627	0.62565	neg	
0.63_540.9128m/z	540.9127729	0.62565	neg	
0.63_548.8510m/z	548.8510087	0.62565	neg	
0.63_556.8896m/z	556.8895781	0.62565	neg	
0.63_557.8126m/z	557.8125975	0.62565	neg	
0.63_560.8865m/z	560.8865481	0.62565	neg	
0.63_563.9272n	544.9093239	0.62565	neg	
0.63_572.8668m/z	572.8667931	0.62565	neg	
0.63_584.8850m/z	584.8849634	0.62565	neg	
0.63_589.8610n	570.8431618	0.62565	neg	
0.63_590.8397m/z	590.8396663	0.62565	neg	
0.63_591.9036m/z	591.9036107	0.62565	neg	
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0.63_604.8153m/z	604.8153094	0.62565	neg	
0.63_607.8813m/z	607.8812937	0.62565	neg	
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0.63_616.8404m/z	616.8404396	0.62565	neg	
0.63_624.8752m/z	624.8751664	0.62565	neg	
0.63_628.8742m/z	628.8741711	0.62565	neg	
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0.63_640.8537m/z	640.8537369	0.62565	neg	
0.63_652.8731m/z	652.8731262	0.62565	neg	
0.63_656.8192m/z	656.8191925	0.62565	neg	
0.63_658.8273m/z	658.8273388	0.62565	neg	
0.63_659.8912m/z	659.8911629	0.62565	neg	
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0.63_702.8222m/z	702.8222282	0.62565	neg	
0.63_720.8608m/z	720.8607526	0.62565	neg	
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0.63_752.8130m/z	752.812952	0.62565	neg	
0.63_768.7888m/z	768.788785	0.62565	neg	
0.63_770.8093m/z	770.8093334	0.62565	neg	
0.65_124.9537n	123.9464713	0.64783333	neg	
0.65_125.8732m/z	125.8732484	0.64783333	neg	
0.65_126.8811m/z	126.8810919	0.64783333	neg	
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0.65_130.8752m/z	130.8752094	0.64783333	neg	
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0.65_136.9837m/z	136.9836659	0.64783333	neg	
0.65_138.9070m/z	138.906951	0.64783333	neg	
0.65_141.9126m/z	141.9125986	0.64783333	neg	
0.65_146.9387m/z	146.9387262	0.64783333	neg	
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0.65_157.8631m/z	157.8630658	0.64783333	neg	
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0.65_162.8392m/z	162.8392249	0.64783333	neg	
0.65_164.8362m/z	164.8362053	0.64783333	neg	
0.65_166.9245m/z	166.9244635	0.64783333	neg	
0.65_170.8710m/z	170.870989	0.64783333	neg	
0.65_174.8651m/z	174.8651223	0.64783333	neg	
0.65_178.9492m/z	178.9492	0.64783333	neg	
0.65_187.8612m/z	187.8611794	0.64783333	neg	
0.65_187.8738m/z	187.8737548	0.64783333	neg	
0.65_189.8583m/z	189.8583091	0.64783333	neg	
0.65_191.9464m/z	191.9464286	0.64783333	neg	
0.65_197.8900m/z	197.8900003	0.64783333	neg	
0.65_197.9454n	394.8909426	0.64783333	neg	
0.65_197.9957n	178.9779026	0.64783333	neg	
0.65_199.8871m/z	199.8871077	0.64783333	neg	
0.65_205.8398m/z	205.8398429	0.64783333	neg	
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0.65_218.9345m/z	218.9345851	0.64783333	neg	
0.65_224.9089m/z	224.9089195	0.64783333	neg	
0.65_227.8947m/z	227.8947042	0.64783333	neg	
0.65_232.9150m/z	232.9150386	0.64783333	neg	
0.65_246.8865m/z	246.8865371	0.64783333	neg	
0.65_254.9441n	508.8727052	0.64783333	neg	
0.65_259.9338m/z	259.9338068	0.64783333	neg	
0.65_263.8889m/z	263.8889164	0.64783333	neg	
0.65_286.9218m/z	286.9218017	0.64783333	neg	
0.65_298.8353m/z	298.8353016	0.64783333	neg	
0.65_302.8999m/z	302.8998578	0.64783333	neg	
0.65_306.8689m/z	306.8689312	0.64783333	neg	
0.65_308.8642m/z	308.8642262	0.64783333	neg	
0.65_310.8577m/z	310.8576964	0.64783333	neg	
0.65_311.8704m/z	311.8704147	0.64783333	neg	
0.65_325.8544m/z	325.8543825	0.64783333	neg	
0.65_326.8302m/z	326.8301933	0.64783333	neg	
0.65_327.9213m/z	327.9212516	0.64783333	neg	
0.65_336.8590m/z	336.859035	0.64783333	neg	
0.65_353.9196n	790.8181985	0.64783333	neg	
0.65_354.9092m/z	354.9091575	0.64783333	neg	
0.65_359.8715m/z	359.8715293	0.64783333	neg	

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2723.345365	3965.370308	2806.973259	2968.36736	2520.545113	4015.080187	4192.476721	4617.795402	3562.389092
2821.453696	3600.599254	2384.600733	2112.292953	1540.677473	2243.214683	3442.032698	3364.768577	2015.29225
8676.140464	7282.833589	6436.11797	7295.479255	13823.93282	8448.759918	8027.349728	8897.842506	12010.03113
2592.684424	3037.397973	1961.957364	2355.653613	2765.198095	2962.139003	3644.133227	2650.296997	3187.255183
16059.39646	18470.908	23126.39645	27663.37508	31402.13788	26804.63284	29105.67392	33718.89836	30717.30034
159.5124325	275.8911597	186.8280284	1019.219573	889.387119	869.2215021	698.9621657	1746.274904	1257.422653
12012.19621	24664.59112	13588.03692	16380.45511	19956.14866	16900.05811	23320.49607	24765.13934	33448.30295
1830.674618	1579.946013	1305.777933	1366.124851	2105.698407	849.6092218	1629.590082	2263.74521	1662.353138
19092.10287	25907.83203	24813.21242	21617.58163	24496.1771	24067.0542	27979.05771	29241.39978	33243.31151
3070.923691	5594.86439	2992.011195	2592.208988	2268.258076	3150.328672	4169.206116	3226.373969	3140.274022
19473.3717	24300.85379	17257.2247	20039.04993	22952.89708	22099.94475	22368.07326	22588.10353	26035.01205
2065.781568	2350.231437	3004.7167	4699.52259	5757.545134	5543.897665	4507.55182	5820.793187	4174.59671
1548.975442	1153.297886	2079.936295	1517.54065	1946.352049	1869.334638	2395.826944	1868.576649	1754.812501
859.4752287	2534.638457	1690.437481	2215.000658	1789.322848	1903.870703	3076.131779	3719.866235	3036.057584
4395.186824	7171.323902	6167.483362	8732.14766	8703.566144	8002.322977	10594.08595	12579.09124	11959.78416
332.8321467	73.64740319	183.5290126	3432.330523	4082.321883	3580.861563	2789.275178	5184.826996	3126.463043
4253.046326	7438.524558	5146.374908	5759.348908	4557.376349	5920.742826	7256.821933	6057.80577	8297.24344
4661.443149	8020.61539	5504.125885	11595.63564	9548.925685	11910.02635	12899.43315	16221.60302	15970.23789
5032.286759	4753.307768	2952.000404	4526.279332	3818.145424	4349.349158	3868.454459	3509.329498	4087.663123
10849.77466	11887.6585	13547.84235	11999.08373	12693.40408	11437.00164	16222.69529	14605.47708	15636.63137
9946.562626	8694.549241	15013.17079	13899.42242	18917.97068	13188.63999	17940.3407	15679.34181	17069.82593
4766.221218	8456.433238	4618.842842	7959.330163	4093.598817	7602.675423	8949.372652	9867.530926	8679.51279
550.9791728	710.9437927	408.2966859	1308.404383	2064.087768	1518.105928	2908.333499	3002.143872	2824.002
13003.32897	19548.22756	14806.46817	12768.20529	23005.63119	18062.38191	16869.05316	19085.13008	22023.51812
2149.62831	3481.778858	2982.455873	3513.817469	2879.973585	2940.167536	3148.231462	2628.798959	3939.170419
1545.338932	1415.995159	2811.140741	4077.951893	5427.322543	4260.954777	3182.569375	5353.329218	5044.17578
785.0029131	2401.57456	1240.538243	1935.888657	2019.89032	2104.454775	2662.790358	2776.246948	2768.010821
3884.174787	4626.239985	2356.797617	2831.498064	3002.507317	3645.941305	3761.804199	4274.939428	4786.254234
4103.161956	5591.303143	5628.357314	7155.787267	8433.61431	6998.756879	6588.907968	8707.188001	8963.090506
4395.061102	3612.604009	6398.769493	5379.607054	6675.443211	4503.957279	8026.134291	10229.24688	5577.666911
2102.438243	6115.376939	2542.742375	3727.890678	2857.787558	4010.30262	7510.212113	5236.274953	7112.047353
3835.139054	5431.964709	5140.951969	8850.499292	7473.382729	8376.583281	6911.51814	11984.54027	9058.026447
4125.870603	6955.948776	6019.705711	3992.218203	5468.64424	3985.174327	7295.24577	4072.555957	7291.041021
11231.22475	16902.99693	12329.17433	11162.47833	16891.32703	14375.78988	15512.65938	14247.17133	20665.67095
1593.060016	2672.976028	2257.981788	2289.489644	2767.716404	2789.789877	2662.517368	3999.594971	5230.927527
1461.30478	2643.167836	2040.994026	4412.457178	3610.526276	3596.814345	4077.35606	6711.309412	4886.690068
7772.489909	8143.269846	6581.089012	5782.310577	7666.007479	6623.439664	7928.090705	6199.322411	8618.800474
1637.861556	2176.464701	1474.496611	1974.001664	2172.361993	2715.136161	2413.958267	2369.086569	2452.504735
0.001403199	882.4653756	1022.164932	2275.509897	2384.482417	1871.177129	1844.133206	1899.888251	2195.496698
1993.1399	3030.023266	2463.754874	1950.18258	2732.353129	2436.454409	2911.969616	2262.285668	3278.461089
1249.182924	1207.395682	2763.317283	1145.96317	3673.215311	3027.051227	3273.650619	2874.179764	3487.102963
1474.202495	1442.694088	2279.345279	1350.906754	901.9296165	738.5053576	1783.229326	1520.584244	513.9387016
344.6364001	1270.290841	1353.113446	1002.139737	771.1908482	1365.670992	1749.916862	2169.720887	2093.933956
738.3934884	1126.012937	1414.175888	2489.435681	2193.202889	3171.464661	3152.456491	3071.780007	3247.866216
698.0549785	673.5885396	702.7144322	901.6544354	956.1319824	905.2262074	1639.151687	1719.250031	1401.97772
1053.630898	2501.674797	2776.546668	4283.759862	3041.947787	2242.877958	2858.649895	4024.420123	4253.438993
354.0863596	0.001403199	657.3137693	843.0516624	1421.280374	547.0139901	777.7131588	564.5496826	1073.371437
1825.061625	3346.988699	2406.420694	1129.014579	3237.995769	3225.338076	3192.611208	4342.976807	4795.825418
1346.86962	3800.032215	1783.780226	1773.235138	1990.186446	1248.245476	2912.166957	2178.340302	3488.300278
755.5782813	843.5767336	501.257191	1765.038609	939.2598502	598.1902459	1730.174927	426.2332679	2256.440057
3070.552891	3123.46923	2519.413511	2786.56405	2524.99059	2780.353259	3110.792592	2599.524094	2434.45908
730.4451295	1013.873853	939.8794229	1033.93409	1029.966464	959.1297865	1166.491732	1167.878443	1064.00947
2372.20442	2270.895972	2052.06559	2479.591956	2033.803296	2556.005522	2399.031635	2430.710092	2113.315126
2146.752842	2506.318587	2586.434942	2106.515866	2086.143298	2194.351628	2732.08388	1983.507635	1956.184097
198.1597435	163.3065472	157.3871309	234.8489117	73.11865906	142.6344899	240.1067231	175.3471045	76.8552792
166.8366913	248.1641015	132.3733226	103.9215091	40.46902341	106.6218189	189.2112533	167.9831742	64.92216344
374.0638007	405.1962666	358.8447542	460.6535097	246.7707612	515.7176263	393.6957237	374.213741	372.8361627
280.3013223	373.1371036	300.9040786	342.4450463	220.1526526	360.8970147	357.6000047	445.6967465	316.5538717
3568.206449	3522.776643	3426.755059	2701.495578	2828.9352	3087.71584	3482.418972	2561.875071	2653.196207
177.8767652	308.2733797	139.7854865	137.3395582	49.58497623	116.4295409	178.6008714	143.8514603	84.19430084
485.7396248	336.2566456	346.5838451	429.5455145	126.990901	391.1068568	393.4404758	398.3270522	209.2781572
1130.313249	1119.540479	863.7497439	895.4625376	671.3600296	902.7180291	1143.423691	924.103575	740.0605403
408.4111717	411.8330068	379.5110221	522.3837527	311.6412208	439.2058566	444.457855	501.2608526	325.9834471
2342.21137	19721.33416	19903.48184	18461.98444	19479.03029	21394.47599	19904.57655	16822.32961	18385.50275
5103.275801	4504.473382	4769.437964	5702.592261	4888.6845	6111.393787	5407.024869	4947.393286	5689.42663
28288.00634	19279.7903	22417.77192	25911.04323	18091.97125	30851.7346	24549.38316	23129.2809	24696.47116
281.706063	277.8215597	312.3147188	409.6474471	232.9685402	312.5361861	439.036378	362.9334984	213.2993868
511.6342093	666.7901721	740.6467829	832.1881403	497.5507853	761.9755075	822.0999823	982.8056869	675.7982262
3295.989598	3944.771981	4600.993667	2891.599791	3164.348465	2795.649958	4382.565103	3051.290844	2991.304114
517.1601791	537.4430069	477.7779817	691.9270911	333.3561587	628.0096605	559.12381	600.3945428	381.2447164
3304.171489	3849.409994	4573.631197	2804.793454	3241.273753	2870.914181	4281.604483	2939.602442	3019.66629
601.8216157	646.4077656	594.2951278	700.7336661	380.2132949	585.936099	729.1248208	640.8342718	410.6131425
842.5425115	1177.728251	852.5906078	737.1980619	651.6370803	798.2048624	1196.627769	897.7700448	828.4497051
3724.466977	3597.168877	3190.673356	4423.009825	3210.328633	3748.385907	3887.699957	3688.285494	3146.004564
320.066563	262.1368026	220.1008409	330.5241051	123.4924182	260.3485357	293.186905	274.2418365	106.8989884
1171.233534	1638.081871	1302.549775	1186.429814	853.0009847	1328.063946	1629.189307	1622.652397	1361.440435
1702.614653	1585.223613	1799.543167	1478.833176	1659.919866	1855.767857	1752.876112	1745.244187	1770.066045
1780.894238	2108.32535	2382.449822	2329.010066	2427.142769	2292.721488	2534.243111	2873.224123	2852.558407
1017.372016	1005.64775	1186.026864	977.5900503	1144.690691	1050.701068	1067.489059	1094.976606	1063.191761
2806.110763	3860.932087	3154.887878	2591.571187	1899.275913	2788.514108	3628.959677	3066.798624	2770.058887
3403.729196	2981.463664	3160.096285	3389.285368	3027.390984	3395.822138	3144.88386	3126.28249	3076.750237
231555.6254	203495.9803	202864.372	167658.7464	175037.6318	182715.4319	210142.1087	170020.8674	183532.186
34780.16544	32476.55931	33807.95715	39265.4076	34079.72622	42231.17162	38771.40527	44794.22287	38600.5136
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752.9108892	818.2885394	1159.561107	957.9129044	601.3581603	1069.506074	1174.344521	1329.391553	793.8266001
7817.094614	7811.242658	7431.464897	8267.390756	7640.685704	8999.821623	8618.320552	7262.20992	8578.420757
6530.945674	5431.42785	5367.354143	5305.657751	5197.014843	5821.946899	5315.69643	5092.624539	5019.902917
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589.0808962	556.7861297	438.564439	508.9225181	281.0862084	610.677666	676.6491224	417.1879496	419.2964594
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693.2956309	1189.766946	762.2177669	831.4590821	683.4627229	805.4969671	1223.217084	1087.581087	992.4067178
37241.61578	35926.57855	35786.94107	31128.0861	35960.58875	33910.94004	37917.93395	33989.78205	38228.29139
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432.1849675	385.4959961	549.5587685	435.6635075	423.6306746	334.8186323	358.4184831	374.0253503	687.5314825
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4983.765563	3618.690008	2908.800695	3448.19972	3081.891028	3187.97576	3121.435123	3197.213007	2805.149377
138.6235212	709.6047628	313.2227767	192.9054718	234.1097357	154.2290271	364.3464446	152.5617758	233.6407953
2146.580834	1649.841121	1531.568286	1649.624356	1411.309875	1783.913587	1415.9102	1241.497604	1417.328749
18093.82947	13609.27279	12105.67701	13621.26921	12283.79151	16072.19943	12229.13679	11032.81288	10802.55435
2178.060987	2559.649762	1508.726467	2007.334648	706.4560882	1454.003512	1984.634729	1479.421198	662.8978324
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9456.550485	11179.73215	9478.472075	7033.630438	13277.28312	9488.644809	12344.09042	7991.807233	12162.73672
1345.726765	1903.607338	1779.798708	1638.063393	1777.872364	1538.835413	2404.39119	1663.186151	1663.910663
2052.181359	2575.817976	2281.631614	1376.313581	1043.875661	1488.467275	2144.442719	1885.814777	1746.169199

0.65_362.8687m/z	362.8686608	0.647833333	neg	1361.94505	1502.638904	2328.776467	1834.125631	1727.323615	1363.185175	1252.047573	861.0228221	1343.476761	
0.65_362.9413m/z	362.94131	0.647833333	neg	46496.50055	48606.05793	53764.0179	51561.06554	56214.96982	51620.10181	65883.43506	54581.93576	59817.00285	
0.65_378.9185m/z	378.9184632	0.647833333	neg	18864.69152	24620.48644	20661.85086	17680.94555	17045.91367	18305.97428	24697.5563	19107.60159	21611.60692	
0.65_379.9316m/z	379.9315832	0.647833333	neg	4040.415678	3629.003515	3785.379996	4545.875835	4116.832807	4850.112789	5885.877606	5230.668184	4531.085662	
0.65_386.8791m/z	386.8790929	0.647833333	neg	823.6220229	1284.80107	979.1734084	635.9592647	505.1137222	395.9780481	505.5423148	581.3049985	319.5594119	
0.65_387.8843m/z	387.8842501	0.647833333	neg	1212.852773	1042.521497	1319.957204	1458.157345	1621.30524	1503.415058	1523.455134	1359.191207	1401.810599	
0.65_388.8746m/z	388.8745836	0.647833333	neg	14603.82113	16134.35721	12462.54997	11232.93112	11653.26963	12658.26866	14209.60378	13063.02654	13259.0501	
0.65_421.8373m/z	421.8373236	0.647833333	neg	1184.485225	1283.61461	956.1481112	941.1898159	482.6363949	962.475036	1342.875307	1125.749542	783.3646539	
0.65_427.8585m/z	427.8585468	0.647833333	neg	2515.528417	2945.466459	1808.833553	1497.838656	1622.858153	1807.036458	2396.221322	1756.398322	2375.564914	
0.65_430.8548m/z	430.8548002	0.647833333	neg	6130.824879	5969.078547	6148.77104	6175.157492	17431.87403	10917.73064	6306.437413	6277.066126	10263.0849	
0.65_450.8439m/z	450.8439433	0.647833333	neg	3387.618098	4645.527904	2487.368934	2801.2825	3224.898818	2890.528717	3936.999295	3446.580967	3861.602979	
0.65_454.8670m/z	454.8670178	0.647833333	neg	790.9555708	1315.558062	845.6432388	878.6588835	399.8819374	747.0410343	756.9219105	632.3221261	213.9733404	
0.65_456.8617m/z	456.8617165	0.647833333	neg	12321.52259	13658.62093	10412.25179	8530.76112	7731.50541	8844.936094	12447.55874	9429.547867	7833.492631	
0.65_467.8242n	512.8136869	0.647833333	neg	4390.903131	3567.786241	1980.678805	2949.764654	1828.938904	2013.551624	2774.319931	2216.947054	1507.337917	
0.65_482.8713m/z	482.8712577	0.647833333	neg	2672.402205	2676.354564	3446.209551	2921.584351	2768.685959	3164.343618	3724.851165	3184.648381	3438.725979	
0.65_498.8424m/z	498.8423964	0.647833333	neg	3487.319663	3701.720184	2866.065197	2258.593816	2090.688026	2588.443027	2984.395563	1518.54311	2157.536637	
0.65_505.8017m/z	505.8016861	0.647833333	neg	1360.830635	1698.011847	1516.512454	1015.411528	858.9261519	817.7560646	1632.324548	917.7870941	541.849376	
0.65_514.8202m/z	514.8201828	0.647833333	neg	1070.424532	780.4730034	607.2162518	540.0829598	752.5128779	556.3825427	828.9502671	558.3411771	582.1959491	
0.65_524.8489m/z	524.8489386	0.647833333	neg	9819.153137	10012.34682	8011.803058	6343.994998	5432.929125	6152.72277	9333.342136	6326.247304	5681.355013	
0.65_534.8049m/z	534.8048808	0.647833333	neg	3023.841495	3282.233972	1375.964752	1864.838436	951.0964203	1661.583964	1755.195058	1742.035339	1077.743385	
0.65_555.7972m/z	555.7972268	0.647833333	neg	2537.667893	2640.067492	2531.618191	2463.369285	1698.500182	1874.823362	2079.540604	1840.516128	1784.084249	
0.65_560.8142m/z	560.8142274	0.647833333	neg	1738.273988	2033.878167	1287.186645	1142.195934	4052.909757	1654.847073	2095.49379	971.6046431	3295.065607	
0.65_563.8341m/z	563.8340745	0.647833333	neg	967.1789817	967.2190572	384.6582093	511.74355	0.001403199	337.7204827	896.6686334	552.5778342	193.3702885	
0.65_574.7971n	573.7898096	0.647833333	neg	3999.664704	5087.334466	3131.870693	3110.489874	2424.010592	3841.718922	4201.503254	2602.784057	3564.24821	
0.65_576.8607m/z	576.8607138	0.647833333	neg	11666.9734	12975.84422	11041.05737	10415.61089	11301.49819	9431.307331	14101.41493	11026.06259	10408.12692	
0.65_580.8039m/z	580.8038885	0.647833333	neg	1202.675275	742.2544205	286.2672755	497.3939407	623.3784811	0.001403199	736.1522675	142.6556099		
0.65_587.8262n	586.8189401	0.647833333	neg	5695.20553	12138.60162	6534.737578	5998.061281	8204.507935	7882.178743	7964.188879	7099.23687	7195.130991	
0.65_592.8364m/z	592.8363594	0.647833333	neg	6650.569504	7765.566264	5235.767116	4651.36275	5153.918729	4406.488764	6812.89391	4854.773346	5582.968184	
0.65_628.8028m/z	628.8028025	0.647833333	neg	2079.380229	1364.488983	2594.775689	999.8464935	3728.975692	2763.908667	2442.718927	2514.765865	3766.965974	
0.65_644.8481m/z	644.8480877	0.647833333	neg	7582.660612	8496.649521	7323.252027	6845.231479	6665.741928	5753.567431	8705.808316	6702.110015	5987.11976	
0.65_655.8132n	654.8059392	0.647833333	neg	6827.894579	10999.17282	6941.083355	6168.599716	8413.990301	8650.185053	7536.068172	9383.931719		
0.65_660.8239m/z	660.8238885	0.647833333	neg	4762.111202	5363.09091	4358.452448	3962.941113	4180.703617	2834.608112	4854.954182	3653.754377	3795.164104	
0.65_696.8616m/z	696.861647	0.647833333	neg	1015.826498	2575.255285	2212.970937	1146.021632	2583.871086	1176.307752	3224.233809	2061.480484	2247.145536	
0.65_712.8347m/z	712.8347227	0.647833333	neg	4372.13751	3391.369772	3935.470387	3457.740643	4050.692442	4259.972419	3873.34144	4175.16153	2716.064863	
0.65_722.7931m/z	722.7931081	0.647833333	neg	2793.298842	3201.960768	2136.031636	2375.811405	3220.401796	2614.763357	3114.518415	2122.395716	2293.834821	
0.67_108.9887m/z	108.9887034	0.6701	neg	213.1362212	126.8868346	149.6270574	189.1179336	80.44591861	166.63872	171.3950078	149.9754024	74.78637415	
0.67_149.9917n	194.9900143	0.6701	neg	2490.896696	2068.442804	2090.456064	2646.077479	1748.144928	2889.619743	2346.752592	1779.734939	2095.809335	
0.67_321.9745m/z	321.9745433	0.6701	neg	1185.262102	1256.720432	1070.433446	1292.323473	2303.056084	1405.684722	2018.297949	1537.426101	1988.173267	
0.67_336.0305m/z	336.0305116	0.6701	neg	378.9427191	385.8370482	484.5246785	711.0330659	797.7319836	445.5501377	1147.466672	528.7686615	1011.607943	
0.67_368.8892m/z	368.8891534	0.6701	neg	1028.780514	1415.445218	1038.212258	788.7587792	863.6854697	482.8880837	1134.63992	535.2595604	749.05869	
0.67_389.9624m/z	389.9623524	0.6701	neg	3091.47369	2915.08405	2920.518397	3975.851685	6262.00786	4914.406572	4112.649874	3631.051468	6501.861878	
0.67_391.1338m/z	391.1338117	0.6701	neg	1270.656982	1489.732431	1305.150622	2013.476744	1509.692214	1515.613707	1303.121812	1035.017706	1060.226329	
0.67_404.0180m/z	404.018019	0.6701	neg	258.4161376	304.0614285	331.466458	663.9123833	805.610981	351.110795	618.3055182	735.0531006	873.2009938	
0.67_430.9285m/z	430.9285291	0.6701	neg	15540.59473	15812.14526	18871.69778	17088.48854	17920.20602	18636.44886	22340.9444	19306.88943	18946.99618	
0.67_446.9059m/z	446.9058538	0.6701	neg	12527.7801	14211.84464	12663.54979	9880.847788	10022.02287	10242.41379	15239.46718	11608.14696	13320.99586	
0.67_453.8479m/z	453.8479247	0.6701	neg	330.6030715	0.001403199	463.7637645	345.9538786	326.0671869	982.0456871	350.7231077	368.6728821	207.9975731	
0.67_459.1211m/z	459.121124	0.6701	neg	961.0700804	552.8089237	1141.218718	760.0848717	1024.212004	1101.303849	702.3442357	673.6317139	744.2824646	
0.67_467.0884m/z	467.0884046	0.6701	neg	651.6007862	871.2831016	1559.367809	1286.418992	2038.147823	1856.188822	1803.417894	2315.292362	2547.191385	
0.67_472.0047m/z	472.0047116	0.6701	neg	258.2178408	436.3187987	775.4391054	1526.551269	1401.464803	1633.916837	1218.112861	1413.064082	1913.596199	
0.67_485.0357m/z	485.0356578	0.6701	neg	1809.120453	1824.342098	2381.961641	2902.025539	6012.340435	7000.159912	3577.310308	4532.441879	5187.239308	
0.67_498.9163m/z	498.9162526	0.6701	neg	10959.17196	10455.3854	11969.00433	11679.11467	11832.45969	11615.48204	13782.26421	12998.58112	12861.617	
0.67_514.8930m/z	514.8930049	0.6701	neg	10710.71818	13339.03324	12256.57057	9170.352378	8177.988038	9531.079255	11766.72608	11454.8847	11387.45852	
0.67_525.9369m/z	525.9369076	0.6701	neg	2295.359555	1819.986113	3901.882726	2226.39531	8005.11892	5719.906073	3369.941249	4533.723257	6569.658275	
0.67_535.0763m/z	535.0763469	0.6701	neg	764.4268383	1038.454834	1282.626893	1759.071518	2591.937812	1559.13067	2032.690281	3049.671894	3220.956912	
0.67_539.9925m/z	539.9924555	0.6701	neg	501.6087715	321.6061104	487.9342221	1426.071862	896.6058491	928.9944354	837.0709521	774.4543228	1726.09751	
0.67_553.1870m/z	553.1870188	0.6701	neg	3904.630792	3777.991207	4316.945017	4215.363161	4011.03723	4568.371885	3416.606525	3841.201097	3970.505138	
0.67_566.9036m/z	566.9035542	0.6701	neg	6342.362683	6478.942824	8401.499599	6699.980693	6793.141544	6769.647361	10033.00624	9346.753235	9751.031936	
0.67_594.0999m/z	594.0998642	0.6701	neg	194.2555639	188.7269477	538.0800857	1057.186607	928.6972742	553.548517	875.4153498	795.0493774	1459.69158	
0.67_634.8909m/z	634.8908772	0.6701	neg	4579.156175	4771.114151	5321.818424	4716.762679	3513.827193	5329.952812	7122.268443	6248.407766	5078.046629	
0.67_662.0877m/z	662.0876891	0.6701	neg	0.001403199	0.001403199	727.5094092	1931.405707	773.3826255	1086.750204	430.1016702	831.8375624	1325.845454	
0.67_675.9670m/z	675.9670434	0.6701	neg	0.001403199	197.6581176	398.7909484	301.461057	890.1464833	688.4554425	391.7592528	823.7841949	953.1260729	
0.67_689.1619m/z	689.161887	0.6701	neg	756.5443993	685.407313	1426.150151	1033.916289	1113.854404	961.0129319	1537.761794	1250.799171	833.9179145	
0.67_691.9443m/z	691.9443165	0.6701	neg	0.001403199	452.1606515	883.8595499	716.6561551	1126.726964	825.2918544	1106.970641	903.1574402	1270.088593	
0.67_702.8786m/z	702.8785621	0.6701	neg	1508.623458	1914.480426	1953.94	1150.411231	1392.071398	1261.838636	1839.477405	3237.303146	3424.029802	
0.67_730.0747m/z	730.0747137	0.6701	neg	0.001403199	0.001403199	591.7935175	1027.81354	1653.22269	1299.048023	0.001403199	1171.17559	999.6167771	
0.67_739.0391m/z	739.0391378	0.6701	neg	932.4388216	774.7946395	563.3131979	1751.323875	1038.760212	1008.391433	1497.910561	3274.597397	817.2873336	
0.69_1000.3378n	981.3199738	0.692166667	neg	8831.086775	9502.392865	8130.89343	0.001403199	7266.619352	7220.373162	15614.19794	5644.123413	11616.1592	
0.69_1001.8580m/z	1001.85797	0.692166667	neg	4995.249546	6214.116926	5556.734077	5227.220352	4553.541502	5879.443552	8026.058147	5954.260437	5072.163286	
0.69_1081.2841m/z	1081.284096	0.692166667	neg	0.001403199	4747.266322	1444.704386	0.001403199	0.001403199	0.001403199	0.001403199	2599.439331	1654.970272	
0.69_1117.2937m/z	1117.29367	0.692166667	neg	0.001403199	2800.844374	2877.658058	0.001403199	4090.290684	0.001403199	5692.680111	5041.759188	3530.876052	
0.69_112.9825m/z	112.9825187	0.692166667	neg	58.55830243	77.80220148	2.473267927	58.91986647	108.3006427	112.2210326	51.31897319	20.03140891	44.42252121	
0.69_126.9793m/z	126.9792686	0.692166667	neg	448.1288858	172.965435	342.5104664	411.0918188	124.3260544	510.5953812	509.1108029	341.5322319	310.9273663	
0.69_155.0656m/z	155.0656354	0.692166667	neg	2759.523154	2710.232946	2985.670764	4298.208611	4584.380304	4125.870512	4222.813439	4531.898064	4246.204997	
0.69_171.0201m/z	171.0200867	0.692166667	neg	955.2761241	698.8172076	832.8771236	832.2957312	839.5837292	893.4916583	1107.751619	980.2879982	797.1780857	
0.69_177.0514n	222.0497102	0.692166667	neg	44476.11994	43878.75847	50240.76745	68386.93531	68926.06246	66931.82168	67658.4859	67467.37227	75137.43544	
0.69_209.9976m/z	209.9975668	0.692166667	neg	326.9190085	499.3290833	408.9872555	478.375109	580.3945014	270.1180707	802.3065894	355.7537825	391.5363931	
0.69_213.0858m/z	213.0858022	0.692166667	neg	1360.970195	1248.695272	1398.177202	5082.842894	4803.447153	4983.959401	3077.286897	3165.971105	3459.966804	
0.69_245.0388n	290.0372483	0.692166667	neg	24462.08065	24569.06539	26318.19193	32241.3318	34009.80123	33373.87086	35589.95951	34053.36261	38949.51363	
0.69_253.9870m/z	253.9870449	0.692166667	neg	3599.288765	3382.178099	3337.738218	3663.881654	4619.02778	3743.243624	4808.590914	3541.516714	3863.557842	
0.69_313.0265n	358.024717	0.692166667	neg	42360.35379	38783.88022	45108.71304	49368.03895	51138.41928	52018.8336	53807.4277	56804.99953	59007.05142	
0.69_331.1138m/z	331.1137741	0.692166667	neg	1521.136433	1635.262636	2727.469632	4852.68256	6080.610464	4801.832094	4186.738304	4912.596333	4917.67038	
0.69_381.0138n	426.0122231	0.692166667	neg	49454.84492	46392.20192	51188.72297	50818.04757	49657.20002	54587.13148	62535.93844	61910.23799	64596.34776	
0.69_392.8960m/z	392.8959922	0.692166667	neg	6745.303611	4579.444054	4930.242803	3764.036673	3850.335211	4147.503661	5377.060907	4042.293732	4237.387398	
0.69_439.8887m/z	439.8887231	0.692166667	neg	3463.750224	3507.617986	3486.395744	2980.963533	2506.197739	2992.621631	3668.959181	3502.696305	2823.396249	
0.69_449.0013n	493.999736	0.692166667	neg	50325.29836	46258.29308	48410.71274	43310.01187	43029.98006	44254.32279	57858.25116	58265.27997	59004.2458	
0.69_457.9492m/z	457.9492201	0.692166667	neg	3204.685845	2869.406199	4391.383235	3985.280533	5751.394697	4083.748954	5171.354999	3456.887284	5457.64351	
0.69_516.9884n	561.9871931	0.692166667	neg	46109.19781	43257.24375	44013.81517	40193.16667	35534.76471	40170.31315	61217.56348	55702.72139	57043.16255	
0.69_527.1086m/z	527.1086101	0.692166667	neg	574.7903777	591.3573118	627.6821988	683.0026866	614.5955546	744.2072591	277.2932017	468.1742249	552.6157997	
0.69_582.8800m/z	582.8800266	0.692166667	neg	7065.560673	8453.900859	8652.715041	5147.733444	4948.783216	7048.692062	8457.558504	8167.080776	8647.535012	
0.69_584.9761n	629.9747345	0.692166667	neg	45005.92654	37401.18413	38013.84068	31548.01278	35085.53463	37052.45804	54025.90317	54383.71611	50518.09761	
0.69_598.8536m/z	598.8536417	0.692166667	neg	51079.31848	43808.64881	47023.80754	35515.07429	35947.69828	39091.68548	44500.86369	38765.99554	41239.59186	
0.69_603.0640m/z	603.0639713	0.692166667	neg	873.7305388	1020.922673	1291.566018	1960.391173	1363.393231	1817.912515	2165.697137	3465.841315	2853.382147	
0.69_621.0105m/z	621.0104671	0.692166667	neg	1490.592	1849.046554	3365.7801	5903.982086	4513.393306	5903.695714	6113.949301	6572.997647	6454.493723	
0.69_636.9845m/z	636.9844838	0.692166667	neg	1847.709954	539.9675622	1011.123209	4277.569652	2610.027517	5060.501732	3553.508074	3322.312017	2259.339688	
0.69_650.8678m/z	650.8677835	0.692166667	neg	5027.548878	5598.707596	5685.331323	5094.463011	4109.886368	4726.455574	6608.371274	6630.074409	5938.815889	
0.69_652.9632n	697.9619588	0.692166667	neg	37448.62395	33661.09028	36219.55216	27954.70478	28036.10035	30559.30551	43655.85923	43983.48829	42059.08017	
0.69_662.8338m/z	662.8337643	0.692166667	neg	11158.5544	12688.12361	10903.1006	15183.80244	8114.881047	9522.478019	13795.1375	16753.76767	14488.56126	
0.69_666.8413m/z	666.8412896	0.692166667	neg	40233.96363	34868.93587	37414.04751	27465.53745	27197.12108	29797.54781	37082.92025	30488.2583	35482.2268	
0.69_668.9377n	713.9359953	0.692166667	neg	42942.05631	39117.36217	35602.5056	35449.23556	35992.95572	38349.29757	53096.57654	41609.25367	45955.90889	
0.69_671.0516m/z	671.0515531	0.692166667	neg	1076.4822	1501.293924	1109.79843	1818.095411	1072.465971	2005.993193	1615.795143	2268.429291	1646.357834	
0.69_688.9980m/z	688.99802	0.692166667	neg	2181.397588	1838.611952	3260.085229	5768.797678	3611.272423	6093.035108	3571.632792	6823.221459	5201.825321	
0.69_691.3811m/z	691.3810664	0.692166667	neg	2804.557666	1275.483735	1324.365446	0.001403199	0.001403199	0.001403199	1423.933181	1550.20745	1029.754266	
0.69_693.3974m/z	693.3973841	0.692166667	neg	1191.224154	1613.759178	3310.868118	2053.657994	2574.917261	2810.864431	3044.41013	2171.182785	1505.688089	
0.69_720.9513n	765.9494086	0.692166667	neg	23703.88307	22221.95376	21837.16109	18939.14108	16591.59646	22052.15699	30714.30878	30150.98098	27851.88618	
0.69_734.8285m/z	734.8285277	0.692166667	neg	29649.88937	28064.32	29403.04966	19533.35005	18558.95749	18825.82696	26860.57373	25767.40186	23862.43445	
0.69_736.9236n	781.9230423	0.692166667	neg	30097.30531	25357.60989	25769.59196	27190.00274	26400.70279	27029.35945	39534.51275	30431.33543	34412.37312	
0.69_756.9855m/z	756.9854504	0.692166667	neg	1621.777002	1390.131279	2197.012143	3303.648904	2752.4663	2706.417413	3185.050232	2191.064819	3976.174798	
0.69_759.3682m/z	759.3682187	0.692166667	neg	1338.948968	2320.341217	3205.307318	0.001403199	112.8256375	66.40624254	2205.801007	1046.347149	3713.282994	
0.69_772.9586m/z	772.9586033	0.692166667	neg	1388.616093	1045.727342	1690.810476	4262.735085	3643.141143	3579.866651	4226.654554	3361.852417	1739.190138	
0.69_786.8422m/z	786.8422167	0.692166667	neg	1661.077396	2689.604143	3203.019526	2128.703972	1280.626611	1097.67523	2848.704861	3282.476306	1737.47001	

0.69_802.8154m/z	802.8154186	0.692166667	neg
0.69_805.8253m/z	805.8252857	0.692166667	neg
0.69_813.8688m/z	813.8687914	0.692166667	neg
0.69_821.8865m/z	821.8865486	0.692166667	neg
0.69_833.9372m/z	833.9371899	0.692166667	neg
0.69_849.9103m/z	849.9103346	0.692166667	neg
0.69_870.8029m/z	870.8029499	0.692166667	neg
0.69_881.8566m/z	881.8565869	0.692166667	neg
0.69_889.3718m/z	889.3718361	0.692166667	neg
0.69_897.8604m/z	897.8604005	0.692166667	neg
0.69_901.9243m/z	901.9242638	0.692166667	neg
0.69_965.3457m/z	965.3457315	0.692166667	neg
0.69_965.8452m/z	965.8451977	0.692166667	neg
0.69_969.9110m/z	969.9110192	0.692166667	neg
0.69_985.8852m/z	985.8852245	0.692166667	neg
0.71_1003.2647m/z	1003.264687	0.714216667	neg
0.71_1011.7476n	992.7297931	0.714216667	neg
0.71_1012.7964m/z	1012.796372	0.714216667	neg
0.71_1014.2955n	995.2776768	0.714216667	neg
0.71_1015.3123m/z	1015.312332	0.714216667	neg
0.71_1018.7448m/z	1018.744847	0.714216667	neg
0.71_1021.2847m/z	1021.284748	0.714216667	neg
0.71_1021.7824n	1002.76452	0.714216667	neg
0.71_1047.7882n	1028.770314	0.714216667	neg
0.71_1055.7759n	1054.777447	0.714216667	neg
0.71_1056.2756n	1055.277982	0.714216667	neg
0.71_1063.2648m/z	1063.264799	0.714216667	neg
0.71_1063.7612n	1044.743336	0.714216667	neg
0.71_1075.3138m/z	1075.313779	0.714216667	neg
0.71_1079.7355n	1060.717636	0.714216667	neg
0.71_1080.7832m/z	1080.783236	0.714216667	neg
0.71_1086.7300m/z	1086.730032	0.714216667	neg
0.71_1089.7692n	1070.751313	0.714216667	neg
0.71_1115.7753n	1096.757471	0.714216667	neg
0.71_1123.7628n	1104.744912	0.714216667	neg
0.71_1128.7055m/z	1128.705471	0.714216667	neg
0.71_1131.7481n	1112.730309	0.714216667	neg
0.71_1132.2480n	1131.252189	0.714216667	neg
0.71_1148.7720m/z	1148.771989	0.714216667	neg
0.71_1157.2576m/z	1157.257592	0.714216667	neg
0.71_1157.7547n	1138.736875	0.714216667	neg
0.71_1164.7448m/z	1164.744777	0.714216667	neg
0.71_1191.7484n	1172.730534	0.714216667	neg
0.71_1199.7361n	1180.718285	0.714216667	neg
0.71_128.9596m/z	128.9596146	0.714216667	neg
0.71_130.9577m/z	130.9576619	0.714216667	neg
0.71_180.9732m/z	180.9732194	0.714216667	neg
0.71_196.9470m/z	196.9470076	0.714216667	neg
0.71_215.0099m/z	215.0098926	0.714216667	neg
0.71_236.0653m/z	236.0653437	0.714216667	neg
0.71_238.0236m/z	238.0236408	0.714216667	neg
0.71_248.9605m/z	248.9605199	0.714216667	neg
0.71_264.9344m/z	264.9344201	0.714216667	neg
0.71_281.9149n	280.9075755	0.714216667	neg
0.71_306.0111m/z	306.0110887	0.714216667	neg
0.71_329.0003n	373.9986093	0.714216667	neg
0.71_332.9220m/z	332.9220255	0.714216667	neg
0.71_348.8959m/z	348.8959459	0.714216667	neg
0.71_350.8936m/z	350.8936047	0.714216667	neg
0.71_355.9112n	400.90938	0.714216667	neg
0.71_384.9355m/z	384.9355472	0.714216667	neg
0.71_396.9876n	441.9861571	0.714216667	neg
0.71_406.8658m/z	406.8658262	0.714216667	neg
0.71_411.9543m/z	411.9543368	0.714216667	neg
0.71_416.8834m/z	416.8834273	0.714216667	neg
0.71_418.8813m/z	418.8812943	0.714216667	neg
0.71_422.8397m/z	422.8396599	0.714216667	neg
0.71_440.0277m/z	440.0276793	0.714216667	neg
0.71_452.9230m/z	452.9230211	0.714216667	neg
0.71_464.9752n	509.9735556	0.714216667	neg
0.71_468.8967m/z	468.8967181	0.714216667	neg
0.71_474.8536m/z	474.8536039	0.714216667	neg
0.71_484.8708m/z	484.8708064	0.714216667	neg
0.71_486.8689m/z	486.8689448	0.714216667	neg
0.71_501.8522n	500.8449102	0.714216667	neg
0.71_508.0150m/z	508.0149992	0.714216667	neg
0.71_520.9104m/z	520.9103924	0.714216667	neg
0.71_532.9623n	577.9612553	0.714216667	neg
0.71_536.8844m/z	536.8843886	0.714216667	neg
0.71_542.8420n	542.8419876	0.714216667	neg
0.71_552.8585m/z	552.8584535	0.714216667	neg
0.71_554.8611m/z	554.8610867	0.714216667	neg
0.71_568.8323m/z	568.8323347	0.714216667	neg
0.71_576.0030m/z	576.0029983	0.714216667	neg
0.71_577.8491n	622.8473368	0.714216667	neg
0.71_588.8980m/z	588.8979795	0.714216667	neg
0.71_593.9353m/z	593.9353344	0.714216667	neg
0.71_594.8509m/z	594.8509308	0.714216667	neg
0.71_600.9502n	645.9486534	0.714216667	neg
0.71_604.8720m/z	604.8719688	0.714216667	neg
0.71_610.8297m/z	610.8297399	0.714216667	neg
0.71_630.8791m/z	630.8791316	0.714216667	neg
0.71_631.3806m/z	631.3805901	0.714216667	neg
0.71_638.8182m/z	638.8182429	0.714216667	neg
0.71_639.3676m/z	639.3676099	0.714216667	neg
0.71_639.8197m/z	639.8197144	0.714216667	neg
0.71_639.8635n	620.8456463	0.714216667	neg
0.71_643.9902m/z	643.9902073	0.714216667	neg
0.71_647.8541m/z	647.8540621	0.714216667	neg
0.71_653.8005n	652.7931772	0.714216667	neg
0.71_655.8375n	636.8196486	0.714216667	neg
0.71_656.8856m/z	656.8856049	0.714216667	neg
0.71_661.9217m/z	661.9217266	0.714216667	neg
0.71_664.8729n	664.8719651	0.714216667	neg
0.71_666.3727n	665.3745135	0.714216667	neg
0.71_684.9111n	729.909091	0.714216667	neg
0.71_685.4109m/z	685.4108747	0.714216667	neg
0.71_691.8775n	672.8596286	0.714216667	neg
0.71_694.7896m/z	694.7895968	0.714216667	neg
0.71_697.8336n	678.8157364	0.714216667	neg

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4449.203288	5730.592479	3379.996127	4040.113564	876.5534664	1005.297886	4592.254346	2856.632111	2591.500774
3755.077726	3058.576639	4911.062903	6387.637508	8534.208106	7747.71276	4565.947784	4502.084778	4412.875319
4351.394448	1337.625687	1530.639326	0.001403199	0.001403199	0.001403199	3686.905559	1192.49448	1441.709919
13354.33112	10898.40999	13396.68726	8069.978375	6798.147224	7640.902872	18836.21268	17637.30481	14082.44202
20534.77367	19580.84234	18535.1	14894.1858	14191.05761	17253.34826	22501.85606	20891.20484	20206.40092
9246.74742	5934.406629	6451.888839	4820.972395	68.74015158	820.3363519	3525.326284	2616.812155	2068.311398
3651.885929	0.001403199	2694.083712	5602.600484	6947.485341	5390.217237	1997.844902	1944.329687	4284.122871
5502.295879	3424.265796	3676.445139	0.001403199	976.7824744	1640.870531	5941.862124	4352.453094	3649.505683
422.3105278	227.9775209	0.001403199	1351.730355	837.2492714	65.92217351	4182.929835	677.4970329	1815.948498
5430.203833	5925.447836	3833.361504	4916.609896	3137.936277	2816.830795	7849.4741	8097.993062	8501.357561
4949.222064	5043.216366	6073.266749	2283.453903	1970.932194	0.001403199	6883.882441	4421.462372	3272.861839
1740.147715	38.60461539	0.001403199	0.001403199	0.001403199	480.5291512	3211.959776	1495.891541	2474.496406
3735.144692	2504.519527	2601.468082	2351.362484	1022.237086	2708.799017	2505.353007	3915.192071	2870.707198
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2464.753891	2584.823976	3753.823138	3976.595543	2068.507315	0.001403199	5276.525227	1671.436276	0.001403199
17243.3157	13725.18817	22563.60512	23291.08484	44874.07044	24036.5276	23143.41703	18766.42749	22303.0582
59544.4225	54692.34349	50650.69522	14188.3382	15944.95525	18211.97615	47500.34171	31561.9681	42152.46254
10337.84807	13263.75724	19075.09286	5003.102606	1766.58836	4470.555439	14171.96044	4189.844636	7618.980627
4672.525538	6006.523633	2475.156303	0.001403199	2437.952247	1827.912825	6828.67373	2791.199707	4559.169
2328.156681	7954.031408	8522.945797	7290.683886	8931.068884	7053.697291	3135.061656	11979.87538	4832.836988
3295.3606	4377.606612	4179.983995	765.3747282	0.001403199	1430.998929	6686.465663	5531.072754	7727.305753
39468.23689	43637.63917	40265.89786	13845.0176	15428.44632	18988.32574	45264.76742	28847.19838	39278.85613
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36577.70576	36036.36976	32722.60119	7313.30874	11667.26649	9396.584942	34090.48547	25706.33814	27239.44075
6576.008113	7835.547123	10496.1716	2984.412007	2993.278608	3891.385787	6110.883201	2780.260148	5678.763896
5270.983526	0.001403199	4201.596452	2822.08499	4039.999668	0.001403199	5782.320313	1467.454773	3480.569565
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2241.880421	5229.628271	4979.737568	0.001403199	0.001403199	0.001403199	6939.804469	3846.276978	0.001403199
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20575.29099	18820.58656	38144.74728	6498.071156	6850.137691	4729.253716	25799.6042	17603.28595	18924.49094
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23490.25609	14965.07393	17636.6796	5037.01048	0.001403199	2937.642376	18633.69845	7617.22394	9531.832293
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26408.51598	23403.36074	32360.82657	4051.89127	6980.982978	11243.16986	24900.77821	18754.41899	19413.69073
31592.911	19027.02239	36007.1424	6689.114658	11650.73167	6198.637561	25841.05638	26080.57353	23446.98651
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57300.74521	54823.51098	61631.12876	64455.76739	69465.34264	65432.87888	59242.23651	57376.87353	59995.38484
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2363.46462	2173.292019	2089.982231	0.001403199	0.001403199	601.0150028	1513.198722	2200.85271	972.9377741
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23358.74795	21725.0109	26711.24028	7829.439635	7775.006966	9270.687726	25180.74988	18508.38863	15963.30913
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17340.54006	14765.34832	16058.74049	21834.00963	26075.36511	22642.31399	21586.09787	19122.86979	17876.66681
3093.904476	2697.940765	1657.516112	1018.866032	1677.132029	1592.610235	3757.410027	3374.331261	2969.166377
385858.7875	352383.1695	366637.4498	201123.2363	227252.69	204088.5704	354152.3899	295850.3789	312832.8129
731.9718187	5553.634812	8538.471589	23503.09543	9897.426305	9822.054812	4229.838193	17391.93311	8758.930644
7445.451137	14697.73733	16831.84152	30845.92064	21143.85704	23808.02343	12161.84947	27689.03013	21057.53239

| | | |

0.71_995.7744n	976.7566051	0.714216667	neg
0.71_996.8222m/z	996.822153	0.714216667	neg
0.74_1123.2654m/z	1123.265434	0.7359	neg
0.74_113.0197m/z	113.019673	0.7359	neg
0.74_115.0513m/z	115.0513491	0.7359	neg
0.74_124.0629m/z	124.0629002	0.7359	neg
0.74_131.0715m/z	131.0714791	0.7359	neg
0.74_164.9571m/z	164.9570928	0.7359	neg
0.74_172.0229m/z	172.0229054	0.7359	neg
0.74_186.0386m/z	186.0386158	0.7359	neg
0.74_186.9295m/z	186.9295336	0.7359	neg
0.74_191.9951m/z	191.9951496	0.7359	neg
0.74_240.0105m/z	240.0104923	0.7359	neg
0.74_243.0029n	223.9850187	0.7359	neg
0.74_248.9499m/z	248.9498515	0.7359	neg
0.74_254.0262m/z	254.0261968	0.7359	neg
0.74_254.9171m/z	254.9170594	0.7359	neg
0.74_254.9266m/z	254.9266399	0.7359	neg
0.74_259.9824m/z	259.9824446	0.7359	neg
0.74_267.0214m/z	267.0213738	0.7359	neg
0.74_270.8911m/z	270.891063	0.7359	neg
0.74_274.0119m/z	274.0118778	0.7359	neg
0.74_282.1073m/z	282.1073296	0.7359	neg
0.74_291.9820m/z	291.9820221	0.7359	neg
0.74_300.0549n	281.0370525	0.7359	neg
0.74_304.0657m/z	304.0656554	0.7359	neg
0.74_307.9980m/z	307.9979625	0.7359	neg
0.74_322.9044m/z	322.9043602	0.7359	neg
0.74_328.9863m/z	328.9863116	0.7359	neg
0.74_335.0091m/z	335.0090501	0.7359	neg
0.74_338.8784m/z	338.8783594	0.7359	neg
0.74_349.0246m/z	349.0246211	0.7359	neg
0.74_358.9669m/z	358.9669237	0.7359	neg
0.74_375.9854m/z	375.9853674	0.7359	neg
0.74_391.9596m/z	391.9596114	0.7359	neg
0.74_396.9737m/z	396.9736806	0.7359	neg
0.74_422.9687m/z	422.9687312	0.7359	neg
0.74_426.8386m/z	426.8386305	0.7359	neg
0.74_432.9867m/z	432.9866572	0.7359	neg
0.74_443.9731m/z	443.9731295	0.7359	neg
0.74_459.9470m/z	459.9470399	0.7359	neg
0.74_500.9740m/z	500.9740173	0.7359	neg
0.74_527.9352m/z	527.9351878	0.7359	neg
0.74_532.8239m/z	532.8238944	0.7359	neg
0.74_552.9872m/z	552.9872171	0.7359	neg
0.74_558.8153m/z	558.8153464	0.7359	neg
0.74_595.9217m/z	595.9217035	0.7359	neg
0.74_626.8032m/z	626.8031571	0.7359	neg
0.74_630.8013m/z	630.8012793	0.7359	neg
0.74_642.7764m/z	642.7764406	0.7359	neg
0.74_753.8977m/z	753.8977332	0.7359	neg
0.74_763.8464m/z	763.8464453	0.7359	neg
0.74_766.7760m/z	766.7760145	0.7359	neg
0.74_769.8722m/z	769.8721602	0.7359	neg
0.74_837.8599m/z	837.8599345	0.7359	neg
0.74_840.3211m/z	840.3211378	0.7359	neg
0.74_841.2839m/z	841.2839244	0.7359	neg
0.74_909.2719m/z	909.2719221	0.7359	neg
0.74_914.7257m/z	914.7257396	0.7359	neg
0.74_925.2448m/z	925.24482	0.7359	neg
0.76_124.0037m/z	124.0037088	0.757316667	neg
0.76_124.0074m/z	124.0073713	0.757316667	neg
0.76_125.0108m/z	125.0107588	0.757316667	neg
0.76_126.0032m/z	126.0031976	0.757316667	neg
0.76_142.0511m/z	142.0511118	0.757316667	neg
0.76_143.0352m/z	143.0351983	0.757316667	neg
0.76_161.9942m/z	161.9941654	0.757316667	neg
0.76_164.9501m/z	164.9501108	0.757316667	neg
0.76_195.8877m/z	195.8877404	0.757316667	neg
0.76_196.8949m/z	196.8949364	0.757316667	neg
0.76_205.0177m/z	205.0177401	0.757316667	neg
0.76_221.9749m/z	221.9748535	0.757316667	neg
0.76_232.9022m/z	232.9022378	0.757316667	neg
0.76_239.0167m/z	239.0167377	0.757316667	neg
0.76_243.9567m/z	243.956711	0.757316667	neg
0.76_243.9661m/z	243.9660689	0.757316667	neg
0.76_259.9306m/z	259.9306269	0.757316667	neg
0.76_265.0115m/z	265.0114955	0.757316667	neg
0.76_276.8472m/z	276.8471597	0.757316667	neg
0.76_285.1061n	284.0992401	0.757316667	neg
0.76_311.9448m/z	311.9448333	0.757316667	neg
0.76_311.9541m/z	311.9540895	0.757316667	neg
0.76_323.8973m/z	323.8973026	0.757316667	neg
0.76_334.1259m/z	334.1259361	0.757316667	neg
0.76_375.0999m/z	375.0998786	0.757316667	neg
0.76_466.1239m/z	466.1239193	0.757316667	neg
0.76_831.2545m/z	831.2545189	0.757316667	neg
0.78_132.9463m/z	132.9463162	0.778533333	neg
0.78_134.9434m/z	134.9434127	0.778533333	neg
0.78_149.0357n	148.0283846	0.778533333	neg
0.78_150.8866m/z	150.8866196	0.778533333	neg
0.78_152.8837m/z	152.883703	0.778533333	neg
0.78_154.8807m/z	154.8806919	0.778533333	neg
0.78_154.9282m/z	154.928244	0.778533333	neg
0.78_156.9253m/z	156.9252704	0.778533333	neg
0.78_160.8421m/z	160.8420772	0.778533333	neg
0.78_162.8392m/z	162.839167	0.778533333	neg
0.78_164.8361m/z	164.8361441	0.778533333	neg
0.78_172.8424m/z	172.842429	0.778533333	neg
0.78_174.0520m/z	174.0519672	0.778533333	neg
0.78_174.8395m/z	174.8395207	0.778533333	neg
0.78_186.8655m/z	186.865503	0.778533333	neg
0.78_186.9650m/z	186.9649702	0.778533333	neg
0.78_195.8110m/z	195.8110023	0.778533333	neg
0.78_195.9538n	194.9463637	0.778533333	neg
0.78_197.8080m/z	197.8080169	0.778533333	neg
0.78_199.8051m/z	199.8050664	0.778533333	neg
0.78_201.8021m/z	201.8021383	0.778533333	neg
0.78_212.8868m/z	212.8867815	0.778533333	neg
0.78_217.9262n	216.9185182	0.778533333	neg

75260.91284	60773.28079	69983.50514	46126.45836	60145.40472	50918.9443	68460.12957	59260.31863	62609.94015
19719.03751	15042.09332	14809.40694	3341.808228	1737.539381	3526.894554	15004.92533	10956.43555	10254.8052
5152.922958	0.001403199	1663.254563	0.001403199	0.001403199	0.001403199	4800.957555	0.001403199	2506.294777
216.764497	102.2376454	152.9521337	175.2806605	79.40214132	174.747673	216.5118445	127.1335836	233.9105988
289.3321929	281.967206	261.1746484	184.8180225	265.4982743	349.4510538	287.9597389	603.1221079	420.4679055
388.3712174	286.6600945	565.9355979	495.8175963	595.6648181	289.438435	506.6893532	368.5480537	531.5629696
253.5054015	171.8020713	92.20016445	132.1645038	102.7650382	216.9627568	169.6229322	123.640289	105.635301
2754.73577	1424.86264	2558.310763	4061.264521	5880.730135	5071.051227	1350.649943	4488.53956	4025.154449
6507.219467	3932.159037	13412.02308	4211.34151	14261.59325	4329.008668	9724.910603	11051.61619	17279.17474
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3885.583306	7917.898449	9988.508792	20447.10966	11280.61565	12248.85836	6276.542555	17687.66586	13064.18564
1038.880526	421.5928927	1072.473233	742.2822055	2733.041197	1506.368011	268.6659277	1733.795895	1540.751154
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2792.108749	2090.246014	5875.450811	3487.177	4694.926144	3344.328848	4654.886631	4201.413944	6107.535107
280.0714049	318.1834195	360.2988766	133.5791743	130.0810532	228.752801	368.1585694	151.9490051	160.6417751
144.0300263	0.001403199	70.61096117	0.001403199	232.0376067	0.001403199	0.001403199	347.8104172	246.9076389
8737.914463	17761.14561	22654.9203	40585.38509	22376.35853	24269.837	14382.32673	36923.06743	26973.04756
1016.882969	549.7415733	4261.255985	447.281421	5009.318246	1336.537317	1141.503248	4094.277513	5598.588124
929.5061654	1011.558029	786.4101412	0.001403199	706.9009069	402.4699354	405.5088006	452.7323914	894.6151582
490.2022829	457.4901403	1114.386964	257.2535055	814.6398948	172.4103213	1299.177368	705.0579408	1459.818437
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507.5232436	1148.405597	1094.677253	2834.82438	2797.937732	1938.848127	723.2011078	2346.918796	2247.209736
642.1455951	516.3369019	605.4758659	720.0521712	820.6849241	613.9624995	485.3058449	464.5433128	430.8388715
377.9603722	250.9434079	638.8766964	525.2606741	2018.28342	919.2742458	1.650441576	1331.113995	1351.689545
1921.038325	909.5141285	4669.570391	648.0483421	4031.293372	837.4318042	2807.428438	3349.076687	5805.206039
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8780.406097	8050.206764	11353.07975	4615.907664	7106.683519	6652.991555	12258.43856	7681.703664	12177.72705
8300.361271	18029.79384	21335.13874	38126.2538	18106.63051	21467.43354	12853.91524	32523.46323	24932.19934
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6690.208614	5866.204315	6768.361628	2170.977645	1978.894053	2423.573597	9762.717358	1741.680084	5284.409129
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1941.495849	1313.1613	2684.753252	931.3325367	885.7944665	1057.216195	3025.30818	1112.870706	2428.387612
5806.869272	3975.843154	4756.248814	2721.12258	1726.663799	2359.536216	6899.30516	1204.833397	3086.231603
0.001403199	0.001403199	297.7659843	5149.780291	4124.904184	5868.982363	0.001403199	0.001403199	0.001403199
2056.215031	1013.905995	3397.401082	492.6982367	835.750573	0.001403199	2901.164832	609.3292556	2572.388434
448.8471458	4203.833911	5968.894156	17070.93196	9153.884086	9134.307549	857.8506788	9785.444247	6799.225432
6662.196434	4384.069813	3047.610754	3445.135372	516.1027753	2424.206051	8419.048441	181.9203359	2352.632751
2321.661518	6537.917077	7899.462292	22246.20435	11238.30488	11856.57718	2916.389607	13570.15698	9021.82583
3841.541563	3508.366233	2514.990497	4872.95237	3186.081514	4127.421557	3753.484812	2556.002411	1832.494182
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3424.116106	4598.488732	1513.989279	454.9792245	660.6560322	1281.67096	1824.543268	2218.216431	1526.424092
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6658.936421	5608.175279	2516.965379	2189.108733	4721.786854	3437.401011	7123.153457	1582.299402	535.0526324
2657.645197	3785.315931	891.0082276	988.1771819	2055.799321	742.1460306	5213.906395	52.10480926	2256.389314
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27.07565574	13.95830031	0.001403199	110.4560485	0.001403199	135.8133555	0.001403199	0.001403199	0.001403199
25762.08657	21664.44636	20485.33412	44381.31782	35617.14304	57147.4247	19274.16509	19863.42036	18966.89582
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15278.34234	19011.4833	21614.78301	46347.85762	34033.20779	45149.55755	21803.08007	21110.22104	20179.67814
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373.8739549	822.4329474	1170.543987	1758.385074	0.001403199	974.3179144	779.2000592	1867.835185	853.2755542
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645.4895132	374.0199842	1389.75933	1696.257654	2777.630734	2143.939592	466.3658924	2147.067461	2415.947395
1421.516265	1760.831812	2142.931645	926.4797459	0.001403199	1.810426132	1906.334605	1349.628459	806.0580061
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3796.016602	4171.133084	4634.808163	1873.773037	389.6512722	976.1742433	3864.428276	4572.355692	1707.635848
2395.523613	2415.674563	2656.184111	0.001403199	452.1513547	131.5028499	2122.047623	2241.192698	1418.902309
2365.276888	2345.119862	2603.217217	185.5735553	316.4715078	132.203347	2087.402924	2109.0887	1491.217337
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21650.18925	19203.3316	20418.92617	14013.88314	15017.58891	13722.52936	22392.85959	11076.76357	20449.49852
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267091.3074	252733.4283	267185.0424	99982.8411	122090.4749	104066.0701	304861.5749	231639.1117	255786.6834
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0.78_221.8345m/z	221.8345028	0.778533333	neg
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0.78_268.8008m/z	268.8007868	0.778533333	neg
0.78_272.0194m/z	272.0194382	0.778533333	neg
0.78_272.0274n	253.0095596	0.778533333	neg
0.78_272.8427m/z	272.8426631	0.778533333	neg
0.78_275.0543m/z	275.054285	0.778533333	neg
0.78_286.0606m/z	286.0606438	0.778533333	neg
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0.78_292.9235m/z	292.92346	0.778533333	neg
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0.78_312.9852m/z	312.985215	0.778533333	neg
0.78_314.8959m/z	314.8959012	0.778533333	neg
0.78_330.9827m/z	330.982726	0.778533333	neg
0.78_363.9066m/z	363.9065599	0.778533333	neg
0.78_368.0882m/z	368.0881554	0.778533333	neg
0.78_437.0412m/z	437.0411545	0.778533333	neg
0.78_439.9009m/z	439.9009365	0.778533333	neg
0.78_701.1910m/z	701.1909975	0.778533333	neg
0.78_752.1546m/z	752.1545632	0.778533333	neg
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0.80_196.9411m/z	196.9411171	0.800366667	neg
0.80_212.8774m/z	212.877449	0.800366667	neg
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0.82_155.8657m/z	155.8656873	0.819566667	neg
0.82_157.8630m/z	157.8629626	0.819566667	neg
0.82_160.0042n	204.9989693	0.819566667	neg
0.82_174.8609m/z	174.8609349	0.819566667	neg
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0.82_177.8600m/z	177.8600211	0.819566667	neg
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0.82_194.9856m/z	194.9855853	0.819566667	neg
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0.82_211.0283m/z	211.0283381	0.819566667	neg
0.82_216.9095m/z	216.9094927	0.819566667	neg
0.82_218.9052m/z	218.9052375	0.819566667	neg
0.82_222.8330m/z	222.8330152	0.819566667	neg
0.82_222.9589m/z	222.9588723	0.819566667	neg
0.82_222.9676m/z	222.9676086	0.819566667	neg
0.82_223.8220m/z	223.8219735	0.819566667	neg
0.82_224.8296m/z	224.8295693	0.819566667	neg
0.82_232.9973m/z	232.9973382	0.819566667	neg
0.82_234.8800m/z	234.8799882	0.819566667	neg
0.82_243.0180m/z	243.0180248	0.819566667	neg
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0.82_263.0078m/z	263.007845	0.819566667	neg
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0.82_274.8683m/z	274.8682678	0.819566667	neg
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3388.390205	3539.707204	2504.178995	0.001403199	0.001403199	0.001403199	4415.134803	2161.100906	527.6022231	
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9836.636974	12820.98878	12704.29007	13289.19446	10307.68241	18036.77518	12780.56804	11665.08673	9880.016461	
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8793.788424	9004.664321	10481.49668	21334.51637	24243.51194	20531.75137	8485.438568	8668.017179	10519.86264	
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7408.534172	8223.078118	8679.674868	5484.454022	2714.112695	4079.202777	6545.275258	6071.791538	4320.14374	
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5611.332089	5211.545411	5405.278514	3332.19715	3554.655025	3660.932437	6372.026528	5986.799181	5888.229398	
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4613.721196	4820.986813	4961.844893	1559.314582	2244.292644	1430.649804	4085.193237	3612.923584	3415.471211	
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0.82_316.8730m/z	316.8730441	0.819566667	neg
0.82_319.0574m/z	300.0395376	0.819566667	neg
0.82_327.0329m/z	327.0328921	0.819566667	neg
0.82_333.0137m/z	333.013698	0.819566667	neg
0.82_337.0580m/z	337.0579994	0.819566667	neg
0.82_346.0815m/z	346.0814867	0.819566667	neg
0.82_350.9931n	331.9752697	0.819566667	neg
0.82_354.8290m/z	354.8290076	0.819566667	neg
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0.82_428.0477m/z	428.0477156	0.819566667	neg
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0.82_472.7816m/z	472.7815822	0.819566667	neg
0.82_481.1105n	480.102375	0.819566667	neg
0.82_497.0340m/z	497.0339923	0.819566667	neg
0.82_525.9026m/z	525.9026455	0.819566667	neg
0.82_526.0154m/z	526.0153625	0.819566667	neg
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0.84_186.8561m/z	186.8561443	0.841733333	neg
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0.84_222.0442m/z	222.0442481	0.841733333	neg
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0.84_236.0235m/z	236.023525	0.841733333	neg
0.84_242.0519m/z	242.0519208	0.841733333	neg
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0.84_252.9428m/z	252.9427825	0.841733333	neg
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0.84_286.8296m/z	286.8296328	0.841733333	neg
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0.84_359.0766m/z	359.0766325	0.841733333	neg
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0.84_379.0693m/z	379.0693035	0.841733333	neg
0.84_394.0674m/z	394.067434	0.841733333	neg
0.84_412.8458m/z	412.8457732	0.841733333	neg
0.84_419.9889m/z	419.9888795	0.841733333	neg
0.84_434.8250m/z	434.8249653	0.841733333	neg
0.84_443.7838m/z	443.7838	0.841733333	neg
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0.84_456.8076m/z	456.8075505	0.841733333	neg
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0.84_494.7642m/z	494.7641638	0.841733333	neg
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0.84_585.7137m/z	585.7136807	0.841733333	neg
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0.84_626.9572m/z	626.9571805	0.841733333	neg
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0.84_667.8348m/z	667.8348463	0.841733333	neg
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7629.742142	9400.179381	11510.16793	2582.686864	0.001403199	0.001403199	9278.317293	4552.43868	6963.830439
10835.25058	11390.56658	13256.30868	12173.79958	15630.55069	13751.5385	4548.839598	4820.852248	6747.334575
2770.89408	2670.901239	3315.482143	2718.277138	2530.232417	2728.29274	3425.983637	3856.524931	3498.220621
379.160459	666.4465344	625.2866988	126.1552808	175.522802	109.1068344	313.6581183	485.347281	284.6663162
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5911.757509	4866.166607	4374.760063	1872.208787	1868.602386	2080.503972	4214.219068	4670.823635	4260.706512
7244.234639	7549.500584	7146.063399	3950.933965	4508.282315	4086.148855	8031.485646	7845.914956	7303.081582
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2267.871439	1967.781427	1681.97889	2038.007911	870.4691839	1243.647924	773.4905553	932.3980079	940.6958716
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2816.626437	2654.406734	2223.708522	2513.176015	2591.55922	2240.193181	4990.554723	4674.654446	5258.776639	
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0.95_256.8406m/z	256.8405631	0.946033333	neg
0.95_259.8394m/z	259.8394086	0.946033333	neg
0.95_281.9052m/z	281.9052322	0.946033333	neg
0.95_289.9944n	288.9873208	0.946033333	neg
0.95_294.8618m/z	294.8618226	0.946033333	neg
0.95_296.9431m/z	296.9431459	0.946033333	neg
0.95_330.7843m/z	330.784258	0.946033333	neg
0.95_341.8988m/z	341.8988118	0.946033333	neg
0.95_348.8096m/z	348.8096461	0.946033333	neg
0.95_358.8410m/z	358.8409879	0.946033333	neg
0.95_359.8167m/z	359.8166851	0.946033333	neg
0.95_361.0580m/z	361.0580294	0.946033333	neg
0.95_366.8008m/z	366.8007749	0.946033333	neg
0.95_367.7884m/z	367.7884162	0.946033333	neg
0.95_368.7962m/z	368.796226	0.946033333	neg
0.95_370.7914m/z	370.7913975	0.946033333	neg
0.95_389.7703m/z	389.7703225	0.946033333	neg
0.95_390.0367m/z	390.0366829	0.946033333	neg
0.95_391.0329m/z	391.0328664	0.946033333	neg
0.95_407.0275m/z	407.0275089	0.946033333	neg
0.95_418.7958m/z	418.7957801	0.946033333	neg
0.95_426.7541m/z	426.7540594	0.946033333	neg
0.95_436.8210m/z	436.8209979	0.946033333	neg
0.95_438.0345m/z	438.0344829	0.946033333	neg
0.95_439.8653m/z	439.8653238	0.946033333	neg
0.95_448.7362m/z	448.7361971	0.946033333	neg
0.95_461.8477m/z	461.8476949	0.946033333	neg
0.95_463.8432m/z	463.8432059	0.946033333	neg
0.95_466.7624m/z	466.7624058	0.946033333	neg
0.95_468.7592m/z	468.7591594	0.946033333	neg
0.95_478.7892m/z	478.789213	0.946033333	neg
0.95_483.8297m/z	483.829732	0.946033333	neg
0.95_487.7367m/z	487.7366639	0.946033333	neg
0.95_488.7445m/z	488.7445007	0.946033333	neg
0.95_509.7192m/z	509.7191552	0.946033333	neg
0.95_559.8150m/z	559.81499	0.946033333	neg
0.95_576.7570m/z	576.7569954	0.946033333	neg

1131.550622	1892.177139	1680.287494	4712.157142	1381.379912	2208.873897	1323.402253	1585.243896	471.7534161
765.6863108	1817.365317	1575.143044	4537.310441	2871.618601	3495.067573	413.6728093	1953.663483	1050.498558
708.7112312	946.4572265	802.5133582	2379.786544	997.7982082	2281.627832	531.2581281	1285.944703	487.2271878
13679.64857	11368.1213	11370.48661	9506.09622	8757.258765	12346.97226	14684.49197	11321.65999	14359.03709
1847.218854	2069.640409	1529.72541	972.7592817	535.4234695	741.4529755	1686.020335	1263.880774	554.4079413
235.3326923	997.4075622	601.1865214	914.3486732	529.5061633	730.4270149	447.63675	144.6584483	266.6573385
2266.615255	2266.981776	1665.746982	503.3846911	280.729235	766.9300465	2049.69113	1125.442059	424.6869919
1415.828014	1236.610136	838.1702275	585.8793012	167.6940169	547.5411821	1263.897384	773.0133382	396.3672247
8541.944239	8273.60022	8248.951883	7338.194498	6185.377312	8081.956721	9365.770434	7090.180231	5625.019568
691.8908049	564.2491147	810.358008	0.001403199	170.4582336	0.001403199	145.8731343	871.8185043	269.7141994
5342.75507	5539.519359	3519.351958	5642.474035	3700.242694	5304.858273	4343.239027	3464.06522	1725.104151
3426.526879	3899.339037	3452.878948	4197.7568	4451.408398	4328.918043	4129.039104	4257.39851	4191.612613
10893.25776	11877.25139	9035.941224	4051.50773	5396.476684	4288.725116	10021.94306	7464.392776	9878.03715
1652.786317	2427.346067	1032.023377	702.8371331	137.2091682	0.001403199	1293.191025	671.2602067	184.3238267
508.2399373	0.001403199	250.5385661	3153.709335	2422.478977	1898.698616	0.001403199	675.7178268	0.001403199
147.9385526	1058.030732	925.5708061	163.6860822	0.001403199	311.4748639	280.2232598	155.9786758	329.3054767
415.3690476	836.8674639	369.7150395	329.335489	0.001403199	0.001403199	222.8512025	190.56884	0.001403199
7344.337848	6996.195324	6685.374335	3990.195803	1600.323403	3735.099084	6256.924394	5798.241535	1780.816065
3391.690769	2942.12216	1757.801514	1023.701931	287.4501804	231.1343603	2282.266889	1197.690093	522.9431937
5367.863976	6730.036761	7130.682142	6758.47271	7818.190217	6557.435057	5485.130827	6443.505924	6923.011374
2355.338393	2296.890535	1384.020387	1132.176856	156.3727155	371.8993614	1643.564176	600.1465225	380.2886519
4428.415919	4400.456368	5091.781239	3539.731704	5119.04389	4218.864383	5159.448516	4072.602605	4949.890646
2684.310306	2530.975537	1984.719666	1132.344096	1031.164848	1293.756596	2891.295301	1659.009605	1556.973449
45329.21057	48556.21017	44080.11022	45699.00171	53834.14089	48597.77422	47021.00693	41588.68248	50289.02325
1362.551948	1741.939105	1842.092356	2801.177448	1879.544449	1874.586679	2062.139692	2189.814094	1297.887007
3198.708343	2757.037114	3692.40158	4038.693311	1925.764629	3787.487359	3249.283697	2936.114447	1298.281188
6458.002548	7278.657167	7848.547072	10836.83056	11292.95581	10581.84671	7626.782856	6565.505707	9014.198417
13944.29063	14132.41864	11636.16834	10413.89286	12884.72835	12451.24069	14366.92197	11106.15759	13808.0609
2602.000564	2146.968477	2592.587083	2612.443416	1343.081226	1473.83011	1675.646868	1618.369995	765.543019
6321.846855	6427.331536	4192.198371	5146.143108	4977.83412	5508.698121	4646.467324	3825.530423	3592.840123
4421.172631	5384.649116	7104.696556	5645.832956	1047.058495	3858.541577	6248.397741	4024.216999	1080.077972
22405.7053	29737.89316	25302.19854	45008.19844	39131.12839	37351.8511	30019.69344	29721.74703	32496.06285
2000.664922	2740.577911	2607.28796	4016.292495	2222.743169	2756.522448	2894.194906	4148.477081	1313.202145
5459.800132	4714.834424	3003.279616	2259.066683	2680.347022	2556.244592	4611.641692	3550.154734	3735.483941
2657.022935	3110.604541	753.2667023	1907.160891	1983.501572	2316.635976	1023.714321	2235.660507	2231.215941
4989.46542	5031.657451	3606.379623	9907.059427	4394.28717	6576.307819	4930.860837	4476.48555	2181.367595
2827.562196	4013.702333	1679.528019	3199.889896	1015.828706	1287.100358	2065.244575	629.4874878	1162.334953
377.4474439	170.3724678	159.5829395	0.001403199	0.001403199	0.001403199	277.287925	163.2941471	92.24450835
749.7911641	392.6348127	568.9140282	0.001403199	0.001403199	0.001403199	713.7499791	330.9439316	400.0333513
342.1874446	435.9787367	146.002303	0.001403199	0.001403199	87.71980448	178.5980668	0.001403199	1.507673627
1596.338726	1481.104721	1382.056372	1816.332349	1427.041276	863.0443762	2081.318166	1205.572928	1355.887148
1539.99137	1192.091805	1014.506557	97.07445239	241.1821556	95.81309086	1451.940819	1056.90445	975.6051441
4438.962423	3728.166737	3601.952852	2168.657045	2394.215713	2608.329447	4209.044439	3504.026631	3981.974281
1124.388784	957.6919288	955.0604294	1327.655233	829.2121257	822.8139352	1064.1997	673.2512481	670.6079139
1111.486857	785.1218677	888.3772996	313.7708098	74.9816707	472.9488587	1019.241595	985.2506218	713.2463384
9905.821041	9478.61249	9715.151037	2948.435672	2950.545901	2791.492667	10262.87859	8744.030396	6898.794798
6522.360144	6559.421685	6213.77228	1603.615323	1695.358964	2115.588813	6926.074101	5947.47665	4467.723565
594.1439176	644.9709394	538.35698	113.7453203	90.7118676	0.001403199	630.645651	641.3548398	481.5427574
763.7193245	811.1323404	1215.083425	1336.367746	550.8185453	863.9195372	920.4506789	771.2845412	489.1931273
4337.696762	4420.051367	4697.927972	3728.61442	6411.351504	5974.464009	5585.410831	5312.369846	6958.877662
7756.072409	7594.10752	8454.316657	5646.137506	5256.011681	4746.719106	8682.48265	8966.108055	8136.640843
1441.010765	1412.29306	1207.557378	1315.009824	608.9903828	874.9228097	1345.563691	1503.880107	1225.815605
813.4348427	912.3301754	690.2574333	499.6921545	430.8116651	114.4101768	394.062203	82.37326311	255.7534021
937.928548	626.3191974	495.1311397	0.001403199	0.001403199	0.001403199	416.2173774	337.8922684	440.6388515
9238.780685	10357.09861	9073.649825	13170.31009	12624.79117	12600.64565	11934.78779	9958.322362	12203.89105
550.5455103	1016.200067	1074.246308	155.6769038	518.7042643	531.7467688	760.4023232	636.689786	486.1011271
20559.87704	17473.86768	17034.48876	11816.69818	12871.11425	13639.93325	21323.01414	18133.61479	18558.71998
2113.940678	3252.492834	2934.581456	2196.560151	2520.766723	2062.917855	3701.554588	3740.866002	2661.098407
34457.46788	35477.15184	36135.15165	74159.64585	54683.76262	59535.08619	44455.8716	52125.99943	42876.79723
1453.493982	1009.256075	949.8030938	0.001403199	0.001403199	0.001403199	1027.906667	922.5012958	400.4598125
2739.997923	3684.059442	3318.054726	2891.023051	2928.505286	3022.981571	1884.527561	2284.875506	2741.881022
1489.206073	880.3399821	1427.726295	1551.722221	889.9829384	560.2453917	1339.872736	1639.889014	542.4877268
890.0216335	640.307438	728.8090544	415.9152023	258.1529022	211.6254987	658.4435163	391.899828	487.7893184
2699.206347	2699.868518	1977.37108	669.8707397	1167.116501	806.2228099	1834.215826	1576.595174	1830.664735
297.6579536	685.1315191	654.9660739	786.3539814	352.4446484	84.42419977	910.7392851	713.577877	380.737791
1131.929229	1242.731616	856.8663772	88.75950946	143.4111483	166.270899	1478.990177	994.8545959	918.8293421
6068.604985	6222.156475	7085.444402	10834.30314	10516.39593	10928.11671	8226.830832	9191.827082	9303.734783
3790.061296	4434.374721	4717.337503	7004.638355	7070.004811	6513.132882	5669.74679	5573.850692	5459.823557
783.8531605	878.9657654	673.8803579	189.4138041	295.8004055	191.027927	519.3846042	451.9496326	477.1186593
1566.949015	2818.960788	3483.714785	12285.0938	12642.50878	12517.95228	2812.948359	6492.022911	5452.121596
54274.1928	50517.94898	50482.58242	71062.04278	72494.51085	72626.84565	63615.5556	61074.88065	63480.53578
772.0394885	855.8218308	755.7195253	168.5349859	129.5886972	106.3459941	538.4470642	771.147885	299.3018504
4623.134967	3695.702374	3284.265751	772.9243504	1270.946587	1003.005425	4454.40002	3510.573453	3202.205795
3051.089044	2594.575398	2243.152416	1476.179856	945.4862561	1288.546964	2470.843315	2201.540238	2059.760865
392.8966374	977.1430086	663.8212783	2386.89222	2161.194249	2082.223601	851.4092542	1472.6395	920.3250135
1757.773541	2073.692851	1728.559195	421.1788616	1106.486941	731.1425436	1818.0234	1684.045527	1741.935383
20366.86044	25635.90483	29441.53411	57483.82808	52450.25886	52846.44935	27968.77314	35882.23211	34176.81822
128.8738965	297.2086163	312.1754882	1278.960505	1521.06298	1019.183864	627.2840342	749.7343566	386.6617064
3428.322871	3434.52043	3886.626215	2667.769513	2340.468342	2551.999444	3240.36012	3571.835581	3129.770859
6590.541687	5255.931173	4792.396272	2769.885733	3448.17801	2688.66303	6007.299251	4667.78451	5136.590139
38478.18627	44608.0207	43303.84712	60192.18635	57349.67952	57554.49873	48417.28974	53133.45699	50670.33937
3297.844557	3716.167211	3839.209374	8670.311474	9575.382617	9256.451219	5694.889571	7453.725508	6655.616909
142401.8068	146435.4062	144841.9424	179131.083	180452.6804	182761.0697	179794.0313	174226.5714	173118.9437
12841.82093	10986.8312	11574.43612	14899.25756	15840.14689	16952.877	14084.72836	13860.50043	14255.77532
0.001403199	0.001403199	0.001403199	1227.707196	451.7567854	521.897917	0.001403199	160.1988602	0.001403199
1546.415972	1647.720932	1330.253535	2672.871335	2199.328301	1794.087202	2258.643499	2246.789992	2039.933549
23502.53834	24777.60719	26480.86755	42158.33467	39009.22293	40206.6001	32189.54228	32533.12693	33470.24231
42159.83746	42237.18238	40213.75504	62225.52794	56777.57884	55220.0757	51064.61309	53678.23739	51715.23202
4273.660502	4462.502229	3558.694964	5622.476167	6032.098102	5552.71657	4741.615727	5233.928531	5137.840082
23276.57822	24643.00463	23283.93339	27939.47888	30149.27435	28274.24693	27982.86976	27191.49687	26702.59781
0.001403199	0.001403199	0.001403199	2484.064149	1063.860136	1579.851717	0.001403199	0.001403199	0.001403199
0.001403199	0.001403199	0.001403199	11992.04291	3340.927871	4226.616455	0.001403199	907.5927582	379.1879868
0.001403199	0.001403199	0.001403199	2169.554375	342.7041355	741.7738133	0.001403199	0.001403199	0.001403199
808.6906835	1548.637704	1513.740447	0.001403199	131.002095	633.9291667	1753.102775	449.6139984	1654.766782
8905.217323	7058.923904	6904.637021	4049.271804	4344.875509	4759.983892	8734.156057	9987.770191	9211.372839
4344.722021	5954.268618	5290.672286	7557.99344	7452.81514	8000.361816	6352.85141	8687.24197	8233.316595
821.9768	1474.21433	1824.494159	0.001403199	0.001403199	0.001403199	1207.304127	2186.256984	1344.886694
6481.987989	9263.985338	11023.72729	18458.85382	14897.53204	15299.89862	10014.02941	13829.66916	12377.49214
5882.840898	5960.266295	5215.274043	3347.159099	3429.52311	3747.450625	6048.840076	5317.982317	6102.430011
16861.12096	22323.73573	21239.39854	30875.19624	29139.99703	27622.56256	24553.40802	26955.07556	26689.00955
195.3788785	382.0486822	923.0284279	1384.521596	949.3405727	890.1455415	421.958216	884.7202638	688.9039091
27777.02217	30674.37704	28979.08564	62650.54844	52926.81396	51561.4848	38574.75337	42273.08703	41259.84683
6290.897589	5006.437176	5665.527021	11163.67764	9531.860415	10242.33114	6137.726402	8081.300559	6400.424313
84776.72377	88634.42234	88354.25584	89765.6717	96898.74079	96792.18668	113039.5017	105662.3009	104522.8574
11619.78121	13931.32776	13585.99276	16498.59059	17562.96898	17607.64859	17183.71888	18842.25826	18309.52917
7767.167709	9582.34309	10463.88388	13027.14544	13823.53169	14195.91552	12685.56768	13643.65817	12729.75194
24588.00474	28194.40693	24976.81264	46144.68786	40400.95591	41795.38763	33697.8765	36421.79956	32217.6986
12710.84601	12743.30865	13871.60071	17138.57101	17608.84494	17987.96344	17389.59232	16762.02575	16307.16607
2114.250287	3758.812157	4719.536004	10957.07351	7171.079014	8525.645595	5429.463062	7348.43673	6347.389853
77006.08427	85605.62656	87669.34578	136899.8289	137140.7037	134286.3828	114180.358	127717.5984	123602.1832

0.95_578.7530m/z	578.7529661	0.946033333	neg							14206.03755	17852.04362	17034.04198	30490.30593	26386.03172	27753.98363	21881.95587	26799.93901	19913.93376	
0.95_581.7974m/z	581.7974297	0.946033333	neg							9204.151004	12047.72112	11010.6103	19476.14472	15806.55084	15326.09736	11926.28691	16356.42096	12647.33776	
0.95_585.7066m/z	585.7066345	0.946033333	neg							0.001403199	1747.15535	878.09976	5670.737885	2967.998921	4036.751356	2111.753944	3109.464061	2354.533249	
0.95_586.7123m/z	586.7123081	0.946033333	neg							6829.711607	10203.03295	9402.653988	26802.84385	21199.20539	21503.22371	13223.47768	16075.66469	13863.97179	
0.95_588.7094m/z	588.7094436	0.946033333	neg							1342.113574	532.7245165	1667.271269	4376.561131	4214.513485	4106.21142	1581.048444	3763.504463	2501.116665	
0.95_598.7392m/z	598.739156	0.946033333	neg							23210.04952	25621.88282	26233.467	36504.38003	34048.61533	35097.0256	32957.28116	36626.21726	31350.3501	
0.95_608.6947m/z	608.694679	0.946033333	neg							12692.01275	13971.1893	15195.2502	25441.22698	24861.2265	23575.22166	17817.10333	21559.51401	17151.26716	
0.95_639.6249m/z	639.6248515	0.946033333	neg							386.3274836	0.001403199	0.001403199	560.2422039	0.001403199	958.8316403	764.0513843	944.2521973	0.001403199	
0.95_674.7290m/z	674.7289749	0.946033333	neg							983.7615337	1825.036307	2579.989783	6352.752252	3310.581829	4300.508766	1797.440425	3008.864944	1217.513968	
0.95_696.7069m/z	696.7069256	0.946033333	neg							23620.96552	26537.35218	29394.28876	52712.38439	47958.71468	51048.82529	38639.98945	44880.00724	40789.66412	
0.95_706.6633m/z	706.663272	0.946033333	neg							2686.21771	5956.414554	5452.030258	15428.60392	12378.22398	11704.66681	5967.192825	8990.826752	5838.692445	
0.95_718.6894m/z	718.6894491	0.946033333	neg							11475.93695	12000.58601	14901.42268	15158.78777	16869.69614	18327.91102	18659.63229	18865.78659	15981.85708	
0.95_727.6394m/z	727.6393597	0.946033333	neg							1743.163391	2521.346037	3244.95256	6394.034622	5441.246647	6621.263806	2431.355658	3717.160558	4483.388062	
0.95_749.6193m/z	749.6193306	0.946033333	neg							1804.343911	2552.632189	2245.725758	4232.84254	4378.96466	4253.16174	3868.10751	3631.891437	2934.854544	
0.95_816.6569m/z	816.6569445	0.946033333	neg							4394.661333	8740.282127	7175.593437	19422.26503	16481.57031	20811.91163	11056.32552	15188.7794	13439.66137	
0.95_936.6057m/z	936.6056962	0.946033333	neg							0.001403199	0.001403199	455.3934358	6907.665066	1692.993925	2124.401398	1264.544205	2045.52684	541.1374232	
0.97_195.8772m/z	195.8772487	0.967616667	neg							2038.47648	2071.422097	1917.201181	2585.633913	2304.755846	2624.768007	2546.655037	2320.564231	2093.064312	
0.97_216.0198m/z	216.0198255	0.967616667	neg							0.001403199	494.2144261	1105.604515	4839.146469	3587.332407	3834.388668	434.608903	2193.803736	1494.515298	
0.97_238.9844m/z	238.9844397	0.967616667	neg							70436.14658	68417.78811	65571.87427	101961.9666	99031.80909	105204.1138	70180.35954	78717.97524	78740.75615	
0.97_244.8523m/z	244.8522553	0.967616667	neg							886.5798236	976.9152266	1003.551097	2052.048493	1750.904995	1682.631683	1315.60749	1450.224612	1290.476018	
0.97_245.9469m/z	245.9469234	0.967616667	neg							3360.713918	3210.3681	3071.701755	3207.766943	2884.167004	3600.576003	3780.144237	2967.207069	2996.285929	
0.97_246.8517m/z	246.8516625	0.967616667	neg							1697.733813	1706.842964	1426.690465	2636.562074	2192.634466	2332.27449	2419.841309	1951.503573	2006.364236	
0.97_248.8560m/z	248.8560493	0.967616667	neg							2526.518764	1609.811328	2164.919038	4047.982504	4372.146356	4374.188013	2431.764279	2593.936314	2331.078567	
0.97_252.9106n	297.9089109	0.967616667	neg							5069.037294	6125.790608	5911.445244	8447.141644	7527.883269	7541.480046	6516.373415	7830.572547	7190.797576	
0.97_253.9191m/z	253.9191276	0.967616667	neg							985.687501	1420.885742	1324.710142	1873.262514	1710.035495	1906.883563	1439.655084	1568.133735	1562.328661	
0.97_259.8162m/z	259.816194	0.967616667	neg							1580.648833	914.9225724	993.1801547	244.1099011	134.6122617	133.776773	1202.74592	941.8426002	722.9668032	
0.97_261.9418m/z	261.9418464	0.967616667	neg							18630.17479	18188.18024	17258.37941	20034.95308	19975.46577	20562.46742	19260.57907	17942.11062	19201.65559	
0.97_263.8337m/z	263.833651	0.967616667	neg							2382.366804	1898.447264	2156.12523	2747.810734	2840.222643	2658.239437	2155.188398	2820.821553	2393.54504	
0.97_270.9219m/z	270.9218581	0.967616667	neg							5402.666085	5321.544226	4633.958251	8377.053146	7556.285559	7357.153788	4215.006828	5334.338447	5211.163338	
0.97_278.8801m/z	278.8801204	0.967616667	neg							1652.286607	2133.747501	1704.720856	1710.713477	2466.364464	2058.009844	2389.336353	1762.629147	1925.260818	
0.97_289.9369m/z	289.9369148	0.967616667	neg							32232.21673	36015.00852	34486.3488	39185.68135	41177.42046	40741.40605	41612.04235	38265.81584	41082.47204	
0.97_290.9835m/z	290.9835151	0.967616667	neg							1337.948072	1334.420468	1575.526926	2162.566383	1395.14771	1804.536096	1299.206466	1270.676948	1149.93413	
0.97_293.9904m/z	293.9903865	0.967616667	neg							3958.804008	4432.080553	4974.369753	7778.11686	7303.572442	6919.923989	4780.405021	6941.378517	6112.321187	
0.97_310.9693m/z	310.9693368	0.967616667	neg							84234.77921	95539.71845	103026.2443	130013.7927	129392.3514	131510.312	100833.7217	107861.5466	111224.586	
0.97_315.8385n	360.836689	0.967616667	neg							32095.5339	32519.01289	33425.81646	40196.06028	42529.87513	40988.44016	41434.351	42202.48711	39677.32563	
0.97_318.9250m/z	318.9249747	0.967616667	neg							2085.651438	2357.264291	2106.230438	804.3890158	1434.923015	2006.630874	2020.792614	1864.452362		
0.97_333.9547m/z	333.9547303	0.967616667	neg							1138.835	1111.016133	1352.065436	1269.104313	1601.141449	1414.217895	851.1294602	1313.872148	1291.112046	
0.97_345.0440m/z	345.044016	0.967616667	neg							0.001403199	0.001403199	0.001403199	304.016663	227.0379431	332.135889	0.001403199	0.001403199	141.9048679	
0.97_358.9341m/z	358.9340562	0.967616667	neg							22189.138	21105.62642	21445.09938	34416.91073	32971.75666	35284.72811	21860.60461	26136.493	25802.57595	
0.97_360.9296m/z	360.9295931	0.967616667	neg							1941.544993	1591.979945	1571.0761	1977.218504	1554.350595	1898.76399	1438.879831	1192.43492	1117.86813	
0.97_361.8855m/z	361.8855036	0.967616667	neg							1159.75248	1295.128173	858.978973	1325.819001	917.3366207	1083.229849	1270.178508	1151.591012	955.745757	
0.97_363.8809m/z	363.88092	0.967616667	neg							46885.75377	47526.84961	48304.81543	57346.75869	55462.65175	56081.99498	54104.70895	51862.71763	53150.91613	
0.97_363.9738m/z	363.9738332	0.967616667	neg							961.7726384	1523.027879	1409.73964	1906.00733	1615.227061	1848.012495	1046.741117	1898.087187	1325.2591	
0.97_368.8892m/z	368.8892235	0.967616667	neg							3185.533145	3053.866012	2514.167783	5763.84206	4969.812352	5242.362485	3042.612665	3480.369279	3411.584467	
0.97_421.8389m/z	421.8389261	0.967616667	neg							1553.013843	1282.631274	1436.472474	171.0981049	441.3890585	377.6547927	1190.435825	1120.423891	1051.313066	
0.97_428.7510m/z	428.7509975	0.967616667	neg							2027.342336	1986.246979	1948.646405	951.0166922	813.8689041	953.2382938	1624.193318	1579.91252	1081.052072	
0.97_430.9182m/z	430.9182217	0.967616667	neg							28409.12441	34981.36662	36139.80567	48809.43228	45476.59204	45771.54529	35714.70123	41891.76376	39548.28532	
0.97_435.7867n	480.7848608	0.967616667	neg							12735.11253	11828.57956	13448.74937	15902.60051	17445.64611	17473.06821	18511.63741	17627.26702	16072.66385	
0.97_435.9584m/z	435.9584065	0.967616667	neg							1770.251583	1845.637438	2779.330106	4432.386981	3557.969029	3659.480016	2373.838239	3017.356564	2464.753202	
0.97_440.8735m/z	440.8735138	0.967616667	neg							4497.078194	5469.240305	5913.417284	10385.35769	8063.660212	7773.927901	5653.198675	9242.634975	6262.561705	
0.97_478.8826m/z	478.8825904	0.967616667	neg							1465.091585	1941.868643	1427.404344	2295.165015	3146.514752	2544.017997	1474.830888	2220.424485	2063.79054	
0.97_490.7408m/z	490.7408226	0.967616667	neg							3416.576748	4267.521723	4106.003334	7291.75924	6770.404934	7389.290229	4491.596066	6048.682358	5399.474547	
0.97_500.8648m/z	500.8647667	0.967616667	neg							4716.524736	4512.525652	4339.147062	6742.025456	7388.317628	7022.829733	4424.615717	4958.356793	5147.955621	
0.97_505.8117m/z	505.8117322	0.967616667	neg							8644.075439	8725.191904	8172.10638	6081.900879	8930.763587	7726.189153	9449.317984	9118.415313	9230.48829	
0.97_510.7266m/z	510.7265569	0.967616667	neg							2434.55101	24122.29107	22644.11377	28757.26612	30855.02887	32876.88244	30454.13925	28114.41188	30289.34752	
0.97_512.7238m/z	512.7238033	0.967616667	neg							2944.734795	3454.381519	2654.208695	4932.182258	4098.40729	4585.774248	4385.084092	4523.236294	3437.239414	
0.97_550.8676m/z	550.8675948	0.967616667	neg							9489.908789	9305.851202	11167.89548	15720.12895	13125.91036	14103.09494	11876.83108	13429.9648	11965.81756	
0.97_555.9077m/z	555.9076614	0.967616667	neg							1001.854787	721.2182104	2267.811486	3020.137387	1305.698726	2095.842022	1365.074938	1425.305112	699.4602063	
0.97_600.7357m/z	600.7356725	0.967616667	neg							4772.722147	4590.436158	6646.771017	7610.633425	6323.98462	6771.084363	7670.594648	6860.991559	5624.769516	
0.97_603.7793m/z	603.7793488	0.967616667	neg							5442.481883	6655.907173	7670.960796	9327.628537	10347.19193	9698.888512	7592.952668	9986.571724	8292.725379	
0.97_607.6872m/z	607.6872251	0.967616667	neg							2171.396882	3276.768271	4525.871771	9779.36831	7912.64286	7795.339968	4248.510584	6789.697003	4833.691433	
0.97_610.6918m/z	610.6918134	0.967616667	neg							1537.164589	2794.652417	2259.361393	3643.851874	2402.473288	2801.562495	2795.269825	2850.623289	2146.878976	
0.97_620.7214m/z	620.7213791	0.967616667	neg							15098.40896	15542.56086	16089.56715	17554.06041	17432.41929	18300.53444	19247.70016	19263.73082	19653.51162	
0.97_629.6691m/z	629.6690947	0.967616667	neg							4194.298472	5496.344656	4937.489341	8918.7609	8159.95646	8499.258383	7935.886924	8634.843767	7639.173354	
0.97_640.6324m/z	640.6324046	0.967616667	neg							904.8506646	1132.890522	1052.681543	1316.793432	1435.35485	2252.96803	1370.488551	1043.777395	1183.996435	
0.97_642.7042m/z	642.7042308	0.967616667	neg							4070.183003	4910.398873	4508.168842	5606.184816	5485.166337	4938.144973	6565.57022	5746.025161	5419.681396	
0.97_698.7037m/z	698.7036712	0.967616667	neg							4178.991221	5362.318139	4224.447081	12644.58981	11719.24269	10457.34702	5684.425609	9923.06179	7750.564449	
0.97_701.7478m/z	701.7477565	0.967616667	neg							1087.489659	3577.973945	2710.795195	5342.495713	4886.365925	4423.371335	2293.930572	5169.643195	3862.413898	
0.97_750.6268m/z	750.6267789	0.967616667	neg							4600.991407	5888.807029	5301.730064	8609.21413	9729.037893	9172.977638	7152.196298	8293.725665	7582.854846	
0.99_168.8900m/z	168.8900081	0.989233333	neg							1407.77903	13516.08618	12201.65955	15342.17148	15708.88113	15446.11365	15710.45649	13818.60608	14743.29298	
0.99_178.8841m/z	178.8841076	0.989233333	neg							780.8011799	698.376641	489.5686471	298.1962682	326.3866833	174.502214	723.0018548	517.5507841	525.1400755	
0.99_188.8618m/z	188.861783	0.989233333	neg							82.97337625	0.001403199	84.95210123	0.001403199	0.001403199	61.04269191	0.001403199	48.54649734	107.6775267	
0.99_190.9452m/z	190.9451589	0.989233333	neg							174.8606695	134.5922421	59.39375126	469.9288413	200.6807159	164.3597545	0.001403199	174.2921391	150.4770892	
0.99_248.9784m/z	248.9783915	0.989233333	neg							2833.845357	2363.164961	2994.841883	1450.309067	1087.828616	1532.003868	2350.259636	2401.946422	2040.150661	
0.99_269.9141m/z	269.91407	0.989233333	neg							988.2453115	1173.460762	1009.223111	1553.13617	1349.977393	1224.409491	1084.890188	961.2465856	887.5072919	
0.99_270.9610m/z	270.9609785	0.989233333	neg							1340.218517	1016.51113	1303.919603	609.7744234	453.7024138	526.5315608	1189.133159	924.7861391	860.1281525	
0.99_390.8716m/z	390.8716103	0.989233333	neg							1262.305651	1939.260405	1365.087719	2963.482081	2673.410759	2191.212951	1797.723733	1746.171273	1489.58028	
0.99_412.8538m/z	412.8538376	0.989233333	neg							3194.942502	2551.945384	2428.291285	3624.466512	4111.696933	4054.420321	2173.168062	2907.733459	2291.807361	
0.99_452.9003m/z	452.900334	0.989233333	neg							15779.4008	15726.23682	17002.63338	16394.85185	18613.49583	16128.27485	18695.19094	17893.3103	19509.77319	
0.99_474.8822m/z	474.8822344	0.989233333	neg							9780.916154	8958.247049	9930.578529	10410.86429	11011.19033	10449.40154	10617.49912	10095.26218	10343.47801	
0.99_484.8375m/z	484.8375245	0.989233333	neg							3509.038823	3741.321698	3763.778811	4837.600489	4179.372105	3929.986871	4925.088449	3249.489502	3561.733007	
0.99_494.7633m/z	494.76331	0.989233333	neg							1187.464432	1634.377727	1725.490267	1799.887071	2479.089666	2717.645512	2093.316605	2602.988357	1473.227282	
0.99_501.7477m/z	501.7476678	0.989233333	neg							7875.228328	8898.800178	8542.282259	9192.774533	9958.310504	10112.91841	10328.49941	9806.654979	9507.468548	
0.99_522.8469m/z	522.8469195	0.989233333	neg							2537.376458	1736.894849	2174.253003	2153.693608	2353.793924	2191.331966	1734.347124	1829.094505	1753.32624	
0.99_572.8497m/z	572.84972	0.989233333	neg							5176.722625	7523.730724	7330.737395	8646.468119	7442.931945	7525.164577	8730.808103	8461.12227	6456.808082	
0.99_594.8321m/z	594.8321451	0.989233333	neg							1369.455891	1781.329622	1616.64007	373.0444816	1046.199637	2227.396366	2032.398461	1562.40375	1680.217407	
0.99_625.7614m/z	625.7613529	0.989233333	neg							3144.943065	3233.951902	2886.215952	1939.19127	2307.96503	2976.652595	3173.042372	3523.129759	3137.147981	
1.01_103.9203m/z	103.9202574	1.0111	neg							9220.24932	8644.073205	8345.444967	10111.90901	10410.26977	10242.74217	10634.53794	9057.125479	9617.702806	
1.01_151.8871m/z	151.8871107	1.0111	neg							502.4057312	752.2940602	603.5176191	762.0194984	926.3779264	809.1535968	946.5712817	910.0832034	934.8245588	
1.01_183.8771m/z	183.8771261	1.0111	neg							11553.65935	11054.77875	10717.44334	11935.65883	12502.90889	12467.56605	13315.80506	12121.97679	12524.06757	
1.01_187.8734m/z	187.873412	1.0111	neg							1036.589593	925.3107221	564.950864	39.1183134	171.7981216	264.3159859	1103.244272	579.4097633	661.9265824	
1.01_198.9006n	243.8997894	1.0111	neg							3692.746239	3930.263925	4054.501331	3497.280667	2984.492449	2756.668355	4380.488746	4176.939912	3173.269663	
1.01_239.8671m/z	239.8670925	1.0111	neg							14095.45968	12818.92763	13531.48251	15883.34145	17998.42126	17248.74314	16438.19787	14938.35377	15644.91248	
1.01_253.0003m/z	253.0003111	1.0111	neg							747.8305713	806.5363156	674.9274696	458.6523102	691.2195108	571.2936051	721.6865155	952.0497488	606.2972794	
1.01_274.8249m/z	274.8249364	1.0111	neg							1631.328379	994.6854187	833.0704641	941.920848	979.9259531	1212.368118	1408.635784	1049.85468	1137.134361	
1.01_276.9633m/z	276.9632943	1.0111	neg							1895.448559	1462.979827	1688.069128	1210.565027	954.2224879	1228.181405	1145.754608	1181.684814	1184.559752	
1.01_286.8929m/z	286.8929338	1.0111	neg							1390.787886	1666.09678	1354.80882	1145.032684	1706.982069	1586.068749	2066.841621	1637.120009	1394.999843	
1.01_311.8325m/z	311.832501	1.0111	neg							2320.826253	1532.887449	1406.380421	1649.975763	1537.407848	1462.272172	1860.274732	1614.214953	1472.070184	
1.01_392.7739m/z	392.7739356	1.0111	neg							4689.648906	4157.305096	4058.620002	5412.898928	4699.079134	5028.772835	5320.04748	4832.246533	4387.200443	
1.01_470.7185m/z	470.7185207	1.0111	neg							5077.376427	3937.59054	3937.182126	2700.640734	2990.805203	2609.494282	4654.942176	4170.432274	4323.555377	
1.01_496.8652m/z	496.8651957	1.0111	neg							2292.909022	2054.570597	1955.174315	1605.630202	2218.750405	2419.658381	1699.389637	2440.471198	2390.518201	
1.01_500.7714m/z	500.7713711	1.0111	neg							29175.9461	30053.26462	28990.22241	29004.24283	33070.73863	31084.77394	37351.85721	34529.11641	35111.82743	
1.01_510.8202m/z	510.8201623	1.0111	neg							564.4258151	752.4789393	656.9172885	929.0702957	630.0743288	654.174769	503.4751107	546.7955399	462.1539815	
1.01_652.6595m/z	652.6594696	1.0111	neg							6741.470044	6962.650554	7263.079436	7797.164864	9530.803808	8902.577743	9459.749521	7935.549916	6920.161198	
1.03_119.9494n	164.9475739	1.033516667	neg							383293.0086	371595.5726	355161.9406	441151.4046	457345.8566	448159.5243	461203.0493	417743.3304	433950.1514	
1.03_162.8830n	161.8758673	1.033516667	neg							3577.801193	2953.51002	2901.059687	1528.522695	1380.039242	1589.216671	3207.991771	2731.819462	2656.375112	
1.03_166.9434m/z	166.9434161	1.033516667	neg							9775.41349	9116.189545	8456.994926	10248.33842	10474.82877	10645.04372	10782.42078	10193.88573	10402.16583	
1.03_168.8893n	213.8878782	1.033516667	neg							13643.2897	11993.33388	10511.41873	12453.55236	12719.60885	12645.58042	14265.77293	11692.08505	11926.69076	
1.03_173.9657m/z	173.9656606	1.033516667	neg							492.6132808	509.1897672	376.7886225	474.1957526	412.4162431	530.3178513	371.5159971	341.7522204	335.191918	
1.03_180.9127m/z	180.9126633	1.033516667	neg							686.3189863	660.4105918	610.2367799	562.9505941	627.0139844	624.1343492	811.196961	619.8321449	736.4720098	

1.03_185.8658m/z	185.8658254	1.033516667	neg
1.03_185.8928m/z	185.892829	1.033516667	neg
1.03_191.8553m/z	191.8553471	1.033516667	neg
1.03_194.8897m/z	194.8896746	1.033516667	neg
1.03_195.8892n	240.8873851	1.033516667	neg
1.03_212.0179m/z	212.0178708	1.033516667	neg
1.03_237.8883m/z	237.8883154	1.033516667	neg
1.03_250.9956m/z	250.99564	1.033516667	neg
1.03_261.8327m/z	261.832703	1.033516667	neg
1.03_268.8335m/z	268.8335078	1.033516667	neg
1.03_270.8288m/z	270.828828	1.033516667	neg
1.03_287.8317m/z	287.831686	1.033516667	neg
1.03_344.7892m/z	344.7891899	1.033516667	neg
1.03_380.8228m/z	380.8227748	1.033516667	neg
1.03_381.7985m/z	381.7985203	1.033516667	neg
1.03_431.8682m/z	431.8682123	1.033516667	neg
1.03_440.7787m/z	440.7786996	1.033516667	neg
1.03_523.7302m/z	523.730153	1.033516667	neg
1.03_524.7501m/z	524.7501446	1.033516667	neg
1.03_532.7090m/z	532.7090013	1.033516667	neg
1.06_150.8998m/z	150.8997746	1.055866667	neg
1.06_152.8951m/z	152.8951082	1.055866667	neg
1.06_154.8910m/z	154.8910092	1.055866667	neg
1.06_154.8956m/z	154.8955507	1.055866667	neg
1.06_157.8722m/z	157.8721952	1.055866667	neg
1.06_160.8859n	159.8787515	1.055866667	neg
1.06_166.9963m/z	166.9963369	1.055866667	neg
1.06_171.0664m/z	171.0664113	1.055866667	neg
1.06_174.8921n	348.7718031	1.055866667	neg
1.06_183.8485m/z	183.8484545	1.055866667	neg
1.06_185.8456m/z	185.845557	1.055866667	neg
1.06_196.8850m/z	196.8850111	1.055866667	neg
1.06_200.8810m/z	200.8809689	1.055866667	neg
1.06_215.8686m/z	215.8686038	1.055866667	neg
1.06_217.8656m/z	217.8656055	1.055866667	neg
1.06_234.9838m/z	234.9837675	1.055866667	neg
1.06_236.8780m/z	236.8780201	1.055866667	neg
1.06_261.8806n	260.873356	1.055866667	neg
1.06_261.8912n	306.8883179	1.055866667	neg
1.06_262.8693m/z	262.8692968	1.055866667	neg
1.06_265.9672m/z	265.9671663	1.055866667	neg
1.06_286.9461m/z	286.9460681	1.055866667	neg
1.06_298.9068m/z	298.9068209	1.055866667	neg
1.06_306.0583m/z	306.0582714	1.055866667	neg
1.06_313.8127m/z	313.8126613	1.055866667	neg
1.06_315.8267m/z	315.8266714	1.055866667	neg
1.06_336.8217m/z	336.8216508	1.055866667	neg
1.06_337.8198n	382.8180274	1.055866667	neg
1.06_349.8624m/z	349.8624117	1.055866667	neg
1.06_384.9133m/z	384.9132776	1.055866667	neg
1.06_402.8047m/z	402.8046661	1.055866667	neg
1.06_406.8956m/z	406.8956021	1.055866667	neg
1.06_412.7600m/z	412.7599694	1.055866667	neg
1.06_464.7620m/z	464.7620088	1.055866667	neg
1.06_490.7031m/z	490.7031211	1.055866667	neg
1.06_525.7453m/z	525.7453272	1.055866667	neg
1.06_534.7065m/z	534.7064793	1.055866667	neg
1.06_544.7358m/z	544.7357978	1.055866667	neg
1.08_104.9539m/z	104.953871	1.072826667	neg
1.08_126.8811m/z	126.8810644	1.072826667	neg
1.08_128.8782m/z	128.8781611	1.072826667	neg
1.08_165.9509m/z	165.950922	1.072826667	neg
1.08_170.8710m/z	170.8709527	1.072826667	neg
1.08_174.8650m/z	174.864989	1.072826667	neg
1.08_181.8819m/z	181.8818631	1.072826667	neg
1.08_181.9379m/z	181.937863	1.072826667	neg
1.08_187.8888m/z	187.8887885	1.072826667	neg
1.08_223.8819m/z	223.8819267	1.072826667	neg
1.08_225.8853m/z	225.8853205	1.072826667	neg
1.08_226.9048n	271.9072843	1.072826667	neg
1.08_245.0672m/z	245.0671514	1.072826667	neg
1.08_262.8773m/z	262.8772869	1.072826667	neg
1.08_277.8546n	554.6912342	1.072826667	neg
1.08_281.8629m/z	281.8629221	1.072826667	neg
1.08_292.9870m/z	292.9869998	1.072826667	neg
1.08_301.0211m/z	301.0211023	1.072826667	neg
1.08_301.8875m/z	301.8875374	1.072826667	neg
1.08_306.8793m/z	306.8793152	1.072826667	neg
1.08_314.9406m/z	314.9406449	1.072826667	neg
1.08_316.8439m/z	316.8439034	1.072826667	neg
1.08_328.8611m/z	328.8611076	1.072826667	neg
1.08_336.8682m/z	336.8682277	1.072826667	neg
1.08_338.8164m/z	338.8164294	1.072826667	neg
1.08_365.0076m/z	365.0076339	1.072826667	neg
1.08_368.9357m/z	368.9356776	1.072826667	neg
1.08_383.8140m/z	383.814026	1.072826667	neg
1.08_398.7716m/z	398.7716469	1.072826667	neg
1.08_449.7858m/z	449.7858079	1.072826667	neg
1.08_457.7578m/z	457.7578005	1.072826667	neg
1.08_460.7633m/z	460.7633353	1.072826667	neg
1.08_470.7922m/z	470.7922278	1.072826667	neg
1.08_480.7474m/z	480.7474306	1.072826667	neg
1.08_484.7465m/z	484.7464609	1.072826667	neg
1.08_504.9434m/z	504.9434298	1.072826667	neg
1.08_548.7351m/z	548.7351483	1.072826667	neg
1.08_616.7229m/z	616.722935	1.072826667	neg
1.10_130.8752m/z	130.8751912	1.10065	neg
1.10_138.9070m/z	138.9069796	1.10065	neg
1.10_141.9126m/z	141.9126344	1.10065	neg
1.10_154.0340m/z	154.0340331	1.10065	neg
1.10_162.9206n	324.8281535	1.10065	neg
1.10_178.9778m/z	178.9778218	1.10065	neg
1.10_182.8968m/z	182.896781	1.10065	neg
1.10_186.9296m/z	186.9296056	1.10065	neg
1.10_188.9130m/z	188.913024	1.10065	neg
1.10_193.8773m/z	193.8773204	1.10065	neg
1.10_197.9025m/z	197.90251	1.10065	neg
1.10_198.9365m/z	198.936546	1.10065	neg
1.10_203.9199m/z	203.9198551	1.10065	neg
1.10_205.9062n	410.8025253	1.10065	neg

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5677.67108	4402.500485	4226.444989	2987.319439	3108.639614	3871.37233	5073.928356	3903.962022	4139.842122	
744.5979607	1459.571266	1247.743198	5793.554755	2043.047833	3243.121169	1138.233959	1790.281706	875.5952447	
3684.366442	2640.760933	2840.410048	2759.775511	2792.007387	2488.649262	3840.64435	2696.241886	2923.607252	
11414.6993	10594.92107	9060.432544	10535.70438	10969.94162	11059.17879	13805.57332	10868.14041	10232.96599	
1186.825314	739.2621981	624.469045	503.0033668	704.2944665	801.9016227	805.8197418	786.3913847	728.5387563	
424.0362075	347.0432182	301.1350122	63.77060316	0.001403199	0.001403199	263.3615718	291.6267756	285.798132	
1731.69242	1515.477856	1697.962112	1205.54911	852.5299548	943.2381648	1600.295203	1641.484681	1296.327495	
1285.326949	1219.362349	1054.657072	1210.659532	1004.462669	999.1510736	1243.394811	1407.685912	1307.68161	
1637.128865	1808.613298	1326.499291	1515.124482	1825.715765	1604.658201	2298.329375	1396.720688	1516.71854	
1864.472989	2209.070535	2217.380234	1742.686704	1255.00651	1901.95406	1679.192654	1429.104134	1367.138494	
1903.115117	1526.049434	1601.759365	2346.586669	2132.005526	2287.096521	2089.352886	1134.641535	1747.393854	
35920.9113	30110.67885	31156.07009	29482.84511	34673.82634	36402.31789	38387.41755	32458.06872	37006.05856	
2392.133546	977.2599543	832.6538669	1184.154201	2545.144256	695.2474893	1959.628616	1272.633972	1168.676847	
40149.87881	34843.05256	32144.49381	34309.89183	38873.64917	37470.30712	41328.72997	36049.24025	39532.52001	
824.9280108	482.7497947	606.5674468	649.1428079	517.8394916	744.3759557	792.8847797	704.4976165	533.0331129	
233.4388861	360.5761628	82.77070785	0.001403199	106.905737	163.4435445	204.4616109	192.9987602	195.6175757	
7736.022221	6600.797807	5930.534149	5814.92477	6829.694271	6449.915238	7445.414848	6440.205074	6845.090747	
1371.744525	1172.813298	907.2569334	503.0957423	655.1988076	854.6928794	1466.72334	947.017128	849.4145716	
7491.857322	6383.161576	6150.542833	5836.026414	6892.86096	7213.382568	8557.160266	6481.438748	7185.867411	
2766.701417	2440.065184	2285.288959	2321.861716	2417.942599	3255.014212	3228.183254	2877.490059	2355.52556	
5845.550684	5117.503694	5424.42098	1983.329622	2792.69378	3198.926302	5963.227879	5008.077329	4678.710889	
8787.612895	8094.700877	8372.532997	8296.686366	8870.499268	9814.769881	10044.99254	8040.600856	8764.183173	
12807.40488	10743.34234	9828.622953	10384.32748	10284.88399	10131.23164	13390.47589	10449.4906	11102.07378	
3762.942173	2761.178077	2692.108688	2578.195129	2931.231332	2569.086509	3386.294645	2816.193192	3017.205091	
3032.789609	2671.345189	2986.988086	3567.543445	2862.065538	3480.640165	3048.726601	2984.201052	2614.28649	
5834.62521	4747.689316	4319.50974	4281.187239	4122.683609	4994.555089	5483.393973	4539.562927	4358.89041	
3262.396862	3497.562709	2391.247452	2304.320058	2262.684428	2230.585499	2951.221447	1841.727864	2623.899117	
433.6494572	316.5706576	317.6960763	164.7593579	163.7243969	169.8680733	394.3955933	330.8034026	285.883627	
432.1464684	300.9290926	235.6493917	163.3682493	180.6848456	152.5341786	334.0817961	250.5716182	192.3039416	
447.0381564	340.7170931	316.0859444	207.2550573	216.4322501	177.2239312	381.8862397	267.0364421	294.1075457	
45.04505091	62.80979708	94.73310688	26.39969356	23.92877374	82.57318188	46.26278753	59.05705166	19.23469494	
4411.555891	2839.929534	2743.614642	1331.647552	1866.06093	1996.367674	2999.673568	2509.688838	2575.31381	
713.8385265	526.4095068	465.8412034	454.3845607	431.6394456	506.6468269	574.9935911	436.112483	554.8948735	
3800.056856	2619.72671	2415.285185	1312.368358	1747.163043	1590.67335	2816.433406	2068.996162	2386.752231	
70393.8937	60523.66692	61073.35054	57389.85798	72232.39367	68933.83396	75606.69168	66504.17371	75447.90564	
1016.31416	740.9312802	693.6331887	675.196456	662.852104	707.5973172	984.5200573	654.2020139	748.6962207	
543.7190251	294.5783022	621.4716461	180.5330903	118.9926509	164.2032127	766.1882751	455.5662003	403.9085251	
1107.332526	839.2786262	857.8908325	474.3357845	449.7332145	335.1199831	882.9647335	706.0958748	666.6369768	
1041.340991	870.1819999	833.4550426	1190.79369	1327.519047	906.5757533	1419.454716	1223.577158	908.9018075	
543.6898641	441.7488484	392.8132206	374.1715705	288.9093086	320.2858756	483.2228804	308.0673097	276.2816117	
3046.796556	2260.14089	1813.769902	1440.591543	1475.114451	1976.79837	2564.808257	1677.531245	1590.904179	

1.10_213.8754m/z	213.8753642	1.10065	neg	489.3987724	288.6543445	372.8646976	275.8708014	327.3992946	352.1275733	389.6167907	272.0787945	406.0715065		
1.10_220.8826m/z	220.8825592	1.10065	neg	751.2693904	635.7130263	524.0474169	542.5577373	474.0561917	557.1039007	713.1087928	548.5684736	494.7713654		
1.10_226.9182m/z	226.9181785	1.10065	neg	963.1717516	826.3155097	663.2431032	778.8101315	731.2107786	919.4954059	1046.456497	950.6424564	760.5661956		
1.10_232.9439m/z	232.9439245	1.10065	neg	1273.22441	632.2383612	761.0705323	930.2379606	927.9067501	1041.305073	1051.795471	899.7003949	931.7185605		
1.10_262.8575m/z	262.8575247	1.10065	neg	1552.523826	990.8315457	1172.649938	1036.848183	1442.202921	1311.452744	1479.63705	1265.770006	1265.980518		
1.10_271.8984n	542.7784642	1.10065	neg	7742.953126	6574.677636	5639.436436	4104.691024	4701.079546	5690.397278	7528.319919	5583.221824	6318.528684		
1.10_281.8749m/z	281.8749231	1.10065	neg	2220.096706	2136.751198	1591.687274	1277.404027	1117.004034	1041.288478	2157.664333	1531.65836	1613.653406		
1.10_283.8903n	264.8724293	1.10065	neg	45860.82006	36782.41214	34209.49798	33984.10899	40219.46086	37798.20342	44364.44324	37538.40013	41391.15061		
1.10_308.8643m/z	308.8642586	1.10065	neg	1548.870151	1054.979084	837.4360535	478.0417706	617.662485	722.727536	1055.189774	851.7787552	802.1932276		
1.10_311.0500m/z	311.0500486	1.10065	neg	10512.8473	9849.211861	11479.65282	8519.396221	8460.889742	10951.75568	11099.21302	9811.304598	9691.068748		
1.10_323.8694m/z	323.8693692	1.10065	neg	4145.630427	4157.127677	3721.081028	3106.740017	3230.43218	3448.295115	4768.855471	4265.855185	3895.599077		
1.10_328.0401m/z	328.0401479	1.10065	neg	1120.710181	765.0535148	919.6754242	946.1569864	466.3948144	861.7819663	782.3586813	708.4656479	455.5656818		
1.10_330.8649m/z	330.8648707	1.10065	neg	4231.750132	3373.135424	2895.33273	2459.437533	2927.162649	2933.351968	4139.08818	3042.910425	3229.646539		
1.10_342.8153m/z	342.8152639	1.10065	neg	4260.672128	2925.699012	2564.089818	2147.495027	2664.39471	2728.967954	3370.092413	2731.441109	3029.903253		
1.10_345.8512m/z	345.8511783	1.10065	neg	2756.651859	2825.045752	2285.517728	1676.624231	2190.359324	2044.14379	2944.078411	2620.858324	2506.592368		
1.10_351.8780n	332.8601563	1.10065	neg	37377.58254	28579.18479	27341.02075	21776.39667	28593.12696	27811.01852	33541.36477	26744.33399	30296.04525		
1.10_368.0310m/z	368.0309671	1.10065	neg	73.43517104	235.5732887	76.624638	236.0364022	176.0408566	79.46407379	162.354134	145.4595394	162.9206249		
1.10_380.8631m/z	380.863089	1.10065	neg	4234.160227	2884.080195	3368.357345	1498.761627	1940.634431	2241.673495	3939.916043	3534.02697	3280.902988		
1.10_390.8190m/z	390.8189872	1.10065	neg	4972.833785	3820.072217	3403.029673	1999.437387	1986.729341	2291.460629	4196.372629	3403.409446	2974.01815		
1.10_396.7750m/z	396.7750436	1.10065	neg	6510.532034	5597.977895	4899.639505	2850.840132	3147.627218	3354.211593	6586.0126	5031.030797	5467.724403		
1.10_396.8482m/z	396.8482213	1.10065	neg	16693.64904	14814.71976	14458.00415	12368.84037	15699.76859	15548.76065	18036.12977	15837.79864	16767.39766		
1.10_400.8473m/z	400.8472718	1.10065	neg	22168.7149	15439.42296	14198.65408	10780.42744	14390.34059	15056.30207	17911.89299	14107.31786	16707.54226		
1.10_406.8036m/z	406.8036325	1.10065	neg	21069.55339	16602.43653	14942.26218	15284.68577	17856.74807	17651.25482	21693.13478	16250.10545	17692.92321		
1.10_407.8827m/z	407.882744	1.10065	neg	1759.234519	1262.049909	937.2254482	985.1005782	1463.454911	1082.833059	1795.952422	1144.004567	953.6754665		
1.10_416.7591m/z	416.7590669	1.10065	neg	5058.884702	3693.321307	3262.080662	3119.006544	3341.97962	3719.538414	4056.677958	3196.598305	3579.274308		
1.10_443.8303m/z	443.8303091	1.10065	neg	5528.439482	3972.144691	4089.820921	2769.913988	3669.817066	3782.067844	5181.557052	3062.954546	4320.338376		
1.10_451.8021m/z	451.8020741	1.10065	neg	2417.195244	1678.991433	1740.026965	1642.454021	1180.16391	1761.526169	2218.923339	1933.194947	1486.472181		
1.10_452.9814m/z	452.9813952	1.10065	neg	2095.018645	1456.417756	1900.430831	2088.195791	1163.753697	1852.284904	2002.34982	1931.120972	1326.673116		
1.10_454.8072m/z	454.8071919	1.10065	neg	2317.866959	1954.120311	1575.948258	694.4789616	1271.050511	993.7717776	2151.053914	1585.455246	1732.573778		
1.10_464.8356m/z	464.8356132	1.10065	neg	8732.483245	7369.149145	6931.553621	5755.177296	7930.7542	6954.520654	9442.850747	7198.656871	8266.113972		
1.10_468.8347m/z	468.8347139	1.10065	neg	12344.17946	8774.679724	8771.962607	6838.861	7973.742752	8413.734904	11435.78184	9189.45233	9923.6155		
1.10_472.8339m/z	472.8339017	1.10065	neg	2236.795569	1724.186882	1161.045464	1006.714031	782.8995291	830.9225225	1608.955832	1148.549863	1050.570563		
1.10_474.7911m/z	474.7911214	1.10065	neg	11665.75644	9450.392693	8587.486328	6798.344068	8123.670225	7483.410642	10485.70499	8040.199642	7809.358686		
1.10_511.8175m/z	511.8174633	1.10065	neg	2328.390115	2031.917599	1497.372084	1362.327898	1869.085434	1593.220567	2100.050233	1037.546188	2190.456878		
1.10_517.7737m/z	517.773679	1.10065	neg	3117.296785	2250.16718	2010.034419	1379.648128	1348.948005	1689.634499	2614.834912	1908.449524	1508.720901		
1.10_526.7929m/z	526.7929382	1.10065	neg	1273.911668	1429.776717	1216.302724	563.9497913	562.428648	874.2188783	1502.038049	1227.33988	834.9842315		
1.10_532.8229m/z	532.8228758	1.10065	neg	4666.062775	3218.415614	3524.063198	3362.923808	3117.170744	3672.69859	4650.722037	2850.362032	3671.061685		
1.10_538.7799m/z	538.7799141	1.10065	neg	3386.251497	2961.528971	3058.743328	2684.175482	2944.915333	3464.29026	3802.425118	3544.720992	3044.301742		
1.10_604.8100m/z	604.8100109	1.10065	neg	4173.97552	2756.249842	2563.165458	1891.281456	1838.030723	1972.970114	3121.132869	1794.499312	2414.185255		
1.10_610.7668m/z	610.7668063	1.10065	neg	3366.510938	2924.757914	2101.051601	1646.560171	1396.62408	2500.389283	2487.660015	1923.694746	1883.585512		
1.12_102.9488m/z	102.9487723	1.11925	neg	175.8401145	129.0288185	108.9372151	84.10373696	103.4310039	112.0692816	117.9405128	114.2985567	93.90245326		
1.12_158.9346m/z	158.9346411	1.11925	neg	232.6778772	182.70591	156.9169103	188.5214241	127.4773166	202.8194986	190.7687606	191.8829193	144.4529198		
1.12_179.9365m/z	179.9364749	1.11925	neg	603.8168271	371.0588664	383.9106636	326.1718638	256.292595	367.477074	506.6251398	325.7350115	236.0966636		
1.12_244.0262m/z	244.0261691	1.11925	neg	516.5461805	393.2739618	466.7523491	99.55427454	269.0606603	208.3235257	407.7910834	488.3664571	504.5768223		
1.12_248.9000m/z	248.8999999	1.11925	neg	1180.252299	953.5250997	983.9775005	978.0796078	864.3088634	932.3340653	1302.806177	1015.582576	955.8955575		
1.12_255.0100m/z	255.0100074	1.11925	neg	2379.349526	1296.962195	1272.341772	1971.840943	2017.714744	2598.156389	1361.877423	1760.7828	1627.80617		
1.12_260.9664m/z	260.9663607	1.11925	neg	3061.589908	2566.420008	2362.568233	3524.19368	3570.314299	4011.937875	2621.504501	2937.233448	2911.575182		
1.12_267.9291m/z	267.9290685	1.11925	neg	312.4470751	250.9021041	370.1310771	337.7686977	286.2819224	248.5057453	414.2277817	370.5539227	513.8239165		
1.12_283.0509m/z	283.0509007	1.11925	neg	476.2789791	377.9390146	419.7450079	380.4407527	402.5406793	493.5305352	297.4874941	554.6423721	389.2859951		
1.12_292.9038m/z	292.9038487	1.11925	neg	3944.95282	3117.96498	2563.320797	4227.218561	3719.43831	4149.895695	2548.869112	3949.120336	2827.597221		
1.12_295.9882m/z	295.9881881	1.11925	neg	856.044021	823.5433752	741.2699894	368.43827	507.0167829	485.1164228	812.2688943	703.3033547	896.7480082		
1.12_305.8760m/z	305.8759708	1.11925	neg	1347.956987	990.7012095	851.0768456	591.2530711	631.6458995	787.4897368	1086.855011	779.7936273	651.0024273		
1.12_306.9721m/z	306.9721352	1.11925	neg	2836.270833	1824.33207	1746.518703	3677.540038	3556.923547	4472.111711	1444.683826	2947.32605	2441.517568		
1.12_307.0222m/z	307.0221872	1.11925	neg	1058.923378	1284.510897	1205.887777	1204.942808	999.8946507	1355.416765	1307.595754	1407.233475	1316.434734		
1.12_322.9411m/z	322.9410945	1.11925	neg	1878.200122	1172.641541	1359.338321	850.9781709	1402.92251	1549.32517	1239.421651	1716.48061	1951.00193		
1.12_322.9976m/z	322.9975847	1.11925	neg	1821.785913	1078.794747	840.3414374	1755.208427	1891.182794	2026.726313	1055.453946	1495.864814	1610.069562		
1.12_328.9540m/z	328.9540267	1.11925	neg	5001.810911	3731.0664	3419.408617	5826.190539	5753.192626	6851.545918	3213.812151	4879.480639	4685.729448		
1.12_332.9697m/z	332.9697396	1.11925	neg	4028.835348	2580.445459	2414.959289	858.566669	2680.446229	1584.194725	2737.339606	2591.274975	3557.063613		
1.12_339.8949m/z	339.8949146	1.11925	neg	3270.502503	3180.400517	2349.724739	2843.777265	2583.275796	2689.316705	3598.582642	3091.326418	3056.055174		
1.12_342.9985m/z	342.9985467	1.11925	neg	2960.33341	2116.212267	1652.07684	1079.916525	1730.81687	1770.735458	1571.36838	1806.105267	2349.679565		
1.12_345.0026m/z	345.0026078	1.11925	neg	308.0909188	110.4806118	186.6614973	71.09053392	162.1089127	83.23144016	72.36621409	329.3343673	163.582939		
1.12_349.9601m/z	349.960113	1.11925	neg	403.1421023	158.7818306	260.320834	238.5616714	318.9399351	310.9136693	188.7612759	361.8754059	372.6272784		
1.12_377.8577m/z	377.8576942	1.11925	neg	2702.452587	2257.344692	1997.307626	1647.014183	1570.007125	1478.372557	2015.991607	1720.08735	1572.236303		
1.12_380.9156m/z	380.9156434	1.11925	neg	12504.34324	10917.36514	10917.81019	14371.76262	16530.77901	15968.26929	12120.1156	12744.77494	12625.11664		
1.12_385.0051m/z	385.0050914	1.11925	neg	1573.284765	806.5551915	780.5640473	1593.615662	1556.006961	2076.481266	1256.648336	1920.625036	1716.234957		
1.12_396.9413m/z	396.9413188	1.11925	neg	2374.175851	1658.973291	1446.551014	2076.208326	2583.989963	3016.150703	1445.622701	2300.719448	2400.517271		
1.12_402.8979m/z	402.8979426	1.11925	neg	2533.996935	1786.905141	1655.679087	3377.33731	2748.048636	3376.387179	1409.678902	2287.390141	2040.555604		
1.12_453.8504m/z	453.8503807	1.11925	neg	1145.184212	515.7341771	805.5695529	636.4874113	722.5400398	711.2866647	660.7534602	369.4388046	659.6794629		
1.12_600.8110m/z	600.8109801	1.11925	neg	1789.417007	1238.25083	1297.038949	915.9228001	1002.552089	1124.173088	1207.004773	995.3941803	1168.08104		
1.14_119.0315m/z	119.0315087	1.1382	neg	6.477579376	0.00140199	0.00140199	18.99778639	15.91642037	16.70828227	0.00140199	11.5712522	0.00140199		
1.14_159.0145n	317.0175509	1.1382	neg	9589.549932	7789.570971	6573.793175	12004.71468	10419.94062	13014.20152	6920.216891	10555.37524	9451.324214		
1.14_218.9599m/z	218.9598833	1.1382	neg	3491.691397	2471.533787	1876.158568	3297.633437	2803.146759	3463.485142	2470.140205	2593.26765	2288.328871		
1.14_231.0484m/z	231.0483839	1.1382	neg	141.8792192	146.9686106	78.71074524	513.010474	211.2656929	411.9835495	271.1492657	174.2105289	143.540186		
1.14_248.0666m/z	248.0665897	1.1382	neg	0.00140199	0.00140199	0.00140199	840.8802528	56.82337203	283.4887403	0.00140199	0.00140199	0.00140199		
1.14_261.9258m/z	261.9257985	1.1382	neg	0.00140199	0.00140199	0.00140199	144.1144685	113.7802481	122.5170293	0.00140199	105.3841534	0.00140199		
1.14_271.9257m/z	271.9257498	1.1382	neg	69.99940908	0.00140199	0.00140199	70.47264393	164.8997497	69.83721383	0.00140199	124.1626434	169.1793343		
1.14_309.0455m/z	309.0455093	1.1382	neg	5283.794382	8851.786182	6784.956846	14171.16604	2959.413644	4903.402156	7951.347607	3330.582645	2439.809268		
1.14_317.1105m/z	317.1105165	1.1382	neg	796.8526601	329.2655962	182.4274786	5095.870453	1452.996065	3733.146567	67.74635114	1555.642097	710.6497408		
1.14_333.0439m/z	333.0439218	1.1382	neg	5030.506535	4587.658645	5225.842468	6052.281704	6223.667121	4838.831181	4863.562101	4665.638939			
1.14_360.8916m/z	360.8915846	1.1382	neg	1157.86604	527.8243668	831.6587189	1020.46842	1003.813316	1211.828857	529.0834007	960.6052362	722.5749143		
1.14_360.9299m/z	360.9298618	1.1382	neg	632.1827543	529.9323548	308.0365145	467.32764	641.4746292	795.0336147	891.9278972	627.8874413	693.9852787		
1.14_363.9741m/z	363.974094	1.1382	neg	656.1847974	617.4936124	824.8813884	943.1852438	379.7510356	819.8096	640.7441621	548.433122	406.5246907		
1.14_476.9806m/z	476.9805526	1.1382	neg	9798.204183	22478.11695	16015.2097	14570.76817	10505.68472	11416.6488	18097.09816	8792.350864	11803.32805		
1.14_486.9363m/z	486.9363237	1.1382	neg	8646.160368	10488.06598	14153.49722	2992.817442	12446.80181	11431.8235	11547.61745	7417.870146	13533.90317		
1.14_525.0593m/z	525.0593127	1.1382	neg	2352.602409	5793.319736	6699.389702	4488.85023	5434.688465	4026.16023	3928.076562	3378.572212	3938.448884		
1.14_553.8913m/z	553.8913071	1.1382	neg	676.7177545	2427.506483	1848.399078	729.5680849	588.0352104	312.4171326	3065.540513	954.5772301	0.001403199		
1.14_556.9973m/z	556.9972861	1.1382	neg	3389.731848	4735.345889	4622.96448	1522.643008	3603.160443	3984.285837	4241.003321	1328.210205	3252.278065		
1.14_620.9288m/z	620.9287624	1.1382	neg	2095.66083	4834.273204	2632.161377	4739.817712	4173.798698	3409.849418	6672.699566	2298.131378	2366.633726		
1.14_676.9468m/z	676.9468108	1.1382	neg	2186.627478	4006.783194	3660.822394	1911.697903	3166.640785	3333.42057	3583.802903	2127.575664	1963.008822		
1.14_717.0871m/z	717.0870745	1.1382	neg	1590.409122	755.909314	4033.689666	4342.576853	7690.43649	3274.557204	2484.658663	0.001403199	3059.52279		
1.16_124.0149m/z	124.0149485	1.160166667	neg	782.35593	1196.54888	1115.510432	984.2853008	197.0593883	657.7350492	336.2528217	736.4033966	156.2178617		
1.16_152.0296m/z	152.0295653	1.160166667	neg	454.4835752	419.4859092	528.0065742	464.0057167	777.1302667	745.9211586	467.1306065	513.2967098	667.3116835		
1.16_168.0244m/z	168.0244194	1.160166667	neg	20796.28992	29205.39144	30426.82239	28134.63821	25958.213	25111.13357	28147.64915	21448.94982	26506.02328		
1.16_168.0284n	335.0495788	1.160166667	neg	745762.9207	1037440.218	1164607.407	894120.3099	1004188.928	849252.7977	1023730.824	757359.5037	977863.0891		
1.16_203.9973m/z	203.9972742	1.160166667	neg	1983.62478	2006.727743	2134.142093	251.5599047	626.9939778	864.0649472	751.2444683	551.2577648	689.8693392		
1.16_214.0092n	427.0106527	1.160166667	neg	39372.97544	39972.36767	45628.24312	43256.37378	47734.80675	45413.05549	46277.81177	43718.437	47040.18291		
1.16_224.9797m/z	224.979702	1.160166667	neg	2228.30514	2585.898418	1944.881504	2086.425072	930.9889773	1293.461745	2556.512732	1753.218205	1576.202057		
1.16_230.0169m/z	230.0169182	1.160166667	neg	1093.936184	2001.559084	2097.32724	1910.052168	817.2923625	1227.470145	1379.83535	1186.737106	743.1838193		
1.16_235.0086m/z	235.0086123	1.160166667	neg	11135.10708	14836.12825	12587.07197	13349.75449	9332.627031	10266.63608	14155.83499	8925.031119	10010.06241		
1.16_243.9890n	288.9873051	1.160166667	neg	16841.00709	19621.07982	22728.42537	26587.96858	26305.36049	25279.35041	23532.98588	26405.72782	27477.69629		
1.16_251.9987m/z	251.9987421	1.160166667	neg	5476.510752	6345.873363	5896.497557	6545.435156	5266.223485	5839.999621	6145.970404	5532.246788	5356.864127		
1.16_257.9980n	302.9965088	1.160166667	neg	7178.760311	7756.789485	6955.157092	7834.865076	5220.001183	5062.777652	7579.657418	5015.788029	5197.811592		
1.16_264.9885m/z	264.9884727	1.160166667	neg	111725.3774	152043.3483	187217.2711	200831.652	199444.4097	171069.9835	165301.0477	154616.555	185480.035		
1.16_266.9844m/z	266.9843814	1.160166667	neg	5142.566642	6103.452703	8561.115687	8689.47063	8401.139569	7814.823391	8463.691743	7133.138466	7853.721858		
1.16_267.9536n	312.9517514	1.160166667	neg	7822.66143	10073.8778	8993.383905	9316.440949	2454.602608	5404.115207	3861.618678	5792.639633	1873.769618		
1.16_268.9974m/z	268.9974293	1.160166667	neg	2788.737984	2939.315543	2798.488413	4144.210089	4613.127594	4694.969975	3002.705031	3173.940928	3088.245803		
1.16_276.9290m/z	276.9289714	1.160166667	neg	521.6070814	466.0122504	356.7557383	50.95493562	335.4929727	182.7844692	474.6258956	249.6249097	358.8096227		
1.16_293.0064m/z	293.0063669	1.160166667	neg	2227.909958	2570.079728	2100.214662	3846.067019	3930.233564	3155.039254	2981.089646	3164.14711	2968.565751		
1.16_309.9598n	354.9578499	1.160166667	neg	9976.958427	11634.0782	9531.362187	13711.88994	6504.578489	10003.21076	11929.25128	7723.367319	7381.298538		
1.16_310.9693m/z	310.9693246	1.160166667	neg	120585.915	142380.9523	148939.8337	183869.2613	170698.6484	172045.7097	157422.4275	154778.7284	167584.899		

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1.20_346.8782m/z	346.8781923	1.202333333	neg
1.20_356.0604m/z	356.0603504	1.202333333	neg
1.20_370.9586m/z	370.9586138	1.202333333	neg
1.20_384.0293m/z	384.0292803	1.202333333	neg
1.20_388.0256n	387.0186613	1.202333333	neg
1.20_389.9857m/z	389.9856739	1.202333333	neg
1.20_399.9411m/z	399.9410728	1.202333333	neg
1.20_404.9099m/z	404.9099403	1.202333333	neg
1.20_409.0006m/z	409.0006	1.202333333	neg
1.20_411.0608m/z	411.060786	1.202333333	neg
1.20_412.9078m/z	412.9077518	1.202333333	neg
1.20_417.0651n	398.0472112	1.202333333	neg
1.20_421.9234m/z	421.9233971	1.202333333	neg
1.20_422.9206m/z	422.9205834	1.202333333	neg
1.20_434.8898m/z	434.8897937	1.202333333	neg
1.20_441.9472m/z	441.9471884	1.202333333	neg
1.20_442.9232m/z	442.9232172	1.202333333	neg
1.20_444.8452m/z	444.8452114	1.202333333	neg
1.20_451.9027m/z	451.9027291	1.202333333	neg
1.20_452.0169m/z	452.0169199	1.202333333	neg
1.20_457.9730m/z	457.9729774	1.202333333	neg
1.20_463.9293m/z	463.9293372	1.202333333	neg
1.20_473.8854m/z	473.8854207	1.202333333	neg
1.20_483.9541m/z	483.9541419	1.202333333	neg
1.20_489.9112m/z	489.9111617	1.202333333	neg
1.22_185.0458m/z	185.0457618	1.224233333	neg
1.22_187.8889m/z	187.8888997	1.224233333	neg
1.22_189.4946m/z	189.4945617	1.224233333	neg
1.22_215.0289m/z	215.0289193	1.224233333	neg
1.22_218.9947m/z	218.994651	1.224233333	neg
1.22_230.9679m/z	230.9678687	1.224233333	neg
1.22_239.0288m/z	239.0287788	1.224233333	neg
1.22_250.0005m/z	250.0005181	1.224233333	neg
1.22_252.9499m/z	252.9499216	1.224233333	neg
1.22_269.0257m/z	269.0256685	1.224233333	neg
1.22_270.9508m/z	270.9508257	1.224233333	neg
1.22_272.0891m/z	272.0891167	1.224233333	neg
1.22_278.9649m/z	278.9649144	1.224233333	neg
1.22_279.9688m/z	279.9688003	1.224233333	neg
1.22_294.8525m/z	294.8524918	1.224233333	neg
1.22_294.9161m/z	294.916095	1.224233333	neg
1.22_308.0061m/z	308.0061207	1.224233333	neg
1.22_308.0871m/z	308.08711	1.224233333	neg
1.22_313.9764m/z	313.9764167	1.224233333	neg
1.22_321.0698n	320.0626034	1.224233333	neg
1.22_323.0195m/z	323.0195	1.224233333	neg
1.22_328.9984m/z	328.9983726	1.224233333	neg
1.22_340.9555m/z	340.9554764	1.224233333	neg
1.22_352.9484m/z	352.9483594	1.224233333	neg
1.22_362.9037m/z	362.9037054	1.224233333	neg
1.22_365.0319n	410.0320966	1.224233333	neg
1.22_369.0419m/z	369.0418565	1.224233333	neg
1.22_415.9667m/z	415.96666	1.224233333	neg
1.22_420.9355m/z	420.9354749	1.224233333	neg
1.22_430.8915m/z	430.8915348	1.224233333	neg
1.22_456.8724m/z	456.8723773	1.224233333	neg
1.22_461.9938m/z	461.9938205	1.224233333	neg
1.22_483.9755m/z	483.975457	1.224233333	neg
1.22_505.9568m/z	505.9567696	1.224233333	neg
1.22_534.1581m/z	534.1580963	1.224233333	neg
1.25_153.0419m/z	153.0418738	1.246333333	neg
1.25_174.0853m/z	174.0853317	1.246333333	neg
1.25_228.0315m/z	228.0315072	1.246333333	neg
1.25_241.0697m/z	241.0696642	1.246333333	neg
1.25_261.0109m/z	261.0109435	1.246333333	neg
1.25_261.0308n	260.0235298	1.246333333	neg
1.25_262.0280m/z	262.0280298	1.246333333	neg
1.25_263.0095m/z	263.0094804	1.246333333	neg
1.25_274.8683m/z	274.8683129	1.246333333	neg
1.25_282.0055m/z	282.0055407	1.246333333	neg
1.25_286.8550m/z	286.8550065	1.246333333	neg
1.25_294.0037m/z	294.0036967	1.246333333	neg
1.25_323.8693m/z	323.8692793	1.246333333	neg
1.25_325.9981m/z	325.9981257	1.246333333	neg
1.25_344.9097m/z	344.9097091	1.246333333	neg
1.25_347.9801m/z	347.9801377	1.246333333	neg
1.25_349.9931m/z	349.9931076	1.246333333	neg
1.25_357.9913m/z	357.9913071	1.246333333	neg
1.25_359.9487m/z	359.948741	1.246333333	neg
1.25_379.9731m/z	379.9730654	1.246333333	neg
1.25_381.0503m/z	381.0502635	1.246333333	neg
1.25_401.9548m/z	401.9548436	1.246333333	neg
1.25_411.9104m/z	411.9104096	1.246333333	neg
1.25_417.9807m/z	417.980677	1.246333333	neg
1.25_423.9372m/z	423.9371622	1.246333333	neg
1.25_427.9359m/z	427.9359197	1.246333333	neg
1.25_433.8920m/z	433.8920267	1.246333333	neg
1.25_449.0376m/z	449.037648	1.246333333	neg
1.25_454.9043m/z	454.9043178	1.246333333	neg
1.25_485.9682m/z	485.9682335	1.246333333	neg
1.25_491.9245m/z	491.9245236	1.246333333	neg
1.25_495.9238m/z	495.9238328	1.246333333	neg
1.25_499.9224m/z	499.9223587	1.246333333	neg
1.25_501.8795m/z	501.8795111	1.246333333	neg
1.25_521.9043m/z	521.9043282	1.246333333	neg
1.25_543.0367m/z	543.0367075	1.246333333	neg
1.25_559.9117m/z	559.9117146	1.246333333	neg
1.25_565.8684m/z	565.8684277	1.246333333	neg
1.25_575.8240m/z	575.8239523	1.246333333	neg
1.27_129.0188n	257.0281781	1.26875	neg
1.27_153.8955m/z	153.8954936	1.26875	neg
1.27_179.9897n	358.9671533	1.26875	neg
1.27_222.9920m/z	222.9920189	1.26875	neg
1.27_274.0183m/z	274.0183311	1.26875	neg
1.27_280.0675n	325.0656773	1.26875	neg
1.27_296.0188m/z	296.0187848	1.26875	neg
1.27_307.9694m/z	307.9694054	1.26875	neg
1.27_309.9974n	290.975688	1.26875	neg
1.27_314.9829m/z	314.9828953	1.26875	neg
1.27_315.8265m/z	315.8265308	1.26875	neg

3567.899543	3611.909532	3434.88061	2688.594219	3246.019443	2901.519777	3013.692376	3433.050883	3504.130994
1391.213063	1605.626449	1331.864857	1503.887375	1200.208997	1390.488326	1106.048203	1568.990603	1186.276882
8057.346625	7985.528404	6735.580851	8230.44706	8922.102906	8281.284567	8668.083072	7475.268566	8328.216413
2301.362902	2317.255329	1789.92438	2139.293365	420.9965416	1573.010913	2598.943955	1299.494408	305.4662479
8792.805929	9600.928981	11227.69528	9746.317704	7766.522178	8629.866833	8824.586869	10912.75358	10105.63837
4145.192137	4303.097804	4587.316366	4315.169379	4062.95211	4469.160586	4684.136948	4233.78741	4319.021439
1403.759608	1047.804376	1410.554349	1072.940712	1430.009298	1585.722357	1303.556354	1688.704783	1339.107003
5542.36734	5502.928867	5146.856438	4779.230895	4417.304353	4438.148208	4734.548614	5080.43895	5253.908565
2404.352069	2344.212162	3207.943956	2535.773066	2114.838157	2513.990192	2518.024846	3038.999773	2504.855258
1582.408888	1380.850449	1868.278038	1678.199943	1643.064265	1295.762631	1540.282662	1657.253768	1729.898989
4260.725606	4214.95176	5030.400309	4549.698552	4344.294787	4131.944962	4213.826306	4755.364256	5102.994025
2610.018237	2388.507679	2784.317889	3241.462251	2645.764176	3078.935209	2376.367874	3168.447485	2756.990861
562.6530608	531.0210837	268.1217439	383.786949	442.9622763	604.0048537	521.0598517	906.394825	729.0919355
7155.615236	7313.014675	6570.338531	6917.892515	8048.399491	7987.182827	8475.095079	6746.262802	7595.605173
5305.208582	5500.852538	4882.391765	4324.706804	4716.009618	4568.158304	5086.182284	5165.904624	5098.756374
1341.233949	1321.479823	1346.023948	1780.144215	2306.118807	2051.862527	1608.684676	2073.217325	2205.57281
1114.347458	1518.52399	1347.421703	1671.135188	1306.103405	1677.434404	1014.575499	1141.065685	1271.640179
937.1054355	1219.545043	940.3507251	1056.62872	1482.062744	1214.836838	1094.95802	1308.042168	1482.429882
579.1995204	341.9819276	425.6478873	689.3348572	831.7707676	793.9697852	763.1618906	764.714039	1094.541186
1253.235213	1013.221736	1140.927551	1606.242445	1727.292153	1466.301082	1598.040874	1336.707696	1602.294703
1087.514978	864.6853834	903.3672128	1143.211914	995.2852604	1335.751603	1674.343585	1284.868458	851.9065278
1168.205459	1232.770646	1398.819773	1910.913529	1231.059563	2212.284293	1523.948366	1893.026192	900.3188318
483.5400074	406.423397	501.4703068	561.7745729	886.3275847	553.1181022	584.7236825	796.5820465	642.3276785
837.4802003	1137.396895	591.3975974	963.464182	466.0686304	729.5541061	1152.226942	861.922544	1253.350444
1618.602835	1062.973183	1325.360871	1712.809339	1937.975176	1553.135383	1202.271492	1582.986755	1518.581563
310.3288807	330.6320163	287.9258894	212.7509886	203.3386395	175.6882233	73.5322953	93.39873793	93.08169871
25933.56495	25067.30824	24384.35911	29874.40379	30842.91078	30127.07984	31604.15334	27128.80633	27749.19268
324.80423	301.3045791	295.4459121	357.9470602	232.7452195	247.2644648	209.715547	233.9111309	218.8029989
380.6395965	478.5854068	508.3078405	452.3085107	517.8064081	543.3985477	376.428992	471.1982478	414.8399252
215.9284422	283.8378689	290.1275419	379.6623332	266.6448403	304.6626213	296.8952133	268.6655384	256.0960673
866.0308847	752.2217661	821.9492971	654.7807045	507.5351026	579.9207187	667.6652318	762.0628042	287.0987818
3085.181915	2916.006129	3129.539979	5647.454486	5724.410975	5884.309744	4180.541991	4422.957741	4222.951194
738.1160974	1007.490435	861.1884887	845.0559925	834.0923341	850.4513941	922.5026589	866.5010376	853.0743748
1043.931628	871.9092551	891.3575546	773.4261517	233.2204565	544.667264	885.5110476	785.5015755	467.6992318
524.3690825	607.4387548	623.6160007	378.780691	4.433892432	291.9496188	273.7925994	248.2619827	0.001403199
2359.702105	2470.871719	2483.762073	1831.651877	2266.119841	2037.260693	2440.111168	2542.214598	2153.902109
498.3648031	597.72348	420.4634501	574.4826123	280.7758458	342.4842696	478.1132242	563.4812431	394.2072982
217.0961891	298.7039126	184.6918874	111.4626119	307.0636046	168.8879638	199.1436372	325.4817785	214.1883392
665.4112751	569.499472	536.3298437	298.9129782	425.7962601	437.9444774	617.4830114	395.350667	364.0299019
1381.025885	1294.561625	1196.638545	1660.702225	1323.117617	1553.803607	1319.478775	1504.634583	1198.107059
3491.483856	3390.247254	2886.710293	1994.629133	2477.14421	2374.354082	2416.831954	2596.687357	2566.770355
1713.477214	2279.320278	2221.92408	3275.944329	3171.346125	3259.902241	2612.043105	3274.85679	3183.291715
909.8464406	821.857081	1083.522861	812.8967523	788.3328612	683.0532697	699.58379	847.693077	770.978745
62.67730283	146.8094245	61.74693095	133.0628932	210.121162	66.2762209	133.3525193	86.60693359	106.6876121
31836.09899	38105.01003	39870.08112	47864.50869	45218.88671	46432.80128	23164.41512	26996.84453	27878.11312
641.8484782	924.2682063	656.1833856	1028.8636	924.1374935	932.3169833	751.2254002	807.7809342	499.5719458
1065.688834	1076.769956	1093.111334	1970.789496	2056.0355	2339.434177	1789.743697	1491.674283	1378.015561
1881.234572	1819.005354	1973.267078	2576.202169	2327.880446	2586.146681	2086.031426	2295.760225	2166.056913
2740.590849	3142.351683	3050.177569	2098.672048	1905.688331	2686.87303	3091.981541	2702.199157	2194.491047
2640.513225	2634.58152	2467.324977	2784.693424	1301.78233	1767.601967	2345.717546	1959.612144	1333.849659
3037.555422	2614.886746	2691.452889	2791.947957	2917.161582	3379.045412	1607.509508	1789.003341	1725.83669
188.7856197	183.2403112	282.1455609	148.0708096	292.3689347	214.5734345	282.1415788	323.7335234	262.112242
1181.754521	703.5499103	1091.052991	1257.267952	640.844634	1242.077113	1176.074794	858.2803749	867.5459721
1729.317543	1708.958506	1350.100477	1099.848482	896.5665505	1325.276146	1588.268462	1529.014009	1257.827685
1736.655453	1234.560646	1228.493475	881.4995363	493.2698923	602.1345819	973.4147097	733.2543564	487.4003897
1407.529767	1752.417017	1211.700402	1412.376917	431.3418312	1191.454791	1076.587847	822.0208591	601.170581
3192.485191	3686.891369	4018.2712	5593.818974	5013.315291	4737.220011	2059.787378	2658.227469	2652.497617
2146.716115	2213.347505	1852.619073	3328.770488	1699.193364	2394.465151	1175.557622	1476.090683	1012.440554
1616.36789	1257.288732	1550.404559	1974.533613	892.3387357	1435.795865	965.003924	391.8922799	661.4787595
1287.027009	1704.853931	1546.72212	1779.618643	1772.235709	1727.805992	1516.94885	1852.795132	1962.468188
0.001403199	33.25454581	36.09428997	31.26586202	28.29181499	28.34016285	0.001403199	33.93315697	57.7884603
248.003479	260.9149846	273.9982961	287.0772002	328.8185122	366.6335003	286.3821108	373.9068356	369.9903151
5210.59591	5855.391333	5561.181448	3105.672872	3470.519774	3194.442519	3599.18134	3801.554394	4038.505961
780.4143121	952.4025144	813.6634223	1128.419401	1296.298529	1262.348405	1136.097986	1289.521649	1220.442107
1921.23816	2281.080676	2359.562914	3859.290654	3088.853988	3827.821063	2925.384966	3324.195208	2198.493243
131326.5553	150738.641	150791.6102	212290.7553	213017.4872	205569.0947	148588.5207	166223.5421	161891.5854
728.4058263	1029.111709	909.5274866	1413.54247	1377.291832	1446.457755	832.8395974	959.5556102	1108.471832
712.8299908	1079.27197	1050.506412	1516.938634	1337.740864	1354.254151	1326.111576	1363.487083	1415.515952
1478.114654	1525.375477	1635.198327	1838.822804	1643.404677	1699.590179	1825.415892	1919.381643	1480.302471
27183.88476	28958.39312	28263.79194	39905.01171	41511.14533	39954.02778	32676.81515	36093.82492	30562.04708
405.7911512	525.0955917	378.4743854	480.8344818	601.971176	590.6989238	699.019356	651.3141841	479.0209336
371.4135286	193.0916787	160.9109985	284.7953164	0.001403199	183.476712	295.3445485	111.8251862	51.5319738
1680.157616	1678.494224	1395.680961	2102.699627	1974.765588	1888.338597	2251.858763	1859.325294	1642.080108
5534.416135	5873.501465	5599.460277	4971.126374	5173.609203	4792.833107	4738.999024	5474.241708	5236.512805
518.0613705	396.7750226	420.1942892	819.3828011	706.900013	829.0731566	524.5279785	516.4463448	436.1282792
3474.054315	3714.462767	3512.649791	2748.839671	2725.9995	2766.459321	3160.607926	3112.150085	3240.986772
8185.573146	7649.040663	7820.73074	10562.39432	10684.09464	10982.63886	8861.1215	8632.834445	8254.621614
3849.088323	4049.97087	3676.026567	7475.500566	6545.264708	6545.081228	4335.184925	4291.474758	4439.98713
2374.208414	2602.186355	2376.113382	3476.599814	3386.070688	3043.477896	2563.267101	2598.882243	2083.066923
14638.88617	16641.13086	16657.2293	28861.54108	26014.49928	25503.76645	17291.62207	19564.95098	18850.10332
12117.92736	13512.25631	12678.564	10226.36635	10076.63875	9702.390549	9502.514973	11017.39037	11131.88491
7268.575861	8764.58521	8480.877527	13305.90447	12196.14673	13641.27676	8644.353362	9940.352145	9552.761172
567.2810862	698.5239981	693.2473787	906.1432466	834.8536888	921.7845815	493.0840241	578.7042465	843.8946308
3367.409077	4236.646793	3727.429479	4316.873974	4669.796764	4296.615302	3436.837443	3182.5205	3591.074392
4122.338677	5187.164847	5313.415218	7129.16405	7510.425479	7430.173513	5225.659908	4950.588473	5191.575943
3410.156854	3155.660065	3041.47347	3502.718428	4209.863148	3110.022788	2899.458459	2891.030514	2737.704904
1253.692251	1622.758817	1093.578799	2409.320207	1838.608701	2188.55647	1652.655729	1737.556816	1469.802251
1240.270563	1351.728712	1198.285913	944.0890946	851.8507336	516.0477232	990.6788208	921.7374315	1057.622623
376.2356389	279.3121392	328.7081829	613.9622886	528.4123496	653.993138	448.2248864	500.7388458	442.9220789
1800.024295	1964.830865	1743.096371	2422.400222	2426.937771	3070.98208	1995.238669	1706.624201	1721.556092
1635.458216	2403.964493	2097.116784	3608.77901	3858.895409	3948.693063	2414.207653	2635.705032	2432.341619
1310.888814	1632.97895	1437.905631	1551.134275	1938.390702	1850.714894	1226.228533	1199.744037	1762.794917
1307.164398	1807.579349	1829.139187	3538.01354	3977.589608	3445.528541	2190.39179	2343.090716	2179.477604
937.7014217	988.6058812	1200.395369	2117.167403	1729.9379942	1855.374333	1444.893004	1187.244292	996.9171207
933.4629277	1784.759107	1629.633423	2867.432384	3102.365721	3710.545489	2104.820676	2734.632556	2524.924905
509.9909408	435.136454	774.5934291	1551.153464	1487.515546	1621.20636	705.5774881	602.3421918	694.8566892
635.9888169	1053.212582	783.6422246	1107.296806	1435.604565	1476.239047	956.0205006	893.3044205	1382.538368
1009.139927	1301.771986	1111.149839	1120.40281	1387.290216	1505.914185	1408.196646	1087.128398	1226.666572
1153.301738	901.6841355	1100.491001	1736.397804	1600.469122	1033.560898	967.8454391	1114.994008	781.002257
1786.036747	2227.256869	2288.916292	3020.244563	3166.567929	3181.325565	2009.253529	2240.829755	2199.699982
136.3993658	97.94066253	64.81307313	118.5504244	157.7441472	79.41680159	128.8692547	212.9497849	117.034438
9133.635156	9692.380739	9419.582027	2644.070359	2556.803633	2497.673097	3176.897844	3131.004051	3199.935393
93742.25098	102120.6826	103018.2861	34604.27223	34533.6326	33118.34683	36638.18881	41207.36693	40432.75836
366.2739646	612.7913503	720.7006829	990.2330447	912.1427657	949.0808927	573.1721162	587.7548398	490.634987
4175.53386	3908.551238	4062.722727	3765.918213	3815.605461	3995.397951	3743.635338	3612.915094	3871.283947
2272.758119	2486.967688	2153.691369	1094.22012	1088.803071	1108.302899	1182.513987	1458.966891	1378.613571
838.6189465	924.9110698	647.2522832	160.0342049	164.6285184	64.41313557	217.1210837	143.0314789	162.3858882
14554.35484	15566.78072	16111.11996	8973.900369	9298.558293	8426.930763	7910.667598	8337.862111	8251.33916
1873.414061	1906.687997	1935.119348	645.2478108	743.3409823	500.6829571	1722.835198	2035.827662	1439.45158
1770.268647	1597.489546	1321.934337	1904.391033	1456.77496	1574.575246	1742.55689	1744.321894	1268.913907

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1.46_591.0174m/z	591.0174249	1.459966667	neg
1.46_594.7808m/z	594.7807732	1.459966667	neg
1.46_594.8553m/z	594.8553125	1.459966667	neg
1.46_614.7654m/z	614.7654063	1.459966667	neg
1.46_808.7719m/z	808.7719179	1.459966667	neg
1.47_146.9615m/z	146.9614792	1.472133333	neg
1.47_152.9046m/z	152.904639	1.472133333	neg
1.47_183.0275m/z	183.0275149	1.472133333	neg
1.47_195.8870m/z	195.8870285	1.472133333	neg
1.47_263.1169m/z	263.1168764	1.472133333	neg
1.47_273.1458m/z	273.1458408	1.472133333	neg
1.47_311.9799m/z	311.9798749	1.472133333	neg
1.47_324.8279m/z	324.8278874	1.472133333	neg
1.47_326.9672m/z	326.9672424	1.472133333	neg
1.47_328.9699m/z	328.9699237	1.472133333	neg
1.47_363.9417m/z	363.9417054	1.472133333	neg
1.47_379.9673m/z	379.9672697	1.472133333	neg
1.47_385.9240m/z	385.9239805	1.472133333	neg
1.47_418.9923m/z	418.9923101	1.472133333	neg
1.47_445.0135m/z	445.0135415	1.472133333	neg
1.47_447.9549m/z	447.954904	1.472133333	neg
1.47_486.9796m/z	486.9796813	1.472133333	neg
1.47_584.8262m/z	584.8262421	1.472133333	neg
1.49_162.0596m/z	162.0595501	1.492933333	neg
1.49_219.0042m/z	219.0042219	1.492933333	neg
1.49_240.9864m/z	240.986385	1.492933333	neg
1.49_250.8841m/z	250.8840595	1.492933333	neg
1.49_270.0329n	251.0150755	1.492933333	neg
1.49_274.9764m/z	274.9763627	1.492933333	neg
1.49_275.9576m/z	275.9575569	1.492933333	neg
1.49_283.0412m/z	283.0412143	1.492933333	neg
1.49_301.9509m/z	301.9509045	1.492933333	neg
1.49_302.9773m/z	302.9772718	1.492933333	neg
1.49_308.9737m/z	308.9737128	1.492933333	neg
1.49_324.9591m/z	324.9590644	1.492933333	neg
1.49_338.0205n	319.0026546	1.492933333	neg
1.49_386.9901m/z	386.9901484	1.492933333	neg
1.49_392.9465m/z	392.9465456	1.492933333	neg
1.49_454.9773m/z	454.9773309	1.492933333	neg
1.52_162.0231m/z	162.0230958	1.515416667	neg
1.52_187.0282m/z	187.0281535	1.515416667	neg
1.52_230.0469m/z	230.0469129	1.515416667	neg
1.52_233.0067m/z	233.0067114	1.515416667	neg
1.52_241.8925m/z	241.8925025	1.515416667	neg
1.52_276.9554m/z	276.9553943	1.515416667	neg
1.52_278.0705m/z	278.0704529	1.515416667	neg
1.52_297.1193m/z	297.1192962	1.515416667	neg
1.53_174.9337m/z	174.9336731	1.534483333	neg
1.53_225.8854m/z	225.8854165	1.534483333	neg
1.53_238.0115m/z	238.011519	1.534483333	neg
1.53_240.0087m/z	240.0086787	1.534483333	neg
1.53_265.0556m/z	265.0556376	1.534483333	neg
1.53_325.9832m/z	325.9832209	1.534483333	neg
1.53_335.0536m/z	335.053552	1.534483333	neg
1.53_393.9704m/z	393.9703742	1.534483333	neg
1.53_419.0664m/z	419.0663786	1.534483333	neg
1.53_461.9584m/z	461.9584241	1.534483333	neg
1.53_487.0537m/z	487.053673	1.534483333	neg
1.53_529.9460m/z	529.9459885	1.534483333	neg
1.55_159.982m	204.981367	1.553483333	neg
1.55_160.9988m/z	160.9988234	1.553483333	neg
1.55_171.0276m/z	171.0276059	1.553483333	neg
1.55_202.9651m/z	202.9650608	1.553483333	neg
1.55_223.9931m/z	223.9931247	1.553483333	neg
1.55_227.9051m/z	227.9051497	1.553483333	neg
1.55_228.9129m/z	228.9128574	1.553483333	neg
1.55_229.9020m/z	229.9019824	1.553483333	neg
1.55_230.9098m/z	230.9097952	1.553483333	neg
1.55_239.0151m/z	239.0151067	1.553483333	neg
1.55_244.9715m/z	244.9715072	1.553483333	neg
1.55_245.9470m/z	245.946993	1.553483333	neg
1.55_254.9262m/z	254.9262107	1.553483333	neg
1.55_262.0756m/z	262.0755522	1.553483333	neg
1.55_265.0305m/z	265.0304562	1.553483333	neg
1.55_271.0938m/z	271.0937691	1.553483333	neg
1.55_271.9599n	542.9024005	1.553483333	neg
1.55_276.9087m/z	276.9087191	1.553483333	neg
1.55_300.0023m/z	300.0022926	1.553483333	neg
1.55_307.0026m/z	307.0026139	1.553483333	neg
1.55_312.9591m/z	312.9591494	1.553483333	neg
1.55_313.9348m/z	313.9347679	1.553483333	neg
1.55_315.9543m/z	315.9542747	1.553483333	neg
1.55_316.0278m/z	316.0277629	1.553483333	neg
1.55_317.0517m/z	317.0516767	1.553483333	neg
1.55_338.9398m/z	338.9397955	1.553483333	neg
1.55_348.8954m/z	348.8953775	1.553483333	neg
1.55_355.9299m/z	355.9299227	1.553483333	neg
1.55_364.9611m/z	364.9610997	1.553483333	neg
1.55_365.0445m/z	365.0444915	1.553483333	neg
1.55_374.9901m/z	374.9900547	1.553483333	neg
1.55_380.9464m/z	380.9464241	1.553483333	neg
1.55_381.9221m/z	381.9221478	1.553483333	neg
1.55_406.9273m/z	406.9272561	1.553483333	neg
1.55_442.9774m/z	442.9774443	1.553483333	neg
1.55_448.9337m/z	448.9336965	1.553483333	neg
1.55_449.9097m/z	449.9096669	1.553483333	neg
1.55_474.9146m/z	474.9146167	1.553483333	neg
1.55_480.8712m/z	480.8711708	1.553483333	neg
1.55_510.9647m/z	510.9647487	1.553483333	neg
1.55_516.9211m/z	516.9210834	1.553483333	neg
1.55_517.8972m/z	517.8971603	1.553483333	neg
1.55_578.9528m/z	578.9527574	1.553483333	neg
1.56_162.9959m/z	162.995872	1.56225	neg
1.56_192.9362m/z	192.9362134	1.56225	neg
1.56_237.9341m/z	237.9340788	1.56225	neg
1.56_247.9627m/z	247.9627463	1.56225	neg
1.56_272.9689m/z	272.9689126	1.56225	neg
1.56_296.9736m/z	296.9735581	1.56225	neg
1.56_298.0617m/z	298.061731	1.56225	neg
1.56_306.0584m/z	306.0583519	1.56225	neg

2504.78361	3414.731253	2754.703323	785.514865	580.7667622	739.728081	1086.825949	607.1537323	663.6967891
3644.644551	3208.293439	1793.19806	3452.807774	2511.836756	2658.806678	3690.383981	2638.020177	2695.873566
96177.05427	98120.01006	88091.16937	116334.7183	129603.0426	126449.9209	124173.8981	102801.7385	111182.8634
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6039.378565	5267.284022	3867.52117	5151.587071	5388.099112	4469.530109	6231.044364	3906.902466	5123.042637
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1140.528536	1228.596748	1240.396401	1412.333948	1197.249202	1242.483933	1271.749187	1109.553552	1237.742654
1968.359469	1770.757192	1491.319843	1840.693891	1998.434814	1717.549556	2340.066966	1570.805729	1830.203249
41.0172478	133.0060633	132.5465797	137.2212892	41.19132479	78.07873318	116.7831438	66.58373586	105.4412861
2327.931151	2451.140005	2284.725025	3240.51577	2596.820222	2643.081312	2698.637947	1737.438221	2526.530039
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1.56_417.0113m/z	417.0112821	1.56225	neg	
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1.58_250.0335m/z	250.0334918	1.577833333	neg	
1.58_270.0962m/z	270.0961797	1.577833333	neg	
1.58_332.0740m/z	332.0739807	1.577833333	neg	
1.58_854.3264n	899.3256572	1.577833333	neg	
1.59_202.0254m/z	202.0254076	1.5934	neg	
1.59_204.0224m/z	204.0223745	1.5934	neg	
1.59_264.0161m/z	264.0161172	1.5934	neg	
1.59_279.9683m/z	279.9682873	1.5934	neg	
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1.59_289.9972m/z	289.9971625	1.5934	neg	
1.59_348.0293m/z	348.0292504	1.5934	neg	
1.59_355.0527m/z	355.0527359	1.5934	neg	
1.59_357.9847m/z	357.9846761	1.5934	neg	
1.59_397.0755m/z	397.075469	1.5934	neg	
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1.59_415.9436m/z	415.9435551	1.5934	neg	
1.59_416.0167m/z	416.0167104	1.5934	neg	
1.59_425.9723m/z	425.9722945	1.5934	neg	
1.59_484.0043m/z	484.00425	1.5934	neg	
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1.62_190.9823m/z	190.9822688	1.615883333	neg	
1.62_224.9136m/z	224.9135641	1.615883333	neg	
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1.63_260.0034m/z	260.0033866	1.631516667	neg	
1.63_286.9846m/z	286.9846193	1.631516667	neg	
1.63_298.0427m/z	298.042704	1.631516667	neg	
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1.63_366.0302m/z	366.030237	1.631516667	neg	
1.63_370.9975m/z	370.9975187	1.631516667	neg	
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1.63_462.8056m/z	462.8055722	1.631516667	neg	
1.63_526.7930m/z	526.792994	1.631516667	neg	
1.65_177.0102m/z	177.0102484	1.65405	neg	
1.65_218.0494m/z	218.0493945	1.65405	neg	
1.65_247.0396m/z	247.0396008	1.65405	neg	
1.65_252.0128m/z	252.0127602	1.65405	neg	
1.65_266.9600m/z	266.9599958	1.65405	neg	
1.65_278.9712m/z	278.9711994	1.65405	neg	
1.65_286.0369m/z	286.036915	1.65405	neg	
1.65_302.0520m/z	302.0520381	1.65405	neg	
1.65_324.0339m/z	324.033907	1.65405	neg	
1.65_337.9993m/z	337.9992681	1.65405	neg	
1.65_342.9985m/z	342.9984986	1.65405	neg	
1.65_354.0245m/z	354.0244588	1.65405	neg	
1.65_374.0780m/z	374.0779847	1.65405	neg	
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1.65_489.9993m/z	489.9992995	1.65405	neg	
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1.67_213.0382m/z	213.0382397	1.66975	neg	
1.67_226.9908m/z	226.9908445	1.66975	neg	
1.67_229.0695m/z	229.0695145	1.66975	neg	
1.67_242.0649m/z	242.0649144	1.66975	neg	
1.67_269.0215m/z	269.0214652	1.66975	neg	
1.68_104.0435m/z	104.0434673	1.68365	neg	
1.68_160.9988m/z	160.9987801	1.68365	neg	
1.68_188.0178m/z	188.0177891	1.68365	neg	
1.68_192.9362m/z	192.9361565	1.68365	neg	
1.68_270.9527m/z	270.952686	1.68365	neg	
1.68_296.9736m/z	296.9736203	1.68365	neg	
1.68_312.9590m/z	312.9590161	1.68365	neg	
1.68_364.9613m/z	364.9612723	1.68365	neg	
1.68_375.9937m/z	375.9936802	1.68365	neg	
1.68_380.9464m/z	380.9464374	1.68365	neg	
1.68_510.9646m/z	510.9646493	1.68365	neg	
1.70_138.0308m/z	138.0308381	1.6992	neg	
1.70_245.9469m/z	245.9469395	1.6992	neg	
1.70_419.0437m/z	419.0437493	1.6992	neg	
1.70_453.0505m/z	453.0505397	1.6992	neg	
1.72_181.0302m/z	181.0301879	1.721216667	neg	
1.72_182.0401m/z	182.0400885	1.721216667	neg	
1.72_234.9919m/z	234.9918714	1.721216667	neg	
1.72_249.0242m/z	249.0242369	1.721216667	neg	
1.72_261.9846n	306.9831275	1.721216667	neg	
1.72_266.0144m/z	266.0144429	1.721216667	neg	
1.72_272.0136n	317.011647	1.721216667	neg	
1.72_280.9618m/z	280.9618179	1.721216667	neg	
1.72_293.0143m/z	293.0142733	1.721216667	neg	
1.72_323.9756n	368.973536	1.721216667	neg	
1.72_326.9672m/z	326.9672226	1.721216667	neg	
1.72_328.9650m/z	328.9649582	1.721216667	neg	
1.72_338.9201m/z	338.9201337	1.721216667	neg	
1.72_341.0271m/z	341.0270849	1.721216667	neg	
1.72_349.9564n	394.9546055	1.721216667	neg	
1.72_355.9839m/z	355.9838884	1.721216667	neg	
1.72_358.0115n	338.9936894	1.721216667	neg	
1.72_385.0630m/z	385.0630148	1.721216667	neg	
1.72_390.9557m/z	390.9556976	1.721216667	neg	
1.72_406.9078m/z	406.9077779	1.721216667	neg	
1.72_407.9884n	452.9866066	1.721216667	neg	
1.72_416.9367m/z	416.9367323	1.721216667	neg	
1.72_452.1678m/z	452.1677629	1.721216667	neg	
1.72_458.9428m/z	458.9427848	1.721216667	neg	
1.72_465.8763m/z	465.8762855	1.721216667	neg	
1.72_474.9688m/z	474.9685764	1.721216667	neg	
1.72_485.9314n	484.9241184	1.721216667	neg	

121.7169596	146.6202788	265.6927373	1320.34112	1085.371168	1206.948833	262.559211	304.5362434	147.1366155	
0.001403199	0.001403199	53.62626614	151.0933044	143.0858296	76.71813941	120.0079529	169.926829	0.001403199	
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951.6213361	653.6409926	678.9597869	162.7401958	97.47839714	41.1576671	347.3545916	453.487587	421.0947835	
970.8285343	629.955288	962.8813377	888.3660108	725.8710804	867.9080008	646.8039619	866.1542816	786.7285631	
1652.424309	1455.130416	1458.046517	2025.190327	2432.711951	2414.485767	1635.023871	1955.499222	1646.180008	
440.2517695	398.2332015	405.6617159	900.5951114	872.352084	805.9413247	275.1529189	413.017473	332.8587349	
146.7302535	204.8689527	278.8412917	484.4108328	256.1426439	441.0886781	307.7056144	380.9978676	309.7003047	
1506.955797	1019.968381	1077.356285	1360.077074	1392.089893	1761.764346	1065.643759	1680.278253	1237.877152	
21650.21583	16670.1534	14989.50801	12862.64737	12755.75278	12867.51577	13039.57779	21124.96762	17130.49644	
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572.4707494	542.7427424	489.0419492	410.998479	430.934371	455.1161857	540.4846819	611.5284633	544.1518406	
2302.974574	2264.778669	2302.061572	2349.084448	2278.823523	2104.290472	2312.681142	2637.591427	2534.546444	
1812.212607	1509.910482	1564.633727	1253.608177	1244.004948	1124.207274	1367.914728	1535.989577	1448.156049	
6087.302609	5370.924445	5519.291847	5615.147377	5811.372569	5753.39564	5771.526999	5812.054826	6237.53527	
4402.903313	3550.394557	3654.171802	2894.578042	2885.919281	3119.817509	3737.616676	3739.353821	3278.101736	
4237.757689	3738.341442	3874.821689	3463.77932	3865.827001	3718.736413	3941.486467	3808.092411	3899.830981	
2636.469377	2306.473508	2588.585969	2943.483483	3027.409385	3028.108422	2655.470367	2664.258468	2744.744263	
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641.9825453	630.23989	659.7077129	488.9086968	573.8553517	506.3108188	613.5717691	611.7755896	540.7970054	
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3226.334776	2678.085145	2389.255883	1999.202221	2222.181411	2047.871809	2458.099244	2275.688103	2729.216002	
3831.842891	3166.645553	2879.382539	3003.073704	3159.374831	2793.728644	3698.823714	3074.912927	3205.90194	
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453.041559	475.7973147	471.1775247	240.9535358	205.0327096	159.2185163	367.8507645	347.3352177	396.9999737	
852.5526256	705.9582008	569.9490549	1049.863877	1039.636079	963.8331205	1544.02	1331.08067	1391.195386	
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938.603282	932.2021139	1203.771782	902.7191606	1013.114022	979.1537412	1199.237067	1031.281583	1139.586839	
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7210.209528	7966.539399	8875.172619	11547.48568	11358.28623	11883.56741	12866.93995	11954.64993	11474.6956	
760.1817897	189.4295795	142.9638255	155.8158309	185.0148194	148.1466935	216.0252426	223.5426598	233.1500226	
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3152.949023	3194.192329	2716.139594	3126.534747	3280.47056	3221.043291	3092.2058	2942.94504	3891.91198	
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1.72_487.0311m/z	487.0311128	1.721216667	neg
1.72_520.9749m/z	520.9748956	1.721216667	neg
1.72_542.9564m/z	542.9563581	1.721216667	neg
1.72_552.9117m/z	552.9117219	1.721216667	neg
1.72_620.8992m/z	620.8991726	1.721216667	neg
1.74_206.9970m/z	206.996957	1.736816667	neg
1.74_246.0443m/z	246.0443249	1.736816667	neg
1.74_377.1003m/z	377.1002952	1.736816667	neg
1.74_384.9988m/z	384.9987932	1.736816667	neg
1.74_604.8722m/z	604.8721624	1.736816667	neg
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1.75_376.8518m/z	376.8518025	1.74555	neg
1.75_516.8375m/z	516.8375156	1.74555	neg
1.75_594.7810m/z	594.7809859	1.74555	neg
1.76_301.0568m/z	301.0567607	1.7577	neg
1.76_304.9035m/z	304.9034531	1.7577	neg
1.76_577.7905m/z	577.7905062	1.7577	neg
1.76_584.8262m/z	584.8262055	1.7577	neg
1.76_662.8427m/z	662.8427158	1.7577	neg
1.77_190.9286m/z	190.9285717	1.769966667	neg
1.77_205.9157m/z	205.9156629	1.769966667	neg
1.77_225.8854m/z	225.8854216	1.769966667	neg
1.77_275.9062m/z	275.9062026	1.769966667	neg
1.77_511.8183m/z	511.8182597	1.769966667	neg
1.77_658.8102m/z	658.8102023	1.769966667	neg
1.77_730.8298m/z	730.8298206	1.769966667	neg
1.77_798.8171m/z	798.817136	1.769966667	neg
1.77_808.7727m/z	808.7727444	1.769966667	neg
1.78_472.8338m/z	472.833786	1.778766667	neg
1.78_713.7654m/z	713.7654306	1.778766667	neg
1.78_740.7853m/z	740.7853296	1.778766667	neg
1.78_812.7718m/z	812.7717999	1.778766667	neg
1.79_264.8819m/z	264.8819203	1.7861	neg
1.79_337.0810n	336.0729529	1.7861	neg
1.79_404.8461m/z	404.8461094	1.7861	neg
1.79_433.8018m/z	433.8017753	1.7861	neg
1.79_540.8215m/z	540.8215064	1.7861	neg
1.80_224.0542m/z	224.0542064	1.798266667	neg
1.80_239.0539m/z	239.0539209	1.798266667	neg
1.80_264.0549m/z	264.0548584	1.798266667	neg
1.80_289.1277n	288.1203767	1.798266667	neg
1.80_292.0417m/z	292.0417401	1.798266667	neg
1.80_308.8642m/z	308.8641898	1.798266667	neg
1.80_390.1278n	435.1260002	1.798266667	neg
1.81_200.1161n	245.1143483	1.808733333	neg
1.81_279.0599m/z	279.0599107	1.808733333	neg
1.81_378.0898m/z	378.0897592	1.808733333	neg
1.82_207.9187m/z	207.9187417	1.820883333	neg
1.82_332.9699m/z	332.9698662	1.820883333	neg
1.82_342.0744m/z	342.074374	1.820883333	neg
1.82_345.9923m/z	345.9923226	1.820883333	neg
1.82_441.8154m/z	441.8154279	1.820883333	neg
1.82_459.0882m/z	459.0882238	1.820883333	neg
1.84_144.9433m/z	144.9433438	1.841666667	neg
1.84_146.9386m/z	146.9386931	1.841666667	neg
1.84_163.9289m/z	163.9288847	1.841666667	neg
1.84_179.9364m/z	179.9364274	1.841666667	neg
1.84_182.8967m/z	182.8967424	1.841666667	neg
1.84_218.0493m/z	218.0493481	1.841666667	neg
1.84_234.9392m/z	234.9392821	1.841666667	neg
1.84_278.0050m/z	278.0049781	1.841666667	neg
1.84_318.9814n	317.9741362	1.841666667	neg
1.84_337.9991m/z	337.999103	1.841666667	neg
1.84_343.0583m/z	343.0583179	1.841666667	neg
1.84_343.9953m/z	343.9952798	1.841666667	neg
1.84_371.0145m/z	371.0145294	1.841666667	neg
1.84_405.9858m/z	405.9858265	1.841666667	neg
1.84_411.9830m/z	411.9830153	1.841666667	neg
1.84_413.9800m/z	413.9800268	1.841666667	neg
1.84_427.9680m/z	427.9680463	1.841666667	neg
1.84_431.9671m/z	431.9671171	1.841666667	neg
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1.84_693.9617m/z	693.9616847	1.841666667	neg
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1.86_210.0384m/z	210.0384202	1.86075	neg
1.86_244.9680m/z	244.9680377	1.86075	neg
1.86_315.0725m/z	315.0725373	1.86075	neg
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1.87_123.9465m/z	123.9464604	1.872916667	neg
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1.87_312.9557m/z	312.9556816	1.872916667	neg
1.87_645.7776m/z	645.7776044	1.872916667	neg
1.89_167.0326m/z	167.0325793	1.885116667	neg
1.89_211.0226m/z	211.0225536	1.885116667	neg
1.89_339.9119m/z	339.9118674	1.885116667	neg
1.89_346.9974m/z	346.9974488	1.885116667	neg
1.89_414.9849m/z	414.9848634	1.885116667	neg
1.90_191.0350m/z	191.0350043	1.899016667	neg
1.90_331.0109m/z	331.0108721	1.899016667	neg
1.90_364.0879m/z	364.0878837	1.899016667	neg
1.90_432.0751m/z	432.0751147	1.899016667	neg
1.90_579.8061m/z	579.806051	1.899016667	neg
1.90_614.7652m/z	614.7651968	1.899016667	neg
1.91_238.9009m/z	238.9009489	1.911116667	neg
1.92_202.9657m/z	202.965739	1.924916667	neg
1.92_220.9928m/z	220.9928267	1.924916667	neg
1.92_227.9704n	226.9631201	1.924916667	neg
1.92_233.0293m/z	233.0293133	1.924916667	neg
1.92_250.0195m/z	250.0194904	1.924916667	neg
1.92_262.9403m/z	262.940282	1.924916667	neg
1.92_276.9554m/z	276.9553586	1.924916667	neg

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315.4425272	249.9049667	320.7760319	843.9220053	686.374793	631.3609792	425.2801942	352.9617995	421.2849892	
2743.715228	2605.979734	2763.619877	5808.423437	5361.925145	4940.368422	3230.187038	3179.574732	3355.4895	
1075.060787	736.2378828	670.8188743	779.5804904	634.6025817	525.5338444	1009.737912	449.4816246	483.4039344	
1397.742803	1349.54534	1352.436231	3413.732911	3071.971334	2751.299467	1849.155136	1697.073572	1621.05647	
1094.936525	894.011729	1000.636165	2659.092518	2549.791981	2128.441655	1417.007778	1148.145691	1369.620883	
1214.587193	1150.567377	1108.144008	1204.323747	1085.530285	857.7012398	1367.711374	1071.325354	1133.87615	
1710.642662	1894.174759	1690.884891	1924.196703	1864.735921	1453.705055	1922.980585	1614.081043	1583.561271	
5868.669556	6337.166234	5456.132695	6241.005978	6603.815044	6077.750665	5947.277912	5171.8572	5598.521984	
1134.296524	919.655022	976.9350887	1344.65401	1522.813479	1218.734328	1295.27602	988.5258356	1044.196557	
94499.50571	75028.71989	65949.90867	70615.0112	74610.91647	71793.03513	86439.18459	67053.12097	69106.21491	
1146.049561	972.3305568	1250.768349	1452.02131	1360.609746	1091.968111	2149.705703	756.1915981	1340.769059	
0.001403199	129.2317523	111.1308489	70.0375153	353.4052568	0.001403199	136.6746486	0.001403199	80.17417962	
21323.81409	22084.80968	22063.02642	1616.55473	1405.754439	1430.037313	15436.03715	16283.73627	15892.49204	
1883.834238	2141.000228	1704.470002	607.8244497	680.8614646	746.8354674	932.2288207	1122.346753	859.2049902	
13716.30552	14582.95233	11321.9487	2755.695611	2808.746822	3221.54771	11449.2801	12129.50588	10617.60312	
10257.66487	10755.91237	6982.573025	10624.49471	12748.25612	12373.65126	9709.406415	10424.62133	9371.862539	
5635.466117	5758.174581	4528.660198	6164.283719	7306.019779	7649.122721	5797.508715	6229.814705	5682.389294	
17636.86001	15773.35883	11543.93695	12913.98787	14337.84961	14560.52821	15126.98361	13520.29265	13587.02377	
2089.587142	2029.273406	1736.702153	1512.173063	1757.669194	1734.232362	2192.514704	1712.662959	1568.39605	

1.92_286.9845m/z	286.9844669	1.924916667	neg
1.92_294.9508m/z	294.9507643	1.924916667	neg
1.92_301.0169m/z	301.0168513	1.924916667	neg
1.92_354.9720m/z	354.9720126	1.924916667	neg
1.92_362.9389m/z	362.9389074	1.924916667	neg
1.92_370.9585m/z	370.9584791	1.924916667	neg
1.92_378.9597m/z	378.9597126	1.924916667	neg
1.92_393.0130m/z	393.0130324	1.924916667	neg
1.92_422.9595m/z	422.959494	1.924916667	neg
1.92_584.8264m/z	584.8264002	1.924916667	neg
1.93_191.0021m/z	191.0021178	1.933583333	neg
1.93_224.9983m/z	224.9983218	1.933583333	neg
1.93_284.9217m/z	284.9216664	1.933583333	neg
1.93_284.9913m/z	284.9913406	1.933583333	neg
1.93_310.9723m/z	310.9722558	1.933583333	neg
1.93_322.9988m/z	322.9987536	1.933583333	neg
1.93_352.0629m/z	352.0629039	1.933583333	neg
1.93_352.9095m/z	352.9094835	1.933583333	neg
1.93_368.9309m/z	368.930914	1.933583333	neg
1.93_395.0106m/z	395.0106318	1.933583333	neg
1.93_400.9416m/z	400.941586	1.933583333	neg
1.93_430.9262m/z	430.9261533	1.933583333	neg
1.93_444.8378m/z	444.8377576	1.933583333	neg
1.93_498.9133m/z	498.913275	1.933583333	neg
1.95_266.9356m/z	266.9355507	1.945716667	neg
1.95_366.8934m/z	366.8934448	1.945716667	neg
1.95_420.0504m/z	420.0503769	1.945716667	neg
1.95_468.9290m/z	468.9290279	1.945716667	neg
1.95_514.8931m/z	514.893146	1.945716667	neg
1.95_530.7925m/z	530.7924522	1.945716667	neg
1.96_360.9745m/z	360.9744619	1.95955	neg
1.96_436.8794m/z	436.8794383	1.95955	neg
1.97_263.0398m/z	263.0398271	1.9683	neg
1.97_462.8054m/z	462.8054389	1.9683	neg
1.97_647.7934m/z	647.7934165	1.9683	neg
1.97_744.7843m/z	744.7842906	1.9683	neg
1.98_258.9159m/z	258.9158732	1.980516667	neg
1.98_568.8405m/z	568.8404885	1.980516667	neg
1.99_221.0045m/z	221.0045397	1.9892	neg
1.99_433.8018m/z	433.8018364	1.9892	neg
10.00_367.9069m/z	367.9069225	9.9977	neg
10.01_454.8502m/z	454.8502351	10.00813333	neg
10.01_794.7876m/z	794.7876462	10.00813333	neg
10.03_524.8344m/z	524.8344497	10.02501667	neg
10.04_332.8967m/z	332.8967163	10.0389	neg
10.04_966.7156m/z	966.7155896	10.0389	neg
10.05_192.9289m/z	192.9288777	10.0511	neg
10.09_590.8247m/z	590.8246512	10.08618333	neg
10.10_660.8091m/z	660.809141	10.10203333	neg
10.13_278.9712m/z	278.9711642	10.1281	neg
10.15_396.8913m/z	396.8913054	10.15425	neg
10.15_415.8768m/z	415.8767704	10.15425	neg
10.17_208.8250m/z	208.8250076	10.16711667	neg
10.17_544.8231m/z	544.8230601	10.16711667	neg
10.17_658.8122m/z	658.8121794	10.16711667	neg
10.18_685.8323m/z	685.8323033	10.17923333	neg
10.20_328.9039m/z	328.9039456	10.19831667	neg
10.20_464.8788m/z	464.8787841	10.19831667	neg
10.20_513.1225m/z	513.1225341	10.19831667	neg
10.21_449.1740m/z	449.1739512	10.20653333	neg
10.21_701.5127m/z	701.5126898	10.20653333	neg
10.22_358.2602m/z	358.2602117	10.21693333	neg
10.22_872.8035m/z	872.803545	10.21693333	neg
10.23_1034.7023m/z	1034.702262	10.22736667	neg
10.23_339.9118m/z	339.9117665	10.22736667	neg
10.24_640.7487m/z	640.7487251	10.24335	neg
10.25_680.7963m/z	680.796273	10.25375	neg
10.26_182.9001m/z	182.9000702	10.26313333	neg
10.26_966.7156m/z	966.7156034	10.26313333	neg
10.28_944.7303m/z	944.7303016	10.28213333	neg
10.31_544.8228m/z	544.822845	10.3081	neg
10.31_810.5280m/z	810.5279557	10.3081	neg
10.33_220.8491m/z	220.8490994	10.3344	neg
10.33_264.9094m/z	264.9093853	10.33718333	neg
10.36_481.8689m/z	481.8689666	10.3649	neg
10.37_174.8639m/z	174.863907	10.37356667	neg
10.37_483.8648m/z	483.864755	10.37356667	neg
10.38_189.8511m/z	189.8511227	10.38353333	neg
10.39_838.5602m/z	838.5601977	10.39216667	neg
10.40_808.7563m/z	808.7562831	10.40083333	neg
10.41_424.8116m/z	424.8115887	10.40946667	neg
10.41_602.8490m/z	602.8490445	10.40946667	neg
10.42_176.8593m/z	176.8593256	10.41816667	neg
10.43_284.8411m/z	284.8410834	10.42685	neg
10.45_660.8093m/z	660.8093296	10.44761667	neg
10.46_507.2131m/z	507.2130864	10.45966667	neg
10.47_349.9890m/z	349.9890235	10.46831667	neg
10.47_452.2637m/z	452.2636631	10.46831667	neg
10.47_657.1603m/z	657.1603075	10.46831667	neg
10.47_721.2044m/z	721.2044168	10.46831667	neg
10.48_286.8413m/z	286.8413306	10.48043333	neg
10.48_601.0598m/z	601.0598479	10.48043333	neg
10.49_413.0039m/z	413.0038904	10.48906667	neg
10.49_458.0011m/z	458.0010745	10.48906667	neg
10.50_313.0788m/z	313.0787505	10.50116667	neg
10.50_396.0010m/z	396.0009682	10.50116667	neg
10.50_422.8164m/z	422.8163911	10.50116667	neg
10.50_726.8002m/z	726.8001661	10.50116667	neg
10.51_1034.7031m/z	1034.703071	10.50983333	neg
10.51_297.0473m/z	297.0473205	10.50983333	neg
10.52_354.8289m/z	354.8288894	10.51685	neg
10.53_356.8243m/z	356.8242615	10.53493333	neg
10.53_382.7927m/z	382.7927044	10.53493333	neg
10.55_524.8345m/z	524.8344811	10.55398333	neg
10.55_670.8368m/z	670.8368307	10.54533333	neg
10.55_810.5285m/z	810.5284501	10.55398333	neg
10.57_415.8769m/z	415.8768851	10.5726	neg
10.57_474.8796m/z	474.8795702	10.5726	neg
10.58_704.8139m/z	704.8139005	10.583	neg
10.60_149.9368m/z	149.9368478	10.6021	neg

8052.605885	8306.315555	6289.927579	3864.827377	4148.448474	3754.425602	4873.265813	4872.641416	4169.87448	
15349.97056	15798.62465	12349.8784	3938.1354	4404.535399	4120.886925	13462.87456	13760.84361	12361.38177	
6350.660089	6701.584126	4763.538598	6577.887708	8265.479767	8033.991465	6016.921409	6548.699989	5883.172789	
2764.667414	2929.854309	2199.687947	1112.962353	1299.935268	1482.615421	1451.746259	1405.26804	1406.514361	
12616.46934	12756.0953	9676.188005	5099.365095	6020.611086	5696.338506	12316.27851	11446.0282	11122.06209	
1195.779873	1127.062895	1001.81947	1163.226731	1511.497474	1410.390275	1467.561643	903.7432218	1140.236886	
3778.288355	3093.777116	2266.7345	3239.788	3653.461664	3457.601052	3023.539842	3108.732844	2320.953751	
5880.213404	6103.186269	3579.323733	4596.947493	5541.245301	6097.57523	4776.524006	5031.396256	4476.924447	
1604.230305	1624.969126	1284.799943	500.8764198	1023.40827	543.2926281	706.2452635	677.6868019	854.0232038	
2551.154995	2231.339279	2054.707934	3939.328125	3728.157905	3600.626754	4032.354403	2930.411758	2975.824379	
2528.497878	2678.539554	1827.5195	3492.658329	3616.139589	3725.206465	6503.696472	7181.720706	6327.740219	
562.5872873	694.734741	485.4417642	656.1603586	584.1442496	625.8649927	603.1116163	645.6495962	595.8699397	
862.0643645	969.2370692	564.5507529	10.75038702	9.722846699	15.22657191	502.1366947	569.6769085	454.0234396	
1681.348424	1784.675902	1130.131926	2130.255005	2610.737313	2264.597403	1886.046046	1795.297126	1360.122048	
3315.439253	3320.665305	2200.02462	3155.552905	3498.536574	3833.091681	2906.063391	3161.820588	2632.267367	
3563.332244	3699.871377	2391.366212	3886.747391	4224.848767	4484.217619	3271.070316	3208.305771	3198.414752	
3858.347783	3756.530136	2806.154017	3433.188841	3815.858856	3633.849833	3478.588094	3136.371944	2913.483414	
1025.967312	970.3985449	499.2308086	0.001403199	32.31970411	0.001403199	521.6145502	721.6477007	553.1311548	
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2043.657367	2080.667843	1691.165501	1805.806477	2118.567659	2268.044237	1983.780494	1646.656515	1413.919879	
3679.311165	3815.74585	2241.470609	3541.56646	3040.127715	3573.860253	2770.534966	2619.486694	1839.134939	
6318.101935	6552.516376	4736.669138	1629.115111	1985.384396	1763.479743	5927.2438	5306.000548	4660.532976	
2494.331381	1740.85588	1805.104146	1156.86023	1732.210104	1474.439756	1781.394067	979.1243037	1205.929915	
2925.003017	3103.184503	2193.797553	316.2795104	419.2414789	695.104598	1861.091076	1744.365936	1826.265623	
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2283.730395	2334.963633	2049.883924	2207.665008	3019.869181	2415.135453	2196.962089	2090.763716	1717.401251	
1428.032288	1609.807435	893.4231425	1683.029546	1204.148651	1500.402039	1120.572801	1309.881682	1106.303766	
2693.080796	2656.244325	1760.022182	2251.673002	2308.947414	2493.816469	2862.128679	2452.081248	2310.142075	
6262.878615	4569.070599	3687.770783	4577.685377	4630.8235	5092.088616	5472.356137	4444.588824	3986.260313	
2347.460245	2084.129653	1738.984234	2516.609074	2946.090074	2717.464328	3057.437153	2716.501941	1937.452178	
1478.04073	1803.825325	1811.342643	1033.656156	1853.416079	1923.76784	2333.46775	1943.750384	1972.489701	
551.5928077	688.3705954	426.2335837	783.527032	709.0052359	811.0120579	590.4969516	675.0888495	413.3916822	
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23522.73546	20264.66591	16720.83242	18103.54519	19273.90766	19845.48703	21456.59227	15357.48229	17665.80257	
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746169.7987	650601.6896	606099.884	653583.9106	680996.2535	652048.2094	754827.4816	625237.1372	656031.5639	
1361.776256	1340.913785	1046.322692	1478.854592	1882.214523	1728.245134	1645.650123	1511.610372	1279.649979	
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23696.65992	23377.27343	20884.05405	21767.33193	22968.17398	20916.19726	25261.30863	23866.9029	26232.44573	
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374466.9093	359205.9453	361222.3768	353298.2009	362405.1928	358347.2092	412743.3681	376902.7051	381949.5985	
559.7697097	442.4693874	243.7677392	279.4211893	701.1974355	631.2738606	349.0258337	514.576923	122.3356434	
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1895.002539	1351.159049	2177.805768	1210.674989	1766.951875	1133.809722	1523.966321	2110.433153	1450.179283	
787.5325388	678.757845	1024.15894	634.0497658	780.0970287	797.2518371	674.7324822	743.0145314	948.1415668	
17959.34611	17056.97808	17137.72908	17710.39615	20384.84475	16158.12676	21302.68808	20641.16046	21315.43585	
9809.766592	9624.922358	11002.7097	7016.173039	9552.937257	9422.13732	11177.91914	10127.45066	8175.782047	
2839.281134	3096.105946	3021.063642	1287.690574	2410.531269	2054.022529	3934.236475	3219.561381	2179.886898	
4147.513015	4713.912963	4258.584161	1887.733526	1591.752762	1997.830546	4851.348882	3449.847839	1820.082495	
1071.860529	1350.734279	1347.295497	1260.21416	1069.026595	1404.058266	1411.632559	1439.918905	1281.855759	
567.561593	589.1945637	778.2952408	458.5881994	692.2056881	579.8442465	700.5023328	699.226219	644.3189567	
2518.61103	2480.445104	2110.900308	3176.30072	3246.335641	3107.554176	1182.52028	3191.141693	2793.276318	
47832.83156	47090.8295	44801.25211	46493.68653	48853.99754	48310.34572	52001.76756	47919.2221	51292.98316	
868.3262627	939.1954595	1061.335561	1223.526554	1415.329182	1489.213255	867.6972946	1220.182979	925.5556181	
7491.223319	7535.705507	7641.032138	7851.469773	8375.513781	7873.248585	9037.49254	8405.840919	9016.585313	
11570.68629	11872.42663	10399.54969	7809.102674	9264.443041	9478.114671	13230.98045	10256.14531	9328.640928	
6865.482106	5955.926498	5950.563534	9175.303319	9704.934258	8698.809281	8562.290095	5871.36179	9391.269557	
26300.08758	27174.29126	25026.6823	26258.91083	28123.14121	26592.97157	30691.73919	27473.46878	28508.65353	
265194.5476	252805.2686	243118.7859	249281.4656	255895.1182	243481.2311	281358.7825	254784.6616	264935.1535	
15642.86974	15800.19075	14721.50966	15450.18784	16625.83631	15622.69057	17305.51502	16101.2873	16915.41937	
735.5828442	707.2492371	554.7403235	530.9856744	574.669823	554.0315735	822.6551216	626.2688	557.2354137	
4723.003506	5332.791713	3829.15705	4697.852143	6031.127517	5091.041407	5990.764858	4201.770062	4871.668114	
1820.52021	1938.762106	1748.063745	2062.036436	2137.306853	1630.528565	1674.742777	1676.543603	2088.594675	
462.7583273	680.4867882	275.4365475	409.9474547	596.1496944	246.4335419	664.8680189	607.3575629	530.698286	
474.1863553	318.8702619	568.8834892	429.9996801	795.8024588	597.6475611	698.8419689	355.3306808	612.918859	
3904.619884	3081.851041	3719.281475	4194.601577	4544.214194	3774.037853	2963.783502	3327.413131	3931.651726	
4614.576631	5025.476971	5451.15583	4984.725939	6071.374003	4473.336577	5177.593089	5937.551008	5466.315689	
81111.67042	83310.00494	79778.45769	81938.89931	85854.37431	83867.9872	93954.75517	84998.77885	89013.17379	
1079.986425	919.6449007	1011.358106	666.9675225	1504.045203	1141.826532	1467.308175	1237.61274	1721.979283	
2014.318876	2015.312702	1333.783452	706.084287	799.6606616	934.5582035	1538.441005	975.1882477	1292.147612	
1863.055754	960.6340342	1210.936531	498.6991143	748.0911925	560.4028946	815.3888195	968.0423317	827.2980345	
12714.77222	12052.23892	11360.59783	10556.48642	12836.84134	11921.89783	13170.69282	13209.2168	12913.67668	
3393.306152	2674.175475	2560.254811	1510.678905	1813.355996	1115.198793	2157.683608	2521.689588	2131.661815	
328833.3645	331267.5032	317513.9455	322029.1998	348139.26	328510.4416	369468.3853	344307.7979	357791.8898	
6376.102058	6332.719811	6518.232316	5634.462521	6007.261908	6714.808057	7501.306106	7535.371652	6577.670421	
5475.621245	4167.110552	6182.279539	4700.706639	6925.879153	7386.036343	7051.374253	8114.518569	8330.364887	
527.4375568	340.6240767	585.3987573	305.5006289	393.1336023	554.8336623	456.5860342	351.8391495	746.8716325	
334692.3916	333998.4041	325100.6052	328816.095	351197.4307	336192.0376	380588.2833	344056.9577	361898.3557	
102809.2313	103334.511	98639.39863	102418.8096	109269.7518	105036.1467	119927.9494	106177.594	113828.2496	
1693.132808	1760.709486	2581.73685	2164.699325	2060.586194	1997.322725	2731.530576	2564.332399	2532.239661	
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4435.474627	2485.54517	2613.611829	3126.011096	1699.995892	2309.702596	4061.468739	5038.293859	3007.727218	
12619.56672	12311.73598	11063.17607	12429.2213	11753.53325	12191.8202	13123.30679	12527.41566	12701.55194	
6774.339719	6204.676153	6472.062366	6469.807652	6233.470707	6801.343448	6499.757963	6045.641277	5991.27845	
2977.370101	2037.338255	2252.845501	2375.230682	2739.50856	3145.099131	1881.719175	3603.09238	3664.272214	
83.32891342	74.18035565	14.62700358	0.001403199	30.31817148	0.001403199	53.33114024	29.95720053	17.99307414	

10.60_660.8097m/z	660.809653	10.6021	neg
10.60_737.1585m/z	737.1585435	10.6021	neg
10.63_116.9640m/z	116.964017	10.63316667	neg
10.63_344.8000m/z	344.7999754	10.63316667	neg
10.63_492.7991m/z	492.7991404	10.63316667	neg
10.64_946.7286m/z	946.7285718	10.6402	neg
10.66_581.1384m/z	581.1384324	10.65925	neg
10.66_592.8212m/z	592.821233	10.65925	neg
10.67_658.8121m/z	658.8120715	10.66958333	neg
10.67_810.7546m/z	810.754617	10.66958333	neg
10.68_220.8492m/z	220.8491735	10.67905	neg
10.70_313.1813m/z	313.1813495	10.69636667	neg
10.71_185.9261m/z	185.9261427	10.70671667	neg
10.71_479.0700m/z	479.0699709	10.70671667	neg
10.71_533.1206m/z	533.1206109	10.70671667	neg
10.71_726.8003m/z	726.8002532	10.70671667	neg
10.73_358.2602m/z	358.2602044	10.73435	neg
10.73_380.8469m/z	380.8469013	10.73435	neg
10.75_265.1481m/z	265.1481261	10.74601667	neg
10.76_1034.7026m/z	1034.702646	10.76333333	neg
10.76_456.8471m/z	456.8471061	10.76333333	neg
10.77_835.7733m/z	835.7732908	10.77198333	neg
10.79_645.1510m/z	645.150956	10.78928333	neg
10.79_658.8121m/z	658.8120954	10.78928333	neg
10.79_662.1411m/z	662.1411005	10.78928333	neg
10.79_717.0814m/z	717.0813949	10.78928333	neg
10.80_648.8173m/z	648.81727	10.79965	neg
10.80_794.7882m/z	794.7882407	10.79965	neg
10.84_726.8003m/z	726.8003428	10.84081667	neg
10.85_617.8445m/z	617.8445352	10.8529	neg
10.85_703.8420m/z	703.841986	10.8529	neg
10.87_297.1532m/z	297.1531637	10.87438333	neg
10.89_809.0881m/z	809.0880583	10.88813333	neg
10.90_1102.6879m/z	1102.687879	10.89848333	neg
10.90_726.1535m/z	726.1534628	10.89848333	neg
10.90_809.8507m/z	809.8507407	10.89848333	neg
10.91_486.9035m/z	486.9035092	10.90881667	neg
10.92_183.0048m/z	183.0047555	10.91875	neg
10.97_1090.7343m/z	1090.734307	10.96876667	neg
10.97_160.9391m/z	160.939073	10.96876667	neg
10.97_312.8363m/z	312.8363245	10.96876667	neg
10.98_335.0960m/z	335.0959689	10.97913333	neg
10.98_773.1759m/z	773.1758565	10.97913333	neg
10.98_790.1660m/z	790.1660232	10.97913333	neg
10.98_873.1010m/z	873.1010156	10.97913333	neg
10.99_703.8414m/z	703.841429	10.98771667	neg
11.00_726.8002m/z	726.8001785	10.99596667	neg
11.01_160.9391m/z	160.9390832	11.01486667	neg
11.01_725.1582m/z	725.1581861	11.01486667	neg
11.03_209.9192m/z	209.9192262	11.02695	neg
11.03_794.7879m/z	794.787868	11.02695	neg
11.04_617.8442m/z	617.8441953	11.0408	neg
11.04_709.1634m/z	709.1634021	11.0408	neg
11.05_854.1779m/z	854.1778852	11.05113333	neg
11.05_937.1134m/z	937.113417	11.05113333	neg
11.05_953.1247m/z	953.1247495	11.05113333	neg
11.06_297.9036m/z	297.903627	11.06321667	neg
11.06_401.1231m/z	401.1231428	11.06321667	neg
11.09_312.8364m/z	312.8363564	11.08726667	neg
11.09_789.1709m/z	789.1708783	11.08726667	neg
11.10_980.6831m/z	980.6830532	11.09883333	neg
11.11_1034.7031m/z	1034.703068	11.11088333	neg
11.11_209.9191m/z	209.9190532	11.11088333	neg
11.11_592.8212m/z	592.8212373	11.11088333	neg
11.11_635.8542m/z	635.8542039	11.11088333	neg
11.11_767.7870m/z	767.7870457	11.11088333	neg
11.11_776.7224m/z	776.7224371	11.11088333	neg
11.11_918.1904m/z	918.1903574	11.11088333	neg
11.12_1001.1256m/z	1001.125608	11.12125	neg
11.12_220.8493m/z	220.8493075	11.12125	neg
11.12_677.7969m/z	677.7968702	11.12125	neg
11.12_901.2009m/z	901.2008729	11.12125	neg
11.15_160.9391m/z	160.9390651	11.14886667	neg
11.16_853.1825m/z	853.1825584	11.15923333	neg
11.18_1065.1387m/z	1065.138733	11.17601667	neg
11.18_433.3456m/z	433.3455851	11.17601667	neg
11.18_592.8214m/z	592.8213897	11.17601667	neg
11.18_685.8317m/z	685.8316719	11.17601667	neg
11.18_773.1756m/z	773.1756308	11.18458333	neg
11.18_965.2126m/z	965.2126174	11.17601667	neg
11.18_982.2021m/z	982.2020574	11.17601667	neg
11.19_297.1531m/z	297.1531421	11.19315	neg
11.20_456.8463m/z	456.8462739	11.20353333	neg
11.20_790.1654m/z	790.1653655	11.20353333	neg
11.22_854.1780m/z	854.1779855	11.21561667	neg
11.24_296.8903m/z	296.8902988	11.23628333	neg
11.24_492.7991m/z	492.799145	11.23628333	neg
11.24_626.7785m/z	626.7785295	11.24485	neg
11.24_658.8119m/z	658.8118966	11.24485	neg
11.24_966.7159m/z	966.7159196	11.24485	neg
11.26_160.9390m/z	160.9390442	11.25696667	neg
11.27_937.1136m/z	937.1135765	11.26556667	neg
11.28_312.8362m/z	312.8362452	11.28405	neg
11.28_830.7412m/z	830.7412729	11.28405	neg
11.29_160.9391m/z	160.9390564	11.29263333	neg
11.29_490.8040m/z	490.8039505	11.29263333	neg
11.29_558.7912m/z	558.7911893	11.29263333	neg
11.29_898.7287m/z	898.7286691	11.29263333	neg
11.30_220.8493m/z	220.8492569	11.30126667	neg
11.30_492.9906m/z	492.9906047	11.30126667	neg
11.30_767.7871m/z	767.7870962	11.30126667	neg
11.30_980.6843m/z	980.6843071	11.30126667	neg
11.31_954.7601m/z	954.7600587	11.30983333	neg
11.32_609.8093m/z	609.8092654	11.32013333	neg
11.32_694.7657m/z	694.7657088	11.32013333	neg
11.32_716.8054m/z	716.8054485	11.32013333	neg
11.33_1001.1258m/z	1001.125812	11.3321	neg
11.33_918.1904m/z	918.1904265	11.3321	neg
11.35_1012.7186m/z	1012.718562	11.35103333	neg
11.35_415.8769m/z	415.8769167	11.35103333	neg

2308.52406	2203.392289	2467.65859	3877.102186	2219.453048	2743.312203	1989.543656	1963.629012	2231.215236
1071.126983	1447.10615	441.8424446	947.9118933	484.5968889	1116.788581	1188.71407	560.1238155	1101.142486
697.6576097	798.7172074	907.6084288	958.180765	711.8476453	987.730938	738.1467573	731.7697563	1014.80345
1498.11097	1811.804128	1715.319209	1730.350635	1282.30064	1385.440888	1246.896328	1305.412205	1502.035529
37098.86709	36982.4109	38087.14661	38099.99395	39496.78973	35890.47677	40293.44245	37792.29176	42727.36683
1632.103874	2236.082054	1764.516174	2112.913893	320.1746097	1849.303747	1426.31912	1497.164536	1699.156063
9175.584762	9276.802044	7895.030304	7578.734119	9169.61489	8097.799437	9481.783644	9525.998265	9040.395427
2754.089173	2956.995847	3145.951022	2960.615346	2200.735978	3380.380788	2472.207209	2470.570737	2618.361484
14443.50382	13815.44997	15104.3722	13285.44768	11500.56221	14864.02513	15179.1238	15665.91801	15005.91129
2702.164529	1796.308593	2849.688754	2980.228505	2764.914843	3306.783082	2229.025736	4729.898478	2675.819469
1178.306587	1058.679058	945.2250735	1183.817847	1230.520303	1087.456161	1150.819087	1163.155535	1338.87376
636.9370247	456.1505692	483.5358448	640.5029223	689.3764549	643.1115793	619.3120102	624.8167829	585.4010448
429.2986451	231.0646484	194.2141904	243.7834108	347.8390508	224.8263724	237.1683303	291.8803832	297.3836757
7068.915663	6405.046654	5881.832176	6295.29236	6694.814906	6713.739226	7441.519197	6071.102921	6295.606805
1383.67268	1194.700035	832.5996485	927.7688925	1001.377232	1038.111619	1140.857186	1199.478065	593.2051258
7860.975977	8403.799021	6728.605217	6683.275241	7628.818002	6726.135394	8169.669502	6170.021214	6327.338991
12790.9884	11443.84307	12007.50509	12196.47205	12660.51533	12673.65494	13746.35261	12077.34698	12764.27425
882.0029853	699.3644739	528.8731005	514.0351376	1138.105616	557.3309776	1210.77095	678.7024117	764.3752864
1016.838239	793.5753599	674.046028	702.1631388	669.8066097	499.326826	1159.059519	691.6577415	784.2005155
27811.31612	24524.7599	23016.83327	27100.55173	24731.96384	25959.9285	26746.62611	23299.6186	20964.67128
5723.467809	4486.789156	4513.638174	5232.757907	4382.516606	4295.562417	4955.113243	4402.948267	5226.928734
4388.417225	3096.228744	3014.402883	3913.34286	3746.531079	4126.970253	4255.323946	3137.536377	4046.840651
15478.01206	14275.01837	12913.05917	13801.58326	13109.9706	14880.56122	15585.29989	13692.86123	15977.38533
9690.142529	9710.968706	8586.509474	9830.214062	10678.58509	9335.01353	11400.06922	6707.239159	10066.84085
3971.022224	3184.346964	2814.578647	2916.931872	2815.307405	2831.192686	4623.436809	2606.443428	3147.612413
919.256933	986.3910087	1157.697774	855.8870568	1084.694856	765.7565085	1457.95869	1299.574959	752.6238946
1692.956391	1250.518233	503.6802307	2616.726268	1938.887739	1571.928393	432.1689135	493.490593	971.1131101
2480.448078	2771.465729	2110.634985	1113.264175	2436.790047	1989.419056	2752.257493	1056.424431	2360.850976
7041.417533	7215.16986	6442.533349	5916.616924	6554.041588	8314.449945	8299.790486	5407.65501	7166.223276
6711.514202	6697.420875	6021.590233	6245.392975	7509.981488	5804.008212	7090.193964	4749.608381	5596.042826
2459.463183	2007.009532	2830.967858	1562.350545	3694.707292	2776.741396	3091.758059	3175.405096	2534.445615
7735.414273	6054.569588	5937.613086	5386.76057	5190.284776	5494.188844	7356.564881	6826.76147	5887.233131
2560.611363	2342.185941	2284.739546	1671.745397	2174.231714	2420.264146	2477.460834	1466.487946	4173.854448
1754.684415	2248.727678	1718.894057	1356.749226	3382.115529	2290.849603	2886.62876	2584.79809	1815.945151
8752.662513	7715.373993	7848.398533	6184.492054	7343.483827	7602.855019	7943.730137	7509.698814	8517.061098
9432.774268	8577.277838	9422.461064	8338.393987	9887.817145	10874.94389	9229.668356	8123.315578	8915.524579
1178.365961	1242.017316	1129.067498	828.3443476	598.1371012	740.7013438	910.3370182	895.8432018	1044.640463
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14162.9936	13391.25715	10809.77494	12765.51496	14010.89382	14809.03089	16155.23068	14321.33756	13376.78271
46.81097905	117.1006801	183.6509395	24.88655984	71.52796878	179.8675837	29.71262609	63.41881371	173.6811641
483.7478707	520.4722659	561.1653624	430.7914036	529.5090513	315.259012	506.6288968	703.8010342	291.0577277
252.5611618	159.796418	267.7303358	72.29707293	218.7879994	0.001403199	291.2878756	56.81633949	70.7256391
14662.39972	11180.24391	13037.10417	13132.70051	14697.92139	13807.00649	14226.46507	13013.22793	13088.14705
10004.01392	7228.752279	7880.681562	8896.805676	9199.985939	9444.69626	8574.602783	7934.623643	8201.257856
7960.704455	7414.670508	8742.575074	8193.063368	7350.058572	8771.349346	9307.172167	8981.795868	8473.175026
3466.148915	3617.175521	2493.024634	3969.693104	3072.828816	4010.079092	3183.365562	3429.237888	2735.269037
11217.57496	10845.26712	10345.7845	10492.61892	10835.69438	12531.0502	12130.24472	13155.62166	10914.17811
66.01491917	26.4330509	113.4616471	76.29398761	62.94204236	117.552291	36.12866875	36.30030823	205.7039923
6471.781875	4470.403207	5145.832271	5636.636745	4411.550088	6002.655069	7197.599812	5371.096526	5285.31159
374.7515666	382.2204793	502.8771032	311.9604554	412.3906242	497.4226809	383.9427455	453.8585795	640.8198848
3724.718714	4072.590579	2566.042905	3391.896978	2744.997528	2538.877911	3333.714894	2712.516903	3156.547014
2556.796111	2403.891771	3427.159188	2338.615199	2703.18887	3352.238062	2779.338389	3139.409279	4504.900044
8267.552601	7463.107663	7991.659309	8254.357966	8274.103212	8387.015404	9917.547241	8396.939763	8143.113352
8873.158262	8968.331702	8336.600455	7589.061237	8313.864864	8967.08742	11537.24728	9680.389624	9335.842997
10637.01252	12534.74488	11780.459	7721.23512	8744.537845	9271.05097	11750.46159	10654.79814	11217.05178
2286.863598	1744.499999	2264.177746	1579.805981	2616.796811	4492.222142	2785.301507	2159.840553	3842.654996
754.753821	700.9800019	603.4994642	411.8927372	838.6520648	795.6272376	711.0758197	777.5617762	880.8354808
1591.61991	832.0566006	2821.965667	1005.345481	1149.965213	676.3426745	1557.090001	1146.946837	789.1754718
659.6943351	763.0373861	899.5594566	671.8466887	813.5197364	957.0161731	841.7155971	1199.452653	995.8230416
3524.03024	4974.458537	3025.829519	2683.415977	3498.552472	3562.679089	2370.411727	4733.064986	3763.51096
3366.537796	2636.929172	3344.478981	3303.475342	3326.124226	4310.387528	3387.312069	3575.547471	2830.791367
57604.37537	48821.88564	51132.08537	53198.79238	54345.57433	57624.44247	59047.40008	57046.82257	61081.48111
460.1846787	601.955285	459.394354	494.8077535	419.3952498	476.2690155	502.3867792	396.3780346	565.6474893
1930.50951	2443.410604	1582.796112	1402.620168	1547.087053	1576.45829	1402.17761	1676.136124	1126.209155
4106.611226	4248.444174	4148.71383	4358.485978	5137.733213	5148.99647	4077.988814	4375.28543	5376.893985
6769.8045	6603.952153	6588.604046	8356.633194	8374.474094	7392.319176	7601.330634	7770.796982	6753.169265
4386.692108	5129.142707	3779.080098	5352.251405	6557.019916	5913.082291	6838.131042	4083.089933	4714.724867
6946.996331	6350.526267	6792.539817	6801.365195	6732.7484	6695.936808	7064.765082	6168.636688	4707.515173
7589.874958	9177.986345	9444.927909	8198.370169	9769.745619	6578.426891	12193.47066	6756.501764	6511.127409
482.6398301	602.5825347	535.2709063	539.3603681	871.8494221	501.502492	764.1018849	423.8650809	360.7663979
2791.059755	4931.596069	2352.194359	4652.302646	4423.52677	3395.172791	4200.773731	2924.220814	3994.139912
7886.7275	8159.904027	7932.899912	7350.663877	6267.012836	5188.98742	8436.946392	5999.482053	6186.153433
107.1177085	307.3963345	439.7487137	547.1783159	213.5319071	357.5107756	75.95845036	185.8997393	121.7708937
1643.741892	961.674056	1209.327511	1532.960857	2000.728552	914.7515057	1376.224767	1031.123006	1311.853143
6301.173205	7109.446482	6426.890186	5973.403451	7002.044245	3662.948795	5340.143375	5467.276195	7129.401739
3551.526387	3658.022268	3713.529087	4397.02936	4322.057309	5147.804873	4859.744709	3752.127106	4627.250602
7397.504855	6273.27483	6463.107001	6177.73673	6825.435925	7669.753687	7797.894202	5277.774049	7185.060589
2443.770804	2591.105832	2976.064651	1861.620501	3082.022097	3588.867793	3942.90436	3355.894335	3297.465583
7523.555197	6384.20701	7615.918566	7239.170753	9707.278722	5980.25562	9019.882428	6585.904397	7172.090877
4229.027719	4465.338277	4295.872245	3503.538293	3489.321033	3667.052771	5344.804319	3887.334259	3648.574386
6996.515952	4702.32406	4218.669173	3867.589327	5328.953321	4558.632029	5002.22936	5831.669224	4704.363023
88288.73334	60366.7713	61775.04545	53980.08817	57616.50767	61158.81282	76531.65731	83601.90461	64356.80822
997.0034395	807.8981038	1461.372344	937.5632818	792.374265	1246.309994	1343.023642	1123.515676	1447.688403
3323.936351	3682.609378	3483.025997	2697.21574	3111.677366	3601.111816	3299.299714	3924.040983	4254.231437
4524.778788	2928.006968	4098.461138	2395.903646	3967.292577	3878.527463	2105.099256	2694.803391	3468.605684
2672.590791	2348.001079	2038.068429	2153.956787	2205.588115	2295.974539	2657.29876	2185.187985	2645.022737
42187.39031	39566.81527	40097.8799	39895.31297	43794.00021	40802.7467	49462.38354	43450.91601	45606.92057
473083.5604	456905.2348	450834.9042	469097.2317	504637.6213	495161.5049	533858.326	478390.9114	504988.5421
17571.98229	15840.52773	15556.71356	14125.20839	16942.5196	16241.66979	18294.9753	16409.88743	16744.45014
238649.8587	216682.7782	209249.7559	227600.779	232430.51	243651.2563	248281.7421	224559.0966	235619.9828
79.98264308	89.31810601	29.0395357	115.1575973	249.4404964	157.1647223	150.3612624	209.5606956	187.0615011
4753.195187	5215.172432	4059.239694	5534.723049	4489.151635	3846.975668	6572.718727	3174.829629	6103.923972
1558.774614	1609.448218	1448.34919	1232.937769	1141.532014	1542.16597	1731.296312	1668.944848	1862.881579
354600.1059	337519.5749	317174.1311	345155.6688	351389.9846	364435.3662	376365.0979	338972.8638	358140.451
104.6448957	45.56014463	0.001403199	84.55311316	129.9741391	80.01160064	88.84960369	0.001403199	73.33258928
359567.3192	350954.29	344051.5618	346910.1879	370430.253	357192.7225	399793.5898	367560.8179	385665.1388
464870.6642	445920.4147	445890.5878	456018.0252	479951.9228	464533.1776	511397.0552	469936.7729	485911.7984
325342.2763	313160.3182	296971.5906	320533.1575	346339.566	343937.73	347205.0365	321556.4168	334678.9775
716.3872977	678.1090156	565.9990088	793.0914777	642.7147756	599.9838269	913.5406233	489.1476667	742.0246137
3760.514595	3004.939201	2390.896169	3386.759915	2284.11039	2896.502525	3509.23805	2026.550827	2802.881397
8965.327409	8532.910542	8438.400511	9687.599664	9913.61565	10269.72383	10636.52889	6922.659968	10463.86648
6426.273001	6292.131351	4997.927197	5345.903671	6711.083114	5848.79059	4019.742337	4951.123413	4308.254938
1011200.834	952068.2449	929949.242	989615.946	1013491.024	1022961.867	1057297.541	950282.5594	1013756.75
11681.71994	10115.04551	8225.429751	10340.60722	9612.127846	8558.478465	9885.891722	7696.90197	11360.84633
423300.6539	412665.4082	403072.967	418071.0128	433399.8275	437843.8588	460710.2228	422658.6612	449567.1378
2816.297941	1637.337493	320.69445	2524.006038	1559.372343	2779.846678	995.5566378	748.3065862	2583.34064
12691.14158	12052.60183	13103.2679	13440.60864	9732.711596	12830.22187	16321.8391	9643.625656	12490.1176
14794.16847	15592.65333	12526.15266	15221.25566	14147.18665	13115.35452	15805.98796	11921.46201	14458.32847
8341.065353	7697.782209	8079.000187	8409.99109	8536.066892	9852.953404	8382.39944	8230.91693	7721.234139
5588.658562	5886.771876	5892.124452	5237.593189	6019.333573	5673.266838	6114.155345	5416.344356	5605.437582

11.35_616.7494m/z	616.7493736	11.35103333	neg
11.35_835.7738m/z	835.7738278	11.35103333	neg
11.37_660.8100m/z	660.8100129	11.37163333	neg
11.38_1022.7477m/z	1022.747663	11.38441667	neg
11.38_1081.1505m/z	1081.150534	11.38441667	neg
11.38_726.7998m/z	726.7998105	11.38441667	neg
11.39_1065.1381m/z	1065.138125	11.39303333	neg
11.39_426.7583m/z	426.7583116	11.39303333	neg
11.39_965.2126m/z	965.2126444	11.39303333	neg
11.39_982.2025m/z	982.2025464	11.39303333	neg
11.42_160.9391m/z	160.9390603	11.42398333	neg
11.42_200.8590m/z	200.8590217	11.42398333	neg
11.42_553.7968m/z	553.7968164	11.4154	neg
11.42_590.8246m/z	590.8245527	11.4154	neg
11.42_809.8498m/z	809.8497915	11.42398333	neg
11.43_1046.2154m/z	1046.215396	11.43433333	neg
11.43_1129.1502m/z	1129.150166	11.43433333	neg
11.43_912.6976m/z	912.6975596	11.43433333	neg
11.44_1029.2252m/z	1029.225152	11.44468333	neg
11.44_476.8528m/z	476.8527813	11.44468333	neg
11.46_648.8176m/z	648.8175577	11.45843333	neg
11.46_762.7533m/z	762.7532628	11.45843333	neg
11.48_473.2828m/z	473.2827892	11.4752	neg
11.50_1110.2273m/z	1110.227317	11.49581667	neg
11.50_1193.1625m/z	1193.162463	11.49581667	neg
11.50_300.8102m/z	300.8101734	11.49581667	neg
11.51_592.8211m/z	592.8211042	11.50611667	neg
11.52_322.8395m/z	322.8394596	11.51641667	neg
11.52_481.8689m/z	481.8688673	11.52496667	neg
11.52_584.7165m/z	584.7164898	11.52496667	neg
11.53_1174.2399m/z	1174.239903	11.53308333	neg
11.53_160.9391m/z	160.9390564	11.53308333	neg
11.53_332.9222m/z	332.9221967	11.53308333	neg
11.53_567.7680m/z	567.7680197	11.53308333	neg
11.53_820.7116m/z	820.7116113	11.53308333	neg
11.57_450.7802m/z	450.7802305	11.5725	neg
11.60_129.9364m/z	129.936374	11.6033	neg
11.61_160.9391m/z	160.9390717	11.61436667	neg
11.61_658.8122m/z	658.8122151	11.61436667	neg
11.62_1012.7178m/z	1012.717846	11.62293333	neg
11.62_660.8096m/z	660.8095978	11.62293333	neg
11.65_576.7033m/z	576.7033054	11.65171667	neg
11.65_608.7375m/z	608.7374875	11.65171667	neg
11.66_643.8018m/z	643.8017806	11.666375	neg
11.67_684.7359m/z	684.7358671	11.67401667	neg
11.68_426.8341m/z	426.8341055	11.68255	neg
11.68_903.7616m/z	903.7615542	11.68255	neg
11.69_1090.7333m/z	1090.733323	11.69456667	neg
11.69_416.8735m/z	416.8734917	11.69456667	neg
11.69_658.8124m/z	658.8124131	11.69456667	neg
11.70_161.9138m/z	161.9138007	11.70465	neg
11.70_844.7103m/z	844.7103278	11.70465	neg
11.70_857.6741m/z	857.6740656	11.70465	neg
11.71_644.6917m/z	644.6916637	11.71493333	neg
11.71_912.6971m/z	912.6970837	11.71493333	neg
11.72_129.9364m/z	129.9363739	11.72353333	neg
11.73_160.9391m/z	160.9390626	11.73378333	neg
11.73_593.7918m/z	593.7917684	11.73378333	neg
11.74_432.8656m/z	432.8655789	11.74403333	neg
11.74_835.7748m/z	835.7748153	11.74403333	neg
11.79_248.0801m/z	248.080109	11.78693333	neg
11.80_426.7581m/z	426.7580514	11.79721667	neg
11.81_473.2829m/z	473.2829152	11.8075	neg
11.81_526.7781m/z	526.7781495	11.8075	neg
11.82_306.8234m/z	306.8234109	11.81565	neg
11.82_677.7960m/z	677.7960169	11.81565	neg
11.83_129.9364m/z	129.9363923	11.82591667	neg
11.83_160.9391m/z	160.9390709	11.82591667	neg
11.83_433.3455m/z	433.3455467	11.82591667	neg
11.84_425.8128m/z	425.8127559	11.83798333	neg
11.84_458.7908m/z	458.7907877	11.83798333	neg
11.84_494.7453m/z	494.7453214	11.83798333	neg
11.86_417.8218m/z	417.8218155	11.85685	neg
11.86_644.6909m/z	644.6909351	11.85685	neg
11.88_208.8250m/z	208.8250453	11.87733333	neg
11.88_844.7099m/z	844.7098527	11.87733333	neg
11.89_390.8270m/z	390.8269793	11.88713333	neg
11.90_1090.7330m/z	1090.733004	11.90426667	neg
11.90_266.8539m/z	266.8538604	11.90426667	neg
11.90_903.7625m/z	903.7625256	11.90426667	neg
11.91_621.7842m/z	621.7842298	11.91278333	neg
11.91_661.7788m/z	661.7788376	11.91278333	neg
11.92_1012.7177m/z	1012.717736	11.92471667	neg
11.92_332.9223m/z	332.9222747	11.92471667	neg
11.92_400.9096m/z	400.9096002	11.92471667	neg
11.92_723.4976m/z	723.4976208	11.92471667	neg
11.92_912.6972m/z	912.6971687	11.92471667	neg
11.94_433.3456m/z	433.3455728	11.94355	neg
11.95_622.7088m/z	622.7087558	11.95381667	neg
11.97_160.9391m/z	160.9390679	11.97435	neg
11.97_454.7235m/z	454.7234532	11.9658	neg
11.99_838.5601m/z	838.5601265	11.98636667	neg
12.00_980.6840m/z	980.6839642	11.99625	neg
12.02_160.9391m/z	160.9390691	12.01675	neg
12.02_609.8089m/z	609.8088931	12.01675	neg
12.03_458.7909m/z	458.7908595	12.02703333	neg
12.03_644.6911m/z	644.6911195	12.02703333	neg
12.03_663.8471m/z	663.8471356	12.02703333	neg
12.05_222.8409m/z	222.8409276	12.04933333	neg
12.05_708.7354m/z	708.7353982	12.04933333	neg
12.06_160.9391m/z	160.9390789	12.05783333	neg
12.06_189.8511m/z	189.8511378	12.05783333	neg
12.06_248.0800m/z	248.0799817	12.05783333	neg
12.06_374.8109m/z	374.8108843	12.05783333	neg
12.06_480.7951m/z	480.7951332	12.05783333	neg
12.06_699.4978m/z	699.4977751	12.05783333	neg
12.07_631.7193m/z	631.7193109	12.06805	neg
12.09_238.8359m/z	238.835885	12.08511667	neg
12.09_432.8653m/z	432.8653478	12.08511667	neg
12.09_822.7268m/z	822.726791	12.08511667	neg

1549.115251	1678.788815	2184.642286	1154.895997	2292.710577	1930.716225	1993.254043	1791.661001	2165.276779
7189.973159	6555.477577	7660.8894	6882.546113	8712.584908	9027.062834	6417.939275	5457.852604	6873.986248
3328.579444	2720.476569	3553.135057	2967.910496	3317.261508	3151.6286	2466.081307	2886.021214	2990.361615
423844.0061	408060.6075	386132.8392	411356.2444	409222.7809	424457.6029	433473.0991	392458.4666	409525.8722
4273.986902	3343.313929	3439.12881	3765.074309	3573.887041	2988.129611	4416.308229	3758.440765	4387.604763
10084.52714	10692.4561	10451.99618	9978.264199	9058.737793	11107.13368	14067.77764	10309.29877	10485.28839
19804.59577	17865.8117	19024.39685	19019.5234	18542.85066	18499.47458	22806.61793	21061.57233	19738.94246
1180.894471	962.2264037	1387.568907	1008.250457	1227.027533	1251.325259	1245.866786	1493.404612	1294.6491
11308.02109	10107.92657	11300.6588	10230.4771	10601.08227	9488.490593	13318.82537	9859.590339	11713.58758
17877.6286	16322.89097	14952.98694	17699.78186	17318.25773	18002.57578	20916.51275	16758.4295	17296.30245
264.8389603	197.4052375	614.5234798	228.5066154	328.4035304	590.813669	450.8572078	826.415251	404.169022
241.183877	325.2979637	290.3467457	355.0147765	333.8269155	314.1713831	517.81778	433.0619637	295.8268214
1066.32618	1087.207503	1461.066314	1297.82589	977.4090321	894.858236	1398.335953	1144.150917	854.8347981
7718.959305	8281.545239	9289.899312	7974.912898	8221.593965	8238.252231	10151.43349	7971.598102	8260.523656
3262.389312	3638.204028	3855.208466	3875.626776	2244.030583	3474.498775	5584.672308	3906.100747	3211.6262
14322.42872	14597.03177	16107.72929	12380.03252	12932.36053	13215.71821	18160.1487	12126.10294	14509.41399
18015.40371	18379.85603	18874.9588	17157.68324	16684.43757	16721.562	18974.27879	18533.72168	15429.02641
5238.651039	4205.184746	5277.27461	5248.489855	6362.791422	5940.905179	10108.08362	5843.897477	4634.296765
10484.77835	10475.01354	11403.52817	9461.661349	9507.59569	9440.525713	13287.66765	8826.440771	8419.338523
3133.402189	3431.761448	3717.736064	3064.022594	2987.665753	3852.092257	5935.298544	3925.751748	3000.295855
1125.205864	975.6370114	1446.860961	488.7423024	583.8223464	1155.444188	2528.71744	1845.50231	1700.35417
365369.9193	346589.8129	337585.2135	368325.3861	385862.2663	382538.2077	404458.2859	359477.0029	394673.6094
1979.603812	1884.452983	1703.890635	1329.676724	1286.189483	1212.94696	2124.426015	1708.110988	1795.07936
13168.33397	14808.55561	12153.79388	12135.69318	9986.504481	11907.03804	16248.75286	11367.86789	11944.86545
10743.93364	14366.27254	12780.95608	11474.36117	11795.39336	9651.389779	13479.20609	11750.92443	13932.51606
1440.596914	1533.942775	981.0479319	1362.501122	1088.612491	1335.827956	1913.019806	1259.768844	1460.561075
2387.82532	2548.321736	929.1792607	1650.845164	1202.637659	1553.010453	1921.133874	1804.003258	1346.33961
493.0648195	966.4172072	469.6277252	562.1356095	347.3054466	481.3466428	442.9508437	661.1310067	997.5707777
8811.857898	8102.359738	8409.656704	8116.891159	8570.533096	6749.552729	11016.165	8611.617053	8263.095556
1233.792851	1248.769764	689.3541418	954.3588938	712.5622429	1143.661878	861.4562673	1034.87505	1282.861951
8527.958342	7418.333425	5212.009707	5824.035252	6101.965748	5623.990092	6585.510473	4931.61233	6367.941688
261.7517952	146.5744004	184.9248203	576.5936503	310.1967952	212.8756874	177.524023	303.7080408	147.0660283
2094.878853	1860.259401	2206.366858	1724.949907	2343.886819	1855.059152	2395.05309	2042.318241	2344.500392
1727.655432	863.5936501	1217.332027	1315.020155	2027.906362	1231.730119	978.0905758	1344.159431	1151.506177
2851.632283	2181.39362	1742.345155	1624.994675	2688.474205	917.0907593	1449.187187	1728.328629	1815.426806
3300.664408	3208.313169	3427.831235	2842.169038	3313.502316	3634.985521	3732.984194	3191.972998	4602.593547
366.3074646	300.1841172	310.2601511	239.5408296	300.8779105	247.0288106	469.4436619	498.6920165	364.805641
0.001403199	170.5681129	31.19696883	34.53114593	85.31860543	117.7540087	384.0962741	115.4087411	248.2033227
3131.401963	2451.84685	2208.830705	2059.151538	3047.823328	2570.735747	3320.644335	3845.965604	3958.743846
7837.785719	8881.706001	6695.846531	8458.139101	9533.425791	8164.849485	10851.59711	10521.86575	10685.65212
1646.829074	1787.409883	1525.116783	1481.350804	2845.725429	1496.092222	2437.315319	3056.282013	2301.819468
1957.871453	1060.06948	1200.711669	2566.36536	2282.176045	1802.866546	1594.214527	2784.878068	1383.814732
1997.979521	1690.618139	1262.603693	1697.688277	2020.358156	2397.022678	1769.938859	3251.203468	2077.023083
2620.799927	1475.486902	3194.51005	1722.462504	3167.507344	4179.061168	2223.552973	3526.885754	1536.77476
1864.519044	1301.69396	573.3008732	1969.403004	1602.550735	1122.51307	748.9129321	1103.428714	585.7456891
1851.712771	2143.117158	1998.300356	1907.217722	2090.525514	2154.143932	1822.252452	2237.616016	2206.782341
7974.369799	7947.723232	7546.230229	8861.553388	9961.073093	9444.379403	8627.530261	11151.47538	9432.357889
10574.94059	12111.26292	9336.117198	7832.199673	11215.37328	12885.11467	6265.958078	9665.4917	10744.71327
1563.746432	1604.777801	1369.102169	1030.297025	1470.630859	1557.804992	1198.877143	1382.680305	1624.843815
2891.162981	3974.239843	3529.748958	2338.969505	3220.306074	4150.168192	1512.756465	2909.155878	3200.339254
487.8584849	575.6628433	512.2739802	603.131727	600.1677949	450.6694401	580.5032183	419.9488659	688.5351431
6266.584365	8589.747919	7156.562608	8467.795523	7181.014772	5937.972275	4556.602324	4528.344238	5237.594572
7008.926914	5806.235343	3235.728723	722.1425792	1803.956917	574.7642474	2043.706692	1397.582291	1679.579473
1805.609317	1747.723294	1428.546357	1527.620126	2333.082325	2599.686671	2090.756515	640.5811129	1718.973875
11010.63702	12644.60077	8283.615107	2916.339199	11417.40606	12914.13643	10733.649015	10546.38622	12761.77075
329.2606319	511.4380641	308.5822117	259.5744822	300.9878274	228.0914505	270.4812076	187.1548834	305.3830406
377.7007586	827.1212951	745.9324586	465.3853392	942.7874072	588.2301103	617.4501066	1041.702479	868.2723793
1184.512192	1494.18139	722.9862056	1644.467986	1694.026379	1646.725631	823.587677	691.6961654	1406.56556
970.034873	1132.049016	711.2681964	932.8084091	882.8041215	685.8266732	597.1640261	667.2426357	1063.899851
12098.49533	13337.42821	9275.875833	12035.06243	11249.84714	11526.59886	13834.19308	10056.47595	12038.18977
567.5426674	420.8388256	433.891197	534.5759695	548.2726033	487.2942638	953.1571341	668.129945	638.5610267
2274.419699	1838.521714	2203.234371	2744.932491	2786.441521	2515.999775	3650.567692	2581.714368	2708.107104
5457.814968	4069.051657	4606.64677	4813.72267	4742.417422	5255.717952	6431.833448	5083.914473	6447.350949
2073.083178	1585.673048	1678.699471	2333.356929	1875.863591	2066.539754	2917.409496	1839.090008	2536.34115
3256.886706	3308.058475	3251.751838	3164.202444	3556.744024	3724.84	4177.89766	3927.694898	4235.605478
1964.787187	1673.732771	2165.343477	2689.784053	1474.148336	4813.943689	3951.234205	3446.421916	3416.995559
151.4421283	95.28978594	229.4966026	108.3616043	118.9993124	117.4784729	181.4712705	142.7964935	159.1095618
156.9230357	218.1281774	648.1934711	71.84414696	120.8917069	243.2210472	323.5235666	243.1527729	500.6534182
1250.937536	838.2539924	1623.691563	1461.840249	1366.510275	1863.176136	2808.983647	1906.749138	1964.19101
200.2480438	142.6278517	257.3306713	0.001403199	115.7619847	202.7473616	0.001403199	184.1013565	90.34447826
912.7687796	873.7165591	1542.931583	362.0898729	1483.12061	1264.757899	1118.601785	933.7939383	1176.542591
2021.032934	1945.018918	2624.44246	2236.019562	2667.271671	2927.499872	2474.320064	2128.603932	3092.478521
1801.442049	1220.876524	1966.227744	1776.957213	1827.798326	2624.323834	1970.592045	2156.130472	2063.231365
1381.809846	1421.542703	1830.850495	2432.908083	2016.578396	3720.889186	2674.472749	2059.025915	1736.360739
492.595621	594.676812	424.2082123	528.0737023	683.0283664	521.420666	528.0480198	271.9805355	467.6592055
22310.46458	17994.4938	20439.48209	25582.16542	21290.83553	23342.17776	21509.42869	18998.82164	22309.61868
908.7344022	964.3066581	471.5096752	1441.846153	1305.831458	821.2998832	1155.438466	772.5662689	1065.756846
6139.34207	9023.55824	5417.455232	7954.68139	6391.0358	4423.989213	6049.5749	5844.931183	5626.237555
1017.676595	1253.380189	1058.336279	1240.021021	1361.589227	1129.621076	986.4125515	910.8476293	1171.244962
7422.836359	8360.42707	5729.97891	8639.10107	8108.91583	7210.986646	5207.147316	4631.203193	6006.814736
2928.464969	2678.156346	2634.084709	2855.739158	3652.661114	2393.695346	1480.275869	2513.917182	4132.095137
1713.609413	2629.215577	1828.117004	2538.389329	1923.615319	1754.839926	1075.658215	1113.232826	1453.277617
9748.958001	11463.80103	8507.255709	11247.74947	10285.08201	6670.275462	9118.810163	6703.158564	8292.445166
2102.864031	2328.811786	1896.516605	2263.202084	2618.161063	1403.346213	1839.709213	1542.22156	1998.369518
2508.106055	2800.871397	1734.683731	2517.429495	2699.862284	1811.64862	1911.266121	1709.222206	1638.648261
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18951.31591	17900.57702	18646.42296	18509.98046	21112.41304	19090.91682	21581.79786	19992.16696	22332.57203
1211.072452	1600.25812	1608.996219	1888.086253	2024.048263	1391.858925	1408.151089	1517.644295	2135.689403
1449.090048	2365.242227	2609.827415	2537.079953	3846.00479	1893.65844	2254.283833	2158.527576	4735.807813
289.0973764	150.2421458	440.3235903	235.0671922	192.6357059	55.2375149	87.52538836	123.2859898	642.2897912
928.2214946	960.7198235	1284.618116	863.642473	1662.039383	849.7029363	681.5814844	805.4267236	1948.151745
2874.407135	2122.803177	3746.584619	655.7497535	2118.312002	618.4381189	2862.532412	4278.354979	2951.226326
22624.13581	16647.07115	18645.73104	19395.25185	19640.649	21842.0844	19254.68716	18025.10391	23728.72025
90.57378233	94.86847239	381.6029323	139.7473634	62.67893565	50.66290052	0.001403199	88.55267149	137.9685504
18253.54914	15310.30395	17249.71924	18230.02546	21678.01747	18359.3332	18332.72827	18527.24093	17057.82574
3018.272069	3013.069767	3843.342832	2879.494036	3594.389262	3026.219815	4008.100817	4019.288913	4751.028643
3722.325662	3500.437657	4562.326728	4957.285443	4837.903435	4607.430476	5936.559869	6442.608208	7535.594662
3490.273939	2647.263144	3362.988398	3310.091984	3187.823476	3022.512501	5010.566595	4001.219699	3103.35025
308.2644358	419.2088088	486.9826432	293.3814157	485.3002118	367.7541436	708.2554484	487.8255745	424.1457615
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175.5408748	267.9329598	732.4109271	473.959297	917.4322472	275.3325879	278.5194119	113.5606537	205.7234898
1057.54916	1036.410367	854.2907379	1096.025673	1105.104177	924.723113	1129.403474	1266.782602	963.9347622
508.7838526	507.0597351	509.6917028	276.704346	280.6231647	374.3898404	1136.721437	674.8838978	333.7889568
1170.007373	1381.953505	1665.771032	1231.946943	1474.218792	1836.450119	2326.354374	2549.415498	1538.117885
1253.111637	1088.070577	575.8820698	1503.438126	570.351147	1336.561854	2119.470661	879.5240793	1074.214863
1143.504662	1902.629544	1271.917234	1035.574631	1682.504602	1449.052786	3841.494017	1345.823433	2057.934903
2812.629122	1860.754603	3928.241134	3720.079007	4193.381607	3225.019963	3075.994425	3228.932404	4218.400911
303.9463424	322.6974292	173.7053483	533.6736359	396.4769134	372.3602534	144.3572404	400.2523441	274.8782054
3238.209444	2541.890778	2300.454989	2546.527212	2285.326134	2198.670898	2718.891573	1501.527218	2394.098114
4346.673941	4087.129586	3812.30552	4417.134926	5157.751538	3612.317328	4178.77654	3471.154778	3579.388254

12.11_374.8108m/z	374.8108182	12.10555	neg
12.11_648.8175m/z	648.8175314	12.10555	neg
12.12_562.7318m/z	562.7318473	12.11586667	neg
12.14_417.8218m/z	417.8218274	12.13633333	neg
12.14_526.7779m/z	526.7779035	12.13633333	neg
12.14_528.7750m/z	528.7749539	12.13633333	neg
12.14_898.7285m/z	898.7284579	12.13633333	neg
12.15_130.9443m/z	130.9442629	12.14656667	neg
12.15_426.7577m/z	426.7577173	12.14656667	neg
12.16_160.9391m/z	160.9390747	12.15853333	neg
12.17_538.8036m/z	538.8035963	12.16706667	neg
12.17_712.6783m/z	712.6783085	12.16706667	neg
12.18_322.8395m/z	322.8394532	12.1804	neg
12.18_903.7614m/z	903.7614134	12.1804	neg
12.20_494.7448m/z	494.7448289	12.1991	neg
12.20_663.8469m/z	663.8469345	12.1991	neg
12.21_380.8468m/z	380.8467672	12.20941667	neg
12.21_473.2828m/z	473.2827831	12.20941667	neg
12.21_776.7226m/z	776.7226094	12.20941667	neg
12.21_971.7483m/z	971.7482983	12.20941667	neg
12.22_526.7778m/z	526.7778062	12.2214	neg
12.22_593.7919m/z	593.7918861	12.2214	neg
12.24_426.8341m/z	426.8341184	12.2419	neg
12.25_621.7837m/z	621.7837028	12.2521	neg
12.25_698.7062m/z	698.706223	12.2521	neg
12.26_160.9391m/z	160.9390869	12.26416667	neg
12.26_350.9285m/z	350.9284698	12.26416667	neg
12.26_844.7095m/z	844.7094532	12.26416667	neg
12.28_640.7479m/z	640.7478686	12.28461667	neg
12.28_944.7309m/z	944.7308598	12.28461667	neg
12.30_327.8524m/z	327.8524294	12.29668333	neg
12.31_380.8467m/z	380.8467127	12.3052	neg
12.31_903.7621m/z	903.7620806	12.3052	neg
12.32_160.9391m/z	160.9390718	12.31543333	neg
12.32_374.8108m/z	374.8107508	12.31543333	neg
12.32_604.7945m/z	604.7944542	12.31543333	neg
12.33_248.0799m/z	248.0799413	12.32566667	neg
12.33_594.7654m/z	594.7653773	12.32566667	neg
12.33_643.8027m/z	643.8026543	12.32566667	neg
12.33_740.7694m/z	740.7694491	12.32566667	neg
12.34_458.7905m/z	458.7905418	12.3359	neg
12.35_349.8344m/z	349.8344084	12.34783333	neg
12.35_876.7438m/z	876.7438201	12.34783333	neg
12.37_160.9391m/z	160.9390541	12.37125	neg
12.39_1012.7176m/z	1012.71757	12.39346667	neg
12.39_473.2828m/z	473.2827658	12.39346667	neg
12.40_322.8154m/z	322.8154015	12.40346667	neg
12.40_893.7325m/z	893.7325327	12.40346667	neg
12.40_980.6839m/z	980.6838578	12.40346667	neg
12.42_573.7675n	618.7663029	12.42398333	neg
12.44_808.7567m/z	808.7567348	12.4359	neg
12.44_835.7747m/z	835.7746985	12.4359	neg
12.47_767.7878m/z	767.7878106	12.46835	neg
12.50_433.3454m/z	433.3453867	12.49738333	neg
12.50_446.8371m/z	446.8370903	12.49738333	neg
12.50_494.7445m/z	494.744491	12.49738333	neg
12.50_594.7652m/z	594.7652461	12.49738333	neg
12.51_121.9440m/z	121.9439943	12.50595	neg
12.51_223.0285m/z	223.0284536	12.50595	neg
12.51_395.8397m/z	395.8396519	12.50595	neg
12.51_480.7960m/z	480.7960386	12.50595	neg
12.52_160.9391m/z	160.9390564	12.52463333	neg
12.52_237.9166m/z	237.9165665	12.52463333	neg
12.53_379.1564m/z	379.1564041	12.5349	neg
12.56_432.8654m/z	432.8653972	12.55815	neg
12.56_686.7544m/z	686.7543933	12.55815	neg
12.57_160.9391m/z	160.9390683	12.56671667	neg
12.57_442.7982m/z	442.7982244	12.56671667	neg
12.57_825.7459m/z	825.7459289	12.56671667	neg
12.57_980.6845m/z	980.6845424	12.56671667	neg
12.58_238.8358m/z	238.8358139	12.57695	neg
12.58_356.8242m/z	356.8241601	12.57695	neg
12.58_631.8135m/z	631.8135147	12.57695	neg
12.58_689.7720m/z	689.7720066	12.57695	neg
12.59_238.9129m/z	238.9128962	12.585	neg
12.60_206.8978m/z	206.8978063	12.60198333	neg
12.61_699.8009m/z	699.8008609	12.61216667	neg
12.62_138.8602m/z	138.8601658	12.62065	neg
12.62_558.6640m/z	558.6639917	12.62065	neg
12.63_698.7064m/z	698.7063801	12.63426667	neg
12.65_244.9083m/z	244.9082793	12.64618333	neg
12.65_526.7777m/z	526.7777015	12.64618333	neg
12.66_730.7399m/z	730.7398639	12.66318333	neg
12.68_578.7028m/z	578.7028446	12.67523333	neg
12.68_657.7374m/z	657.73744	12.67523333	neg
12.68_757.7584m/z	757.758391	12.67523333	neg
12.68_766.6938m/z	766.6938125	12.67523333	neg
12.69_161.9433m/z	161.9432514	12.68546667	neg
12.69_442.7984m/z	442.7984133	12.68546667	neg
12.69_480.7959m/z	480.7958686	12.68546667	neg
12.69_557.7395m/z	557.739459	12.68546667	neg
12.70_121.9440m/z	121.9439657	12.70418333	neg
12.70_246.9053m/z	246.905284	12.69566667	neg
12.70_432.8655m/z	432.8654769	12.70418333	neg
12.70_612.6801m/z	612.6800649	12.69566667	neg
12.70_689.7714m/z	689.7713522	12.70418333	neg
12.72_433.3454m/z	433.3454378	12.71786667	neg
12.72_473.8560m/z	473.8559645	12.71786667	neg
12.75_160.9391m/z	160.9390653	12.75476667	neg
12.75_630.7191m/z	630.7190537	12.75476667	neg
12.76_265.1479m/z	265.147891	12.76415	neg
12.76_446.8371m/z	446.8371477	12.76415	neg
12.77_423.7389m/z	423.7389112	12.77263333	neg
12.78_351.8314m/z	351.8313736	12.78108333	neg
12.79_160.9391m/z	160.939067	12.793	neg
12.79_657.7376m/z	657.7375607	12.793	neg
12.79_844.7098m/z	844.7097593	12.793	neg
12.82_186.9198m/z	186.9198208	12.81851667	neg
12.84_160.9391m/z	160.9390869	12.83713333	neg
12.85_442.7984m/z	442.7984117	12.85075	neg

2048.878055	1580.818891	1509.285459	1947.349358	1852.55091	1727.786969	896.1976996	1839.826982	1911.664045
3164.188673	883.2351707	2057.62858	1480.192841	1905.195666	771.2764783	1482.966471	1080.332165	0.001403199
3685.018135	2410.506399	2200.624177	2123.320955	3479.128909	3148.392822	1318.355063	2497.463701	2524.055881
4140.853755	3768.887165	3111.088689	4025.464388	4141.082436	4043.435005	2651.524808	3434.267255	3410.923612
1655.411783	1655.314733	1714.944588	1410.738162	2297.944729	2260.84226	1070.443077	1470.194913	1567.067402
1184.960333	824.459349	540.0242284	1112.252767	1533.736145	1206.537746	696.0783661	782.4187104	1085.254259
9257.584609	11198.68498	7877.173532	10717.55708	8103.319225	10747.5069	8934.154379	9604.324501	8705.964592
558.5230631	354.9398692	396.8743301	357.9936359	543.3249262	431.3274684	275.5598851	499.5781139	388.764493
2635.31012	2447.638812	1916.166442	2761.27057	2973.0206	2184.380817	1259.836354	2019.340179	1812.412166
183.3658628	216.9123933	732.0868836	270.6442446	1160.308016	312.9247368	199.0071952	545.7374417	290.9871967
12322.78875	11562.90184	9829.010893	12159.59433	12871.61267	12561.79184	10057.15083	10451.41712	11533.82505
3390.440691	2465.296863	2295.42387	4447.180747	3602.363098	4498.021517	3107.168256	2980.624981	2656.233001
1477.046587	1539.568873	1728.506754	1657.289129	2090.157066	1889.267399	1775.619223	1787.946968	1784.102714
13534.33017	11363.52509	10347.8762	11730.89571	12695.85146	11300.75622	11277.92891	10773.44025	10956.99385
4443.368296	4542.513809	3680.878333	5431.922076	5116.567797	5332.419924	4682.056505	4501.785472	4923.181718
12146.97938	8607.197717	7521.960768	8448.789762	9849.506855	8435.862004	7722.209245	8643.874222	8751.670163
1990.787911	1827.379363	1558.266403	2235.750346	1821.37999	1977.128145	2424.029495	1885.112877	2438.812547
2003.964274	2256.271514	1723.894851	2432.306683	1888.793456	2135.458591	2511.759984	2828.27484	2702.466674
117035.9667	114500.6796	105740.7723	133634.2819	130407.8679	138762.8243	136896.5135	119454.2154	128655.8486
8258.737472	7457.267575	5401.948035	7210.158716	4898.290211	10031.23838	9648.784323	5582.729321	9886.338485
3159.536421	3459.672853	2780.268358	2373.939832	3100.810984	3514.500224	4507.399345	3477.522766	4505.397279
2097.611238	1831.364944	1707.563067	1839.352623	1394.135953	1227.72316	2365.110078	2077.296443	1202.273715
3374.32809	3473.833325	3537.998098	2687.124836	3187.470125	3898.26529	3271.604544	3366.544408	4147.622855
3260.725104	2962.853093	2051.749777	2219.803017	2887.544818	3254.586912	2999.087402	2331.853408	3210.076625
7048.62749	7322.208418	6545.06002	6331.150511	5105.135583	8019.806526	6492.705444	7278.28408	7510.918922
0.001403199	66.62370168	120.3743356	42.01855	170.3049063	97.84894516	248.8810667	110.7509911	251.5558053
846.4909294	901.7472294	694.4915589	539.8553992	779.851789	934.429976	721.921986	867.2690011	1482.275858
16325.27472	16389.87948	14329.6287	17858.81197	15609.6565	19747.56264	17497.13386	15622.83767	15620.5477
304794.3317	296663.4599	291190.2714	323243.2306	326650.7407	343203.9768	330478.0707	306256.0101	332620.0016
248892.0962	235265.6256	210670.4062	240241.5348	217379.3561	241135.0169	251813.3491	226146.6944	237134.806
441.6593529	866.5064022	868.9347498	429.8402645	760.9730804	818.0686645	535.9833127	753.7839322	897.8226753
3053.904049	2640.164375	3603.269878	3151.84355	2300.15197	3419.055122	3486.621556	2972.753929	3219.074298
10903.88858	9113.411819	12519.85757	8299.920357	8943.947234	12544.21475	8325.209096	11510.3001	11223.25789
150.3050573	139.6818055	907.344339	171.2878386	534.6664541	217.4464226	45.43373543	216.2212769	167.3635508
1419.267096	1572.947912	2079.052502	1398.656938	1604.936235	1849.260883	936.7453879	1415.636434	1381.699352
6357911.4131	616329.7325	594644.3884	628616.5313	643495.8734	645829.6799	682085.5624	652474.7269	669381.9913
363.8017126	537.4502931	862.3339815	472.8146139	398.555231	416.7834959	337.0830192	562.6345421	308.2342097
2011.672061	2208.720322	2961.249607	2294.186264	2277.825635	2114.354224	1074.805688	1584.751241	2334.707241
1689.70154	1068.748196	1337.25742	916.0855737	568.287457	1836.570773	1513.257726	549.8069611	800.2826637
501349.1341	468754.2054	450651.388	480183.3233	495108.4046	506325.6333	522948.7443	478542.8307	499128.9917
3779.814128	4283.688931	4647.892172	3092.104502	4009.628712	4978.766616	3576.410381	4208.391944	4182.993614
1397.772372	1030.739529	2112.724161	859.5203095	1192.75816	1542.067519	1050.983974	1247.484429	964.4210723
378604.5376	350547.6396	334599.0971	357777.2385	352287.2423	370216.6914	384738.1945	344168.833	380268.0059
138.7257575	208.8154508	187.6251296	268.8807967	707.871024	178.6572303	336.7638297	184.414814	170.3665652
12941.67044	9659.528422	9172.885842	10008.28143	11640.10387	11537.61753	13702.98671	10139.89359	11528.09554
930.2795344	812.3873017	900.4076169	827.915869	1063.36348	1307.971638	2576.234462	725.1141502	1070.369428
786.0914216	731.4437893	707.9981263	939.3265891	687.3763982	816.2426938	907.0891854	851.2927043	414.1049776
3061.788277	3917.029269	2447.631853	4093.86264	2086.694297	2509.437995	4995.64612	2960.06373	2181.393433
9214.05841	7293.888953	9098.966268	11263.32917	9440.810794	11023.0545	10678.257	7074.833801	7835.677606
664317.5037	652339.8999	646224.2154	710000.0609	720100.0678	730753.0432	750471.4767	678539.9103	723818.5517
463535.2627	432749.7487	414103.0226	442759.5707	449783.5286	463770.3488	478203.2905	431702.5724	459888.2765
11267.56333	9420.586787	8734.612025	10858.87081	12670.66469	10383.20823	10295.96399	9209.275242	11781.97148
67654.85669	62356.41622	58559.10315	63163.66516	64416.39899	66370.58345	66641.3302	64599.76193	64825.74098
1920.637961	1679.229857	2101.849183	1744.166662	3032.996994	2423.122597	3644.969901	2593.506062	2668.916617
2327.508983	2096.74944	2305.166682	2345.866648	2706.904825	2353.130826	2960.876714	2495.751223	1972.742041
4656.97486	5200.515221	4509.730979	4149.554723	4957.610431	5018.95788	4668.881743	5485.342676	5958.927892
6207.662144	5455.740695	6494.439725	4886.033501	4963.769263	5331.4777	4452.234843	4781.380303	5086.391319
212.4481978	301.6149441	210.7441617	241.0627234	266.7999166	192.7278414	214.212148	251.2418726	116.8708445
1234.545746	1015.191809	886.9979763	1202.503429	584.3537935	411.3527675	786.7863931	739.5757313	673.449663
2621.971081	2377.645608	1850.315787	2760.320583	2527.885275	2163.22972	2161.01755	2542.927612	2077.199915
7204.559097	6951.704036	7318.997283	7748.422332	7399.098436	7919.036885	8970.527925	6926.354374	8115.211786
340.3772127	115.6437047	228.2662977	201.1923073	169.6575582	240.2207584	483.546463	329.4260597	322.1049799
2064.62728	2015.936771	1686.635835	1811.094247	1922.047642	2194.076668	2044.140148	2073.058614	2419.694695
3842.109435	2465.146732	3130.55907	1910.456161	1722.05498	2073.436081	2413.101914	3937.696845	2602.17784
3893.34483	3281.275532	4038.201801	3261.6061	1804.719531	2473.550429	3070.081916	2901.213731	3380.830187
60103.56077	59032.86035	58637.90173	65022.85989	56765.49931	64921.27127	67497.69909	62219.68497	60538.28102
168.2663458	230.4772369	740.9745418	136.7663143	108.9042386	54.44678461	144.1285555	542.4888039	306.3823499
1910.751522	2118.008251	2395.871284	1917.823299	2008.370182	1486.462161	1697.873032	2165.947502	2595.652322
2343.772685	2008.200565	2027.986943	2280.890092	1268.58942	3193.830546	3097.852842	1991.607059	3386.029445
3430.906496	2270.303669	2771.669128	3233.505382	2333.397261	4752.056568	3768.767645	3653.968124	3986.497712
581.8980017	583.364876	819.4966401	600.1221588	331.5523842	587.4369756	628.6106245	580.4017525	709.9076834
1368.211154	1577.530219	1564.703047	1424.148129	1051.963535	1319.507434	1478.814793	1457.454675	1823.783056
298391.6626	286015.663	269775.1428	291332.8725	291362.4736	296963.2873	321932.5741	284741.9373	308645.8251
4065.50722	2829.085485	3819.718136	2982.066038	2051.7303	2616.193158	2366.254977	2660.167841	4242.693592
151315.5888	148658.5308	144862.4839	146688.3697	152473.997	157386.8635	163836.911	146675.7306	158884.9748
119888.112	119065.2317	115827.4309	121583.451	128475.2985	125709.9897	134968.1397	121774.3847	132774.6801
148543.8357	140273.1284	138801.4605	142502.738	141919.829	143570.8567	143940.6002	132590.6136	145097.2601
354.0718156	321.5628118	291.1008315	355.2547515	379.7824159	273.9571187	308.5402996	273.5435064	360.8830899
656.3803243	1268.28477	1163.200128	929.8139094	2369.346297	612.1417358	1977.033494	1039.656581	1662.09494
13580.24146	16228.37635	12253.06612	17825.07939	11952.70233	15432.99152	14984.39703	12963.81902	14676.52694
289.8463425	227.5494185	126.7401932	245.0442204	485.6382587	127.4051706	226.6519323	120.2676009	389.9948502
16247.69817	14571.48163	15535.00719	15129.79924	13305.5667	13236.43246	17960.91804	12916.01106	16507.86362
2604.787852	2941.850649	1232.572815	2041.7436	2804.363294	2369.096756	2777.31041	2325.98082	1588.658117
243.2101924	519.4768632	0.001403199	322.4790938	325.2033448	186.6790691	444.4950994	337.2756959	531.2955252
2943.510894	2619.306124	1521.142341	3721.034208	3076.697424	2574.326389	3310.467594	2567.70916	1854.808596
7192.401935	8284.093814	5716.067652	8272.009346	6741.752556	7917.549819	11536.6107	7393.251057	6785.454413
2950.967631	1916.9648	1287.785209	2521.565918	2628.88233	3390.688329	3708.529722	1344.984788	1742.582158
366.1339633	195.5265191	176.5659322	415.6146014	364.2305012	401.8351358	290.291527	300.2144368	226.93176
1253.17648	1823.66529	1236.349505	2019.267457	1886.528765	1934.800402	2424.74796	2060.651172	2097.842285
2201.523222	2184.412104	2257.392856	3272.620692	2823.873374	2902.811569	4036.681669	2684.019515	2580.564663
1817.621024	1957.152601	1112.85499	1602.712374	1514.780972	1623.56835	2448.088023	1391.697574	1506.818103
329.8227	338.1657295	344.1514943	413.5778984	351.1076619	348.4525732	386.6378742	375.2260901	518.1873126
623.030903	571.0446468	444.5581989	723.6466187	557.1734416	627.9810716	712.2768742	631.712596	597.353546
2434.327921	2694.531709	2029.687607	2914.345023	1819.125827	2566.223166	3783.312277	2882.627611	2602.283777
917.0078535	1188.251883	562.5002203	1137.11727	1074.317591	1595.874663	1560.087469	1358.583044	1164.79983
4181.058099	4168.153479	3032.962546	4569.376537	3642.248009	4963.507027	5379.805374	4003.476095	4434.443893
1399.887475	2000.799596	1344.884269	2483.704182	2157.152385	1630.072652	2599.551214	1961.070445	2435.372874
1047.652436	1286.378254	1044.029613	2301.132704	2121.468705	1050.253257	2256.19805	1446.449373	1471.638827
41.73502559	118.5279108	84.54578474	118.4747318	52.16059067	628.0526828	202.8157474	134.4083157	151.5257498
42398.95715	43640.48656	43181.82227	48109.82905	41556.12155	48810.59855	51685.65447	44052.07575	46748.73099
882.0844322	969.5866628	1089.780902	634.8346374	766.3072957	735.6954359	1144.512927	767.3298371	1556.219073
2318.301658	2650.369522	2189.242699	2601.921723	2594.895111	2974.507064	3258.561442	2288.915889	3039.223785
958.6835887	1168.190948	1042.757637	748.9092641	811.9945338	1036.607052	1452.154956	633.2919273	1661.800788
678.7190429	265.6606555	424.7586358	197.8412792	346.1913241	490.5740794	452.8425972	297.7735748	523.9265117
142.4367981	116.6972714	220.7620149	124.8936488	185.9107498	607.2412257	227.4056316	117.9633216	231.5922694
2102.958426	1849.203018	1868.980661	913.2786677	1870.505171	1488.806501	1449.719162	1689.729628	3512.767648
2667.395149	1573.771242	1721.567159	883.2912724	1546.012408	2079.417889	1216.238711	2921.607361	2391.476299
77.34761694	0.477528676	122.471272	1.028915789	70.80861954	222.9907135	4.723455393	169.969174	72.96531664
167.4985881	134.5846626	107.1606295	111.4114871	57.45465587	300.1343835	153.7291573	105.9329529	61.68238367
1350.928455	1712.691222	1453.61636	1054.15868	2531.569863	1489.074902	1940.71387	1956.18569	1285.513261

12.85_955.7609m/z	955.7608692	12.85075	neg
12.86_250.9090m/z	250.9090485	12.8592	neg
12.86_663.8463m/z	663.8462837	12.8592	neg
12.87_160.9390m/z	160.9390411	12.86938333	neg
12.87_563.7389n	608.7374704	12.86938333	neg
12.88_116.9252m/z	116.9252377	12.87953333	neg
12.88_432.8653m/z	432.8652838	12.87953333	neg
12.88_740.5247m/z	740.5247273	12.87953333	neg
12.89_293.1791m/z	293.1790783	12.89145	neg
12.89_300.8099m/z	300.8099325	12.89145	neg
12.89_341.7595m/z	341.7595489	12.89145	neg
12.89_504.7726m/z	504.7726265	12.89145	neg
12.89_508.7157m/z	508.7156609	12.89145	neg
12.89_635.7561m/z	635.7560778	12.89145	neg
12.90_246.9053m/z	246.9052528	12.9033	neg
12.90_712.6777m/z	712.6776899	12.9033	neg
12.92_353.2005m/z	353.2005094	12.92306667	neg
12.92_644.6906m/z	644.6906321	12.92306667	neg
12.92_698.7062m/z	698.7062185	12.92306667	neg
12.94_218.9862m/z	218.9862382	12.94191667	neg
12.94_414.8033m/z	414.8032975	12.94191667	neg
12.94_494.7443m/z	494.7442789	12.94191667	neg
12.94_540.7494m/z	540.749433	12.94191667	neg
12.94_594.7654m/z	594.7653908	12.94191667	neg
12.94_627.6522m/z	627.652172	12.94191667	neg
12.96_320.8909m/z	320.8909447	12.95623333	neg
12.96_436.7850m/z	436.7849504	12.95623333	neg
12.96_495.8381m/z	495.8381395	12.95623333	neg
12.96_563.8257m/z	563.8257295	12.95623333	neg
12.97_472.7620m/z	472.7619806	12.96981667	neg
12.99_462.7336m/z	462.7336133	12.98508333	neg
12.99_487.8063m/z	487.8063496	12.98508333	neg
13.00_402.8284m/z	402.8283664	12.9986	neg
13.00_484.7394m/z	484.7394177	12.9986	neg
13.01_476.7042m/z	476.7041942	13.00831667	neg
13.01_492.7484m/z	492.7483589	13.00831667	neg
13.01_554.7209m/z	554.7209119	13.00831667	neg
13.02_201.8494m/z	201.8493537	13.0167	neg
13.02_416.7045m/z	416.7045081	13.0167	neg
13.03_174.8638m/z	174.8638258	13.02853333	neg
13.03_393.8214m/z	393.821357	13.02853333	neg
13.03_458.7905m/z	458.7904754	13.02853333	neg
13.04_199.9465m/z	199.9464812	13.03821667	neg
13.04_530.7203m/z	530.7203375	13.03821667	neg
13.04_580.8154m/z	580.8154243	13.03821667	neg
13.05_360.8704n	359.8631722	13.05003333	neg
13.05_368.7974m/z	368.7973662	13.05003333	neg
13.06_577.7105n	576.703263	13.05843333	neg
13.07_218.9862m/z	218.9861763	13.07201667	neg
13.08_419.8188m/z	419.8187752	13.08211667	neg
13.08_460.8089m/z	460.8088818	13.08211667	neg
13.08_492.7481m/z	492.7480927	13.08211667	neg
13.08_528.7747m/z	528.7747163	13.08211667	neg
13.08_553.7968m/z	553.796783	13.08211667	neg
13.09_626.6517m/z	626.6516508	13.09211667	neg
13.09_100.9258m/z	100.9257676	13.09396667	neg
13.09_145.9268m/z	145.9268152	13.09396667	neg
13.09_336.7870m/z	336.7869762	13.09396667	neg
13.09_418.7462m/z	418.7461741	13.09396667	neg
13.09_427.8504m/z	427.8504246	13.09396667	neg
13.11_312.8593m/z	312.8592848	13.1084	neg
13.12_264.8565m/z	264.8564684	13.12023333	neg
13.12_374.8107m/z	374.8106873	13.12023333	neg
13.12_405.7818n	404.7745394	13.12023333	neg
13.13_172.8926m/z	172.8926398	13.1299	neg
13.13_390.8030m/z	390.8030108	13.1299	neg
13.13_539.6998m/z	539.6997567	13.1299	neg
13.15_351.8311m/z	351.8311447	13.15131667	neg
13.15_612.6798m/z	612.6797994	13.15131667	neg
13.15_620.7673m/z	620.7673492	13.15131667	neg
13.16_648.6334m/z	648.6333924	13.16311667	neg
13.17_123.9019m/z	123.9019166	13.1749	neg
13.17_621.6602m/z	621.660228	13.1749	neg
13.18_160.9355m/z	160.9355496	13.18458333	neg
13.18_194.9059m/z	194.9059073	13.18458333	neg
13.18_202.9491m/z	202.9491191	13.18458333	neg
13.18_469.7676m/z	469.7676412	13.18458333	neg
13.18_485.8092m/z	485.8092159	13.18458333	neg
13.18_487.8063m/z	487.8062571	13.18458333	neg
13.19_281.8467m/z	281.846695	13.19295	neg
13.19_368.8208m/z	368.8208228	13.19295	neg
13.19_530.7205m/z	530.7205105	13.19295	neg
13.19_687.0064m/z	687.0063586	13.19295	neg
13.19_759.5176m/z	759.5175801	13.19295	neg
13.21_390.8268m/z	390.8268293	13.21166667	neg
13.21_567.7681m/z	567.7681153	13.21166667	neg
13.24_502.7994m/z	502.7993975	13.23833333	neg
13.24_558.7389m/z	558.7389319	13.23833333	neg
13.24_559.7375m/z	559.7375432	13.23833333	neg
13.24_616.6227m/z	616.622682	13.23833333	neg
13.25_336.7870m/z	336.7869652	13.2484	neg
13.25_393.1719m/z	393.1719034	13.2484	neg
13.25_444.8405m/z	444.8404927	13.2484	neg
13.26_433.3449m/z	433.3449145	13.26018333	neg
13.26_499.7811m/z	499.7810624	13.26018333	neg
13.26_594.6409m/z	594.6408574	13.26018333	neg
13.27_397.2266m/z	397.2265753	13.26855	neg
13.27_506.6738m/z	506.6738143	13.26855	neg
13.28_219.8576m/z	219.8575707	13.28175	neg
13.28_425.1098m/z	425.1097907	13.28175	neg
13.28_500.6610m/z	500.6610098	13.28175	neg
13.28_625.7268m/z	625.7268483	13.28175	neg
13.29_446.8371m/z	446.8370532	13.29488333	neg
13.29_462.7335m/z	462.7334741	13.29488333	neg
13.29_468.7703m/z	468.770263	13.29488333	neg
13.30_306.8233m/z	306.8233287	13.30496667	neg
13.30_644.6908m/z	644.6908448	13.30496667	neg
13.32_213.9638m/z	212.9638205	13.3158	neg
13.32_244.8715m/z	244.8715226	13.3158	neg
13.32_412.8087m/z	412.8086807	13.3158	neg

1052.068661	1210.142062	490.5761262	545.8004652	1543.489132	0.001403199	539.1196953	1277.998352	0.001403199
761.1437139	1095.621274	760.4032521	961.6979917	1077.131306	685.7771686	1149.827392	1075.114187	382.6087498
3107.70971	2416.676074	2199.071126	3638.706587	2104.272459	3502.717868	5024.353863	2458.104634	2490.56107
65.70092022	118.1916236	46.05876484	461.0568176	70.53656876	349.4158246	131.6290273	135.6638012	130.1729429
83341.18038	83808.69802	82901.83342	85203.92425	86160.04564	88376.4183	92860.41128	82489.29544	90754.02023
118.8897866	64.71544751	494.0404342	474.3940973	201.9674211	1051.298609	0.001403199	350.3514595	658.7734717
2740.963207	2463.610431	2194.759889	2508.126797	1908.773987	2538.180691	2707.729778	2877.852066	1659.346589
3279.611703	4357.868101	3923.921442	2180.020799	0.001403199	0.001403199	3508.487797	2484.754913	1905.236503
1465.628014	1643.753895	1511.077684	949.7596656	774.6139755	696.7864223	1738.805781	1912.44766	813.4243677
6588.172657	7305.816293	6737.753409	8162.207495	8515.443412	8145.290624	9645.535369	7619.463649	7670.786151
110.6595543	191.4162381	193.8839121	106.4251154	0.001403199	144.086934	0.001403199	0.001403199	0.001403199
251754.3495	246991.5148	246429.2372	269443.7397	272518.6497	274075.1007	290213.4961	259619.2804	280130.7493
8306.234675	9257.949446	9771.800885	10135.51409	10324.8449	10592.32732	11432.3389	9397.544543	10111.19926
23699.15988	24644.10397	23645.15481	25135.56265	23687.74109	24946.77463	29714.30794	23724.06005	26758.96986
1270.438273	1147.910693	1507.0402	1402.857803	1574.762081	1165.234964	1923.103618	1416.601538	1792.28504
4498.036632	3842.735457	4910.730144	5311.713764	6517.314172	5684.599891	7044.839645	7302.168765	6464.888009
25097.86119	9767.385116	16664.48087	8805.779957	11483.20192	8777.973319	12395.81242	30789.63374	8427.942424
35177.87718	38697.5328	38573.83979	39165.52624	43809.06254	40664.25219	44516.54468	35463.28461	45132.77652
7539.946513	6507.51487	7352.329305	7548.921542	7196.176737	6545.206915	8481.203171	9248.963674	7980.775508
281.7733792	440.510423	484.0739341	371.7235868	418.5633123	526.385723	282.1055204	570.690289	595.3935959
127987.8833	125170.5086	135647.7453	132573.4929	140067.6288	138981.8445	146050.4314	131471.1584	139394.1075
5208.648971	6461.746169	6942.868804	6930.314304	7187.479525	6867.619067	7933.148919	7115.758941	6430.88865
201518.2475	206363.6258	198719.3727	209849.2487	213317.1902	218041.9985	226924.0505	204804.1746	219540.5797
4965.367573	4103.534001	4270.128387	5161.236818	4735.040217	5570.731417	6424.486452	4874.611229	4104.547962
1796.3851	490.071299	1634.887115	2254.248603	1691.396907	1469.732683	1633.200814	1707.511934	1195.918024
1219794.572	122804.03	1212939.773	1242127.749	1307669.332	1267785.457	1409226.848	1278295.815	1370557.446
142286.0217	137955.8561	134403.8165	146795.673	152119.6931	153826.689	160173.9795	145335.9181	150201.4766
470649.1197	462289.557	438870.5856	458533.5906	470609.6204	471566.5185	505501.3647	452829.3163	494372.2972
337616.7833	324933.1769	318906.2246	333274.61	332363.6334	347528.4132	361181.065	322693.5848	354876.268
308627.417	300928.7949	307521.5	313378.8492	335546.3057	321490.5102	351922.5958	311275.2164	334093.8122
1432.629829	903.050334	1876.200057	2661.339787	997.8359514	1356.03464	1355.537871	1967.116875	1935.973983
2706.555545	2162.861178	1247.928799	1670.530462	2234.172859	1909.696489	2196.442074	2353.425867	3339.067287
7469.10043	9429.959572	7851.422937	7317.51811	7822.888997	8477.73234	8735.312239	8974.462773	9167.310289
799.1984	1350.133705	1594.663197	2618.018449	3216.557515	2822.658133	2681.412866	2552.673795	1848.542764
17417.21247	18378.37075	18418.57685	22143.61445	22196.479	22134.21122	19555.10506	18818.21647	18965.85078
373.5916334	229.7959508	199.5433659	199.3576803	456.6566642	256.826706	487.7335054	0.001403199	170.6123306
286795.0292	295867.8351	296510.2046	314440.2039	336412.1945	327729.6758	347134.0122	309561.3937	336081.9217
60.42836881	0.001403199	50.2418935	65.17098152	115.5711095	0.001403199	0.001403199	0.001403199	0.001403199
7629.570506	8594.915306	9530.753484	7998.103654	10060.35448	8167.933027	10915.53007	10205.69524	10612.40905
244.9216559	182.9522314	0.001403199	142.2244746	173.0531786	265.4961311	90.78664801	214.6483208	182.1601996
88330.96898	87533.86363	87918.10401	97465.96336	95337.78435	94425.21046	102016.1138	88768.15539	95592.67487
29235.95281	28073.38977	27772.32287	28112.3169	25310.15213	27133.85919	28699.4888	27367.537	28459.40364
33394.97382	33913.62645	31466.07103	31291.53706	32881.62436	31900.32006	36320.61721	32795.51773	34550.52704
1969.812428	1324.960674	1343.769301	491.1016114	1764.442896	1363.225667	1886.147743	1827.939575	1866.560878
2240.868514	1696.336228	2660.433811	1887.039209	2397.972331	2558.499882	2526.913696	2246.963494	2007.954052
396984.1968	383532.3774	379391.5968	382726.7056	394220.1209	390346.1625	427832.2966	376948.5632	407883.8462
9014.911336	8880.42309	8012.139552	9012.744236	10418.58452	9949.452476	8711.363264	9629.653701	10367.07273
98681.77518	96717.52115	103138.338	115713.6599	118026.0384	122856.0072	112804.4179	105436.784	114181.827
1194.703402	1216.759795	1212.981984	1226.017318	1157.814212	1164.622015	1186.166723	974.2698431	1215.931736
4139.735704	2902.536563	3090.590833	3333.039107	2890.13178	3121.981107	2392.334478	4297.447773	3525.880427
368446.8947	374075.8956	374244.8632	389564.614	413401.0963	409847.7425	436960.2178	391137.1096	420100.2138
502.7438248	204.5925349	685.6644852	0.001403199	470.8134004	939.7823007	607.0405363	0.001403199	0.001403199
3283.22147	1643.886366	2052.919781	1956.816023	2603.552403	2413.521025	658.1267326	821.8874741	2460.814876
26414.02714	25661.59171	24356.15514	21821.55219	26761.95488	26365.51518	24090.04789	22995.26495	24312.71804
20034.3717	20640.69684	18799.7738	18731.07447	23002.18131	23211.33425	23394.25284	20943.94638	23007.29591
304.7609453	280.0574969	334.4040476	375.378113	250.1585346	474.200664	314.957895	268.6759424	334.9022558
0.001403199	138.7519397	51.9744294	0.001403199	0.001403199	105.5161791	0.001403199	95.85514832	77.78355462
674.6312526	650.8067485	850.3809253	645.1116049	651.949466	1449.455097	877.23216	465.3173904	565.6638696
8662.700889	8713.492677	9536.881725	10086.69824	9367.77836	10691.19671	8447.244928	8174.637179	9262.880112
417793.8658	408363.0484	398221.2807	429159.5993	422844.2789	418471.0746	453255.5181	406571.7994	439763.7926
1411.348888	1518.82519	1317.536173	1542.64137	1794.792815	1872.917194	1764.608414	1522.303185	1374.514945
8859.558734	8860.074356	7618.421526	7568.228002	9485.940036	10665.5604	7652.982616	7290.533674	8404.400902
3442.556593	3588.897456	3203.043881	3122.782337	3581.863401	4427.741049	2359.805061	3082.398994	3771.81556
327497.3425	328766.7855	325598.5267	340810.6759	348539.1185	346805.7653	379183.3947	326082.4757	353329.6529
1400.755736	873.8224329	982.8249902	831.9647	1215.52753	1292.281622	1047.040818	1115.082882	1195.035527
34388.46307	32612.87464	30532.90912	33267.87415	31866.80323	31362.17279	34454.1619	31739.55013	35829.83317
1531.405519	1081.805341	1421.944636	1625.741321	1461.224656	1306.816054	2672.361785	1411.703102	1760.799523
1906.77271	2023.927754	2184.6581	1496.867719	2535.217215	2223.199046	1862.29581	2557.321038	1551.41935
3258.398627	3646.533292	2235.166121	3127.127416	4923.937738	5363.353847	3585.108348	3469.794016	3103.914183
244.7953856	0.001403199	278.814872	0.001403199	265.7179173	356.7092017	0.001403199	753.8136292	319.9993437
1670.932521	707.1897461	1688.641507	2029.441489	2760.102668	2916.091906	2612.648521	1203.744851	910.0341824
853.1244438	863.8609459	675.6572267	634.2114867	789.3474937	807.3303627	728.3959573	544.5100956	540.8062712
287.445339	1462.208302	556.1244097	365.5769759	2417.927316	2181.268166	1673.335948	1362.976319	1574.678236
6072125.372	5767858.379	5591079.05	5972666.682	5897359.256	5974521.441	6337759.737	5738145.292	6057671.85
95621.08469	91623.57775	91334.83725	91732.38296	96953.35614	94451.43759	103903.9583	94092.02956	99553.90551
454.4189667	596.602796	280.6101273	403.4879146	465.1248114	449.9869154	272.1486756	290.3173993	343.4235935
1073.31683	423.5747977	766.7151429	683.0884955	1202.53206	1845.873712	239.3812833	526.3522932	342.9133723
35313.76913	33748.01411	30844.84324	32349.59253	29866.41039	32204.43775	30981.05767	29167.17245	34113.28096
3218.14872	3395.132542	2550.275931	3540.092414	2693.49901	2035.724555	3780.419313	2481.188866	2138.220726
379.4571464	644.9574437	609.2491742	387.9187059	1047.569378	462.8953635	431.7064207	262.041905	790.3885512
1755.956445	2205.366161	2388.88152	2089.682602	2342.594866	2271.021444	1438.241403	2242.785747	1946.946475
4384.790077	3874.186159	3703.333952	3416.90127	3615.837519	2889.028509	4739.344493	3225.71799	3482.506663
1507.627865	1183.226038	1191.828165	415.1920275	1189.837795	369.0441442	2441.347576	1634.387573	1405.008946
6123.555776	7332.030555	3111.790717	8370.099424	7019.036838	491.3985758	6370.276525	5396.696977	2526.65221
35397.07842	36111.92998	35529.17764	34654.23826	38091.99522	38132.36999	39886.63643	33523.51691	37109.69315
142905.284	142086.9957	140271.7963	151228.6911	149892.1763	153621.9506	162475.4691	143592.5193	159026.8041
1092.676255	1226.052059	1392.596544	1189.042736	898.0436769	907.1028275	2136.099766	1617.205452	440.349942
347.3089794	260.4216636	248.4352166	542.2484624	494.0667038	0.001403199	454.434256	0.001403199	287.7537599
1244.295779	1206.048831	2143.045396	1222.518912	640.4130608	1536.225815	1421.831263	1833.926256	1576.335828
4167.898289	3616.710616	3740.79382	4255.111417	5392.652037	4713.589197	6217.954563	5188.908034	2361.18817
760.0548223	674.6480618	2026.658939	1330.530237	1048.459843	1120.453654	2115.891475	1831.953695	1442.850288
9323.464785	5244.901769	4918.915397	3425.094972	3036.125233	4620.506195	4485.640814	10500.97397	4542.931267
58889.21747	56907.92499	53480.41645	54839.33874	57840.26065	56436.27612	64878.74258	50596.05543	54889.84184
1482.257979	795.4302621	1626.111262	1383.682436	560.6452639	1247.301344	3049.480662	1844.264841	1481.547013
268556.2109	265704.1482	258398.5165	266373.7124	287175.945	274073.7292	298187.8074	261481.9105	283224.8151
4272.820598	6900.409408	7128.988158	6292.630761	6913.641957	6017.096632	7195.523905	4291.005803	7138.561314
20576.63577	5318.835287	7738.991625	4842.936114	6431.52409	4144.472479	4545.865229	21724.75002	6163.781509
1614.512242	2192.175926	2436.231076	3028.637758	2298.029088	3121.054501	2388.892693	3028.468321	5179.527881
163.5007837	210.6386956	249.2617973	219.2050849	200.9089052	243.1300596	94.48703546	271.9780593	414.9288177
4497.855593	2061.118729	1850.774296	1928.431605	877.0231662	1012.256349	2210.196448	5183.206691	1915.954153
4214.170669	3816.913465	4633.953252	3940.327745	4750.040693	4282.907625	5472.606657	4951.740035	5387.162738
7072.687922	6434.892824	6854.925973	5720.524563	6482.675832	7316.818669	7600.0016	6818.843814	6335.98394
1052.962497	1693.165128	1566.575032	1564.369465	444.5868014	853.4564406	1857.644399	1431.782475	1258.551643
10484.76743	11555.75721	12293.84131	12148.28689	13333.70259	13500.07854	12224.82246	13457.12697	13986.64228
656.8814672	269.1955534	1043.13161	1436.487757	0.001403199	796.1713805	1990.857851	1107.521179	444.4183591
52835.16659	54285.48285	54294.48137	55384.5692	59431.4731	58853.21076	61517.59109	53963.64123	59299.50464
1729.225922	315.2612029	1185.228065	818.2021404	1209.152087	1349.334881	1184.742463	808.5881852	1342.229849
1322.496131	1033.228671	1497.075185	1271.521825	946.2613215	873.4935682	1362.184142	1061.927554	1652.487616
679.8468666	815.5788003	486.7589097	631.1906296	378.6838603	456.840903	484.0044195	329.2895775	699.7121121
2318.063043	2052.129317	2249.990296	258.9462528	2072.824512	1624.041178	989.6163362	1277.169258	1795.629594

13.32_432.8005n	431.7932538	13.3158	neg
13.33_300.7765m/z	300.7765137	13.32586667	neg
13.33_350.8416n	395.8396629	13.33423333	neg
13.34_420.8172m/z	420.8172175	13.3426	neg
13.38_325.8339m/z	325.8339276	13.38228333	neg
13.38_337.8813m/z	337.8812786	13.38228333	neg
13.38_417.8216m/z	417.8216345	13.38228333	neg
13.38_476.7042m/z	476.704165	13.38228333	neg
13.38_544.6925m/z	544.6924542	13.38228333	neg
13.38_648.6335m/z	648.6334664	13.38228333	neg
13.40_557.7395m/z	557.7394926	13.39756667	neg
13.40_618.5967m/z	618.5966558	13.39756667	neg
13.41_172.8927m/z	172.8926728	13.40935	neg
13.41_242.8745m/z	242.8745308	13.40935	neg
13.41_244.8717m/z	244.8717439	13.40935	neg
13.41_440.9981m/z	440.9981067	13.40935	neg
13.41_506.6737m/z	506.6736644	13.40935	neg
13.42_468.7703m/z	468.7703465	13.42113333	neg
13.42_584.7585m/z	584.758519	13.42113333	neg
13.43_300.8533m/z	300.8532747	13.42951667	neg
13.43_434.8115m/z	434.8115517	13.42951667	neg
13.43_629.6699m/z	629.6699165	13.42951667	neg
13.43_676.6003m/z	676.6002928	13.42951667	neg
13.45_580.8154m/z	580.8153929	13.44803333	neg
13.45_612.6800m/z	612.6799528	13.44803333	neg
13.46_116.9640m/z	116.9640939	13.45946667	neg
13.46_272.8203m/z	272.8203149	13.45946667	neg
13.46_441.2530m/z	441.2530168	13.45946667	neg
13.46_468.7705m/z	468.7704821	13.45946667	neg
13.46_534.6870m/z	534.6869767	13.45946667	neg
13.46_571.7113m/z	571.7112833	13.45946667	neg
13.47_140.9305m/z	140.9304985	13.47473333	neg
13.47_300.8333m/z	300.8332714	13.47473333	neg
13.47_319.7775m/z	319.7775065	13.47473333	neg
13.47_382.7925m/z	382.7925426	13.47473333	neg
13.47_558.6639m/z	558.6639111	13.47473333	neg
13.47_598.5917m/z	598.5916869	13.47473333	neg
13.47_639.6986m/z	639.6986378	13.47473333	neg
13.49_433.3451m/z	433.3451311	13.48825	neg
13.49_465.1020m/z	465.1019916	13.48825	neg
13.49_484.7909m/z	484.7908942	13.48825	neg
13.49_616.6225m/z	616.6225079	13.48825	neg
13.50_126.9294m/z	126.9294101	13.49953333	neg
13.50_563.6565m/z	563.6565446	13.49953333	neg
13.51_368.8208m/z	368.8208462	13.5096	neg
13.51_489.7522m/z	489.7521504	13.5096	neg
13.52_384.7666m/z	384.7666271	13.52308333	neg
13.52_762.5368m/z	762.5368456	13.52308333	neg
13.53_140.9306m/z	140.9305609	13.53481667	neg
13.53_176.8842m/z	176.884218	13.53481667	neg
13.53_244.8717m/z	244.8717024	13.53481667	neg
13.53_504.7727m/z	504.772659	13.53481667	neg
13.53_594.6409m/z	594.6408933	13.53481667	neg
13.55_452.7284m/z	452.7283905	13.5479	neg
13.55_576.6105m/z	576.6105434	13.5479	neg
13.56_256.8464m/z	256.8463596	13.55923333	neg
13.56_485.2792m/z	485.2791654	13.55923333	neg
13.57_116.8930m/z	116.8929904	13.5693	neg
13.57_351.8312m/z	351.8312242	13.5693	neg
13.57_454.7231m/z	454.7230707	13.5693	neg
13.59_254.8519m/z	254.8519121	13.58755	neg
13.60_197.8565m/z	197.8564805	13.5994	neg
13.60_212.8649m/z	212.8648666	13.5994	neg
13.60_223.0284m/z	223.0283879	13.5994	neg
13.60_563.6566m/z	563.6566384	13.5994	neg
13.60_643.6418m/z	643.6417827	13.5994	neg
13.61_195.9058m/z	195.9057812	13.61116667	neg
13.62_158.9755m/z	158.9754771	13.62125	neg
13.62_419.8192m/z	419.8191683	13.62125	neg
13.62_441.2529m/z	441.252921	13.62125	neg
13.62_503.7239m/z	503.7239022	13.62125	neg
13.63_244.8717m/z	244.8716866	13.62963333	neg
13.63_270.8619m/z	270.8619308	13.62963333	neg
13.63_409.8114m/z	409.8114271	13.62963333	neg
13.63_418.8220m/z	418.8220227	13.62963333	neg
13.64_126.9292m/z	126.9292153	13.64228833	neg
13.64_174.8871m/z	174.8871074	13.64228833	neg
13.64_458.7902m/z	458.7901893	13.64228833	neg
13.64_467.7700m/z	467.7700307	13.64228833	neg
13.64_658.5896m/z	658.5895604	13.64228833	neg
13.65_453.7757m/z	453.7757135	13.65066667	neg
13.65_546.6895m/z	546.6894881	13.65066667	neg
13.65_676.6000m/z	676.6000168	13.65066667	neg
13.68_372.7636m/z	372.7636183	13.67551667	neg
13.68_598.5916m/z	598.5916093	13.67551667	neg
13.69_269.8936m/z	269.8936029	13.68553333	neg
13.69_327.8523m/z	327.8522698	13.68553333	neg
13.69_352.8287m/z	352.8286787	13.68553333	neg
13.69_491.7498m/z	491.7497839	13.68553333	neg
13.69_508.7160m/z	508.7160037	13.68553333	neg
13.69_588.7013m/z	588.7012771	13.68553333	neg
13.70_212.8650m/z	212.8649632	13.69686667	neg
13.70_700.5112m/z	700.5112031	13.69686667	neg
13.71_138.8601m/z	138.8600772	13.71038333	neg
13.71_199.9117m/z	199.9117463	13.71038333	neg
13.71_216.8538m/z	216.8537624	13.71038333	neg
13.71_309.1741m/z	309.1741089	13.71038333	neg
13.71_374.7609m/z	374.7608947	13.71038333	neg
13.71_478.6789m/z	478.6788833	13.71038333	neg
13.71_494.7889m/z	494.7889125	13.71038333	neg
13.71_536.6819m/z	536.6818917	13.71038333	neg
13.71_538.6117m/z	538.6117096	13.71038333	neg
13.71_553.7968m/z	553.7967649	13.71038333	neg
13.71_578.6047m/z	578.6046894	13.71038333	neg
13.71_643.6416m/z	643.6416492	13.71038333	neg
13.71_741.5045m/z	741.5045488	13.71038333	neg
13.72_159.9192m/z	159.9192142	13.71835	neg
13.72_394.7696m/z	394.7695921	13.71835	neg
13.72_457.7408m/z	457.7408292	13.71835	neg
13.73_314.8051m/z	314.8051337	13.72668333	neg

311202.1269	319091.2474	307481.8438	315552.8215	334240.2515	320861.5241	352573.7369	310775.7996	333608.3307			
108.2921242	295.5139238	0.001403199	0.001403199	117.4424535	0.001403199	142.8067434	95.15864563	138.8442998			
145825.2038	140545.5236	139092.2355	137662.7538	139557.0859	141650.9001	155922.0308	138801.1673	148909.8713			
251.861791	0.001403199	196.1312924	150.3425569	0.001403199	174.532058	0.001403199	0.001403199	537.1804453			
55989.70494	57994.46058	61034.73507	61588.48584	64184.70369	64522.79819	67371.97222	56464.625	64501.20682			
137240.25	140195.0055	134751.8537	136286.4564	140289.1114	143168.6749	154519.3115	133312.7705	145617.2677			
28002.54128	26304.16849	26535.95925	26629.25209	23785.72856	26867.48999	31075.09454	26984.91824	29410.71806			
12625.22803	11716.21416	10094.18802	8843.755503	11355.37505	8582.747562	12355.20934	9195.892246	12729.94439			
56139.52642	64865.1407	61970.38795	61655.77913	72211.75419	68303.42004	68923.12401	60814.34027	69350.90398			
872.7337657	1336.724167	1505.6479	777.0185914	2262.077825	685.0701506	3838.681265	2628.054434	2793.150806			
13059.8497	16037.02483	15665.8131	13489.97357	16809.86134	15597.82362	14847.01053	14068.49125	18349.86625			
1861.388734	2334.575579	2660.342034	1950.646046	3674.353519	2670.320913	2179.523986	3030.792045	3378.066446			
544.0861016	526.9604002	842.3718457	689.5495053	485.4636561	497.9064166	741.1900009	512.8388601	1134.282361			
1865.939195	1463.552617	1771.016629	2081.780263	1502.869266	1440.880093	2831.31799	1523.349167	1965.033211			
593.1990482	397.5894201	699.1628435	547.9336582	386.2918745	500.8789356	933.5340447	590.7053104	392.6474441			
166.2516514	208.6793371	545.1869131	446.6491712	415.9391327	0.001403199	0.001403199	515.0251312	222.141496			
2430.340907	916.6992358	1526.050948	2173.33855	1294.647514	2436.158346	2712.47353	1203.345552	1835.644726			
1710.770389	2290.318865	2085.370818	1900.201529	939.7079333	1894.875639	505.7541297	2397.273293	2612.579725			
2058.131939	1426.801077	1800.738434	1381.728874	1799.349763	1550.720752	1636.826308	2568.49038	1931.896319			
1782.398815	1756.37601	2203.475113	2208.256816	2021.205174	1657.750698	2675.171344	2291.653307	2174.441351			
1607.461088	1221.051627	1202.857219	1063.420136	647.7623496	620.5617263	1739.351936	1118.332298	488.2238777			
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6474.782579	4144.133812	8184.864151	5904.455215	8744.655584	10393.86535	6595.393854	9107.763633	10718.96311			
2606.22156	1975.587177	2640.586174	2312.325578	2544.93099	1519.142855	4026.084272	2034.390319	1693.437612			
1981.837717	4873.39546	4468.091838	2182.113263	7648.990388	4208.736285	6392.13779	4236.349928	4890.746694			
39242.7341	39123.98095	40712.99144	39567.03465	42754.38457	42705.61695	46738.64616	40226.07456	41553.8199			
2635.231543	3363.618203	3463.979192	2992.699253	4383.16672	4513.87634	4065.198952	4096.373217	3548.469979			
8713.653106	1548.795756	2420.173228	1437.808018	1997.292494	439.4688786	802.9227176	12113.621	712.7829503			
469.3518771	698.6712631	503.524107	750.2052312	1353.598486	1015.489052	820.658589	825.2155788	286.7619451			
26238.01794	28673.85271	26674.46312	25953.26588	31461.61841	28612.80685	30177.48297	28394.43776	33630.59314			
32707.0252	34264.42901	31720.61408	34462.61594	41723.98233	35556.36542	37858.7587	34480.23571	39265.78926			
311.6681612	393.1547863	316.7607777	292.0942274	428.7024609	362.783658	386.0613964	405.4589088	405.0424111			
22361.08113	21727.33858	22018.56778	22772.9412	23754.3207	23148.02682	25490.05351	20029.47034	22095.00653			
0.001403199	139.5322135	0.001403199	0.001403199	261.1070811	111.7029996	276.408647	178.5978928	0.001403199			
372197.5995	375182.6014	379429.518	389679.2206	407109.342	398670.6448	426650.2159	382444.7601	408583.7789			
139628.8223	142163.3342	148559.8186	153023.0936	155662.7758	155853.9107	165442.2136	150224.5011	165816.8404			
3807.447429	3674.038852	4634.66528	3380.355756	6431.280814	6083.396061	6455.950045	6084.401797	5122.22127			
2143.57315	1174.389641	1834.081244	723.8060806	1604.596145	1636.576506	2525.670601	2487.992527	1745.523543			
1110.658363	1661.524346	1420.168536	1760.452864	584.4999301	1559.784042	2146.229279	1399.737315	1370.744306			
3387.359536	3179.329203	1327.664899	1084.180471	1766.649498	1031.543036	1954.352566	1733.256577	1790.602327			
269.5242085	446.9280942	0.001403199	0.001403199	283.7121806	0.001403199	564.6356698	0.001403199	0.001403199			
4229.248462	3884.056316	4217.343363	3113.928349	7738.352223	4395.594798	5386.855444	2897.458572	3734.466283			
36.4819726	70.56850646	64.67124121	28.41647517	32.36838505	118.2355656	44.22270007	68.39109152	29.9384001			
2477.697893	1973.059111	1815.57348	743.8217238	1363.386637	1043.201459	2379.024082	2515.657941	1250.459327			
2411.30096	3009.377551	2946.275609	1756.186802	3079.770716	2203.627866	1890.514169	3287.445234	2621.974351			
103325.7363	96496.7709	94303.56988	97985.99015	103544.9621	100680.38	108265.9766	96353.98213	104854.3556			
4337.159295	4792.514428	5253.79669	3649.747389	4511.929587	4051.602528	5545.113667	4613.626754	5792.60854			
1500.263996	1017.922119	1368.825444	0.001403199	424.6768719	495.4075502	1241.480517	529.6370239	559.9174003			
516.1109833	572.7284201	412.7039254	354.9382585	459.2004172	360.6117602	555.857838	322.272888	484.7077247			
83277.6607	82554.22849	80479.24788	81779.18537	83147.88157	83627.18353	91825.16245	83405.92562	87273.10829			
637.2513695	610.3980814	711.6224475	295.6809488	571.4909384	328.4434345	520.9049826	553.3243369	552.1966045			
1320.444091	1930.256116	1118.953663	1375.922192	1609.191696	1313.771392	1605.388242	1812.227846	1082.90749			
22849.43051	24507.53036	25440.7818	25282.27109	23527.75319	23341.97124	30168.81544	23313.25461	23141.6418			
513.5104839	581.148968	1212.823775	521.9403705	873.8183585	487.5954399	1004.726042	585.6644804	512.4605919			
1248.661622	2684.405644	3295.048447	1428.104873	3949.751679	3541.635663	5480.952853	2584.371812	3391.647015			
6044855.661	6131087.497	6108874.802	6166165.756	6637103.445	6490227.243	6890678.248	6200928.687	6517139.172			
4315.928314	273.61704	1247.641814	242.6624166	314.665717	0.001403199	0.001403199	7034.315906	0.001403199			
4196.515106	4667.760802	4673.49564	3999.613271	5851.545535	5033.780592	5282.994389	5113.106999	5388.110601			
385.9625256	512.0401512	723.5729968	473.7543708	722.0605394	399.3989699	746.4103441	310.3792912	739.2473958			
332614.1207	336571.5373	339520.4098	343327.4256	363682.7734	360604.8101	381073.3863	342506.8833	363571.4738			
446105.4104	449819.5019	448290.4596	457290.536	482358.4376	481719.8302	493382.0548	459642.6293	472122.8534			
411.0706779	273.0617778	162.1632017	402.0085535	549.9268835	440.3686514	384.5817582	422.46019	473.8725413			
524.7836333	283.9007584	164.62231	251.8283022	352.8677459	405.5600117	526.3561379	393.6595544	413.9424682			
770.4509683	309.314877	232.4446751	1409.230859	386.1863502	478.9399046	276.2489861	187.4810944	92.94683205			
1000.306527	1339.50081	910.4706877	707.5497	1726.243758	2707.149808	1353.346212	2219.848106	1691.022928			
3284.563991	1458.415354	2509.115066	2129.995802	4077.484105	4563.132478	2989.380966	1636.872391	2235.741041			
75.53593596	109.0941769	0.001403199	148.887558	51.59667485	138.8723317	0.001403199	69.11069107	156.3585047			
344.5587879	177.774014	182.2100716	268.5825943	299.3957553	242.5334706	419.6674541	192.0123964	214.1672781			
1104.896986	169.4737132	1160.009602	1323.914636	854.9521581	523.6407616	795.9091453	515.2079697	705.2748419			
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125720.8423	126972.4195	123988.8949	129913.3627	140839.7527	139229.5188	148581.7147	126897.2583	138242.607			
568.5253046	558.2332238	573.0615565	588.7566573	935.2929998	645.6279176	1033.116943	296.5410785	587.8520946			
362.910494	421.4439372	557.9932613	870.7240922	679.0773166	678.7319509	834.8185303	659.8011608	587.5373624			
398761.9054	401988.3067	387393.8626	403821.511	418261.096	419566.7761	444290.2815	398927.1119	418168.4184			
398.3046095	0.001403199	144.9376445	391.9613247	195.7866317	172.5633925	169.7720122	0.001403199	0.001403199			
31.92276691	0.001403199	60.64539632	25.92666043	41.02264658	35.2173843	95.84184634	32.07971774	31.36876356			
199896.7367	195721.2125	191398.3234	189856.3439	201713.4211	205162.397	218322.1699	192071.7579	201462.6555			
816.4674456	1135.811048	258.1672336	1242.863701	1208.232191	497.0713192	843.038069	883.7140427	855.8172682			
17409.1525	16131.88018	15493.84424	14164.72005	20993.01593	18665.56787	19126.6573	14919.53943	15662.23553			
143273.0275	154979.4125	164252.0759	160992.5752	176928.0451	163251.5288	187880.7196	159466.6136	167850.0442			
476.7368646	212.3539219	450.2226387	864.9972612	363.4871492	589.6362171	1070.072392	944.4191742	439.3135403			
1510.645606	834.5116036	696.3451482	926.7594601	376.5475813	363.8333836	393.615784	312.8119202	955.1255126			
1793.835054	1776.412255	2352.473639	2198.490175	3404.000443	2809.907498	2926.452345	1021.444597	383.1349669			
4026.687123	3375.671937	3734.429812	4900.042136	4754.212171	4004.729542	5320.876695	2280.917755	3930.194561			
4838.733088	5191.445673	5260.318139	5661.070123	6695.484008	4042.960215	7407.463091	5285.128568	3849.710981			
71653.28746	70987.77849	70482.13567	69435.60548	73518.45794	74827.90505	80510.02129	70742.37566	75387.7122			
46985.90098	50159.08159	46656.50898	45372.70897	49916.24489	51115.84083	53211.82556	45919.29645	47346.51256			
353.8981947	192.087206	0.001403199	451.8597082	133.8955571	715.4634506	232.9816666	0.001403199	0.001403199			
870.087986	1528.34133	1839.727549	1871.049889	2017.397698	1551.299119	2127.51391	1428.005029	1164.920973			
1188.141795	968.8250047	1547.628046	1643.126236	1466.638774	1042.488674	1474.47227	1013.258601	1339.505216			
1877.879649	1139.643616	1738.733983	2058.64187	2196.353239	1514.310739	1237.746498	1054.892545	956.4148664			
491.4470773	240.9047373	837.6942876	543.2461632	679.352155	329.5671862	523.3580422	166.3065835	440.0539857			
185270.6842	213507.6296	225246.2647	216356.6989	270249.9263	252026.45	260724.6074	232401.9809	246459.0152			
289.4913813	203.8822719	37.31613399	155.0504889	188.868811	133.2078566	116.582347	187.3720729	0.001403199			
63482.18166	62162.57577	61999.97333	60755.86888	65915.51555	67264.75913	70189.03562	62034.98484	66521.49125			
6598193.06	6849876.095	6824975.924	6654145.965	7554022.872	7085800.677	7776893.82	7079468.234	7270778.374			
922.6391257	414.9591723	903.8311213	598.6824853	756.4455985	499.4785904	647.3661995	708.5463832	231.0872561			
3193.843605	2223.586862	2551.836202	2652.196917	2826.669812	1947.668652	2940.07382	2071.160918	2388.095472			
975639.8356	1010378.017	1019115.665	997347.5587	1138564.806	1072285.276	1148707.289	1030981.631	1091836.725			
3492.048884	3110.650073	2429.914921	3318.726635	3491.166172	2914.729911	1653.922544	655.065094	2757.793301			
661105.1767	673607.7721	684560.5389	678960.3938	749657.6763	710210.56	763482.3456	666305.11	722708.6231			
39437.84433	44486.10416	46636.92887	44196.82514	54713.52124	48353.89491	54546.63925	51975.08188	48657.16321			
2349.068241	3067.583052	2611.93228	2296.360832	2769.48145	2295.473777	3939.544156	2778.366565	2986.188251			
284057.4955	299148.0999	323729.1346	294119.5078	362772.8828	324833.9312	363732.5595	317678.6782	340425.1224			
2496.632616	2970.563823	2985.756228	3215.490157	2609.295319	3830.268823	1926.662843	2096.370622	1941.931766			
20777.21543	16838.25778	18306.15576	11696.96511	13012.62396	9908.941528	19745.70811	12985.98719	9462.859691			
517.081689	579.7097119	529.5316291	438.4028535	541.5970898	473.1960875	664.0784369	564.301502	337.9991947			
143839.1622	151474.059	145756.362	147447.3501	158571.5624	152904.775	165459.0552	148006.3115	162322.4342			
1211.122634	1711.306279	1396.323423	794.9828657	991.3688605	1580.259553	677.2336973	282.0149197	580.6423939			
253792.8154	256519.8306	255341.7018	260261.6007	269383.0478	268612.3373	284448.7976	258182.1333	280496.2977			

13.73_400.7020m/z	400.7020021	13.72668333	neg
13.73_438.6863m/z	438.6863128	13.72668333	neg
13.73_539.7000m/z	539.7000342	13.72668333	neg
13.74_100.9258m/z	100.9257657	13.73631667	neg
13.74_138.0026m/z	138.0025842	13.73631667	neg
13.74_336.7666m/z	336.7666497	13.73631667	neg
13.74_340.8994m/z	340.8993981	13.73631667	neg
13.74_397.7713n	396.7640902	13.73631667	neg
13.74_576.6101m/z	576.6101313	13.73631667	neg
13.74_600.5864m/z	600.5864045	13.73631667	neg
13.74_676.6006m/z	676.6006238	13.73631667	neg
13.75_506.6736m/z	506.6736247	13.74978333	neg
13.75_512.6813m/z	512.6812523	13.74978333	neg
13.76_474.7589m/z	474.7588576	13.76163333	neg
13.76_476.6851m/z	476.6850927	13.76163333	neg
13.77_316.8020m/z	316.8019848	13.77343333	neg
13.77_397.8366m/z	397.8365899	13.77343333	neg
13.77_618.5971m/z	618.5970812	13.77343333	neg
13.78_132.9235m/z	132.9234729	13.78351667	neg
13.78_144.9235m/z	144.9234548	13.78351667	neg
13.78_209.0043m/z	209.0042849	13.78351667	neg
13.78_214.8595m/z	214.859458	13.78351667	neg
13.78_292.2283m/z	292.2283361	13.78351667	neg
13.78_357.7788n	338.7609314	13.78351667	neg
13.78_401.7797m/z	401.7797367	13.78351667	neg
13.80_100.9336m/z	100.9335653	13.7953	neg
13.80_151.0149m/z	151.0148907	13.7953	neg
13.80_153.8686m/z	153.8686235	13.7953	neg
13.80_218.8581m/z	218.8581135	13.7953	neg
13.80_238.8356m/z	238.8355774	13.7953	neg
13.80_312.8363m/z	312.836296	13.7953	neg
13.80_316.7790m/z	316.7790336	13.7953	neg
13.80_566.7192m/z	566.7191806	13.7953	neg
13.81_519.6787n	518.6712626	13.80541667	neg
13.82_384.7666m/z	384.7665972	13.81721667	neg
13.83_130.9289m/z	130.9289035	13.8256	neg
13.83_201.9062m/z	201.9062055	13.8256	neg
13.83_286.8837m/z	286.8837442	13.8256	neg
13.83_481.7418m/z	481.7417504	13.8256	neg
13.83_506.7419m/z	506.7418896	13.8256	neg
13.83_561.6822m/z	561.6821963	13.8256	neg
13.84_247.9600m/z	247.9600099	13.84356667	neg
13.84_433.3450m/z	433.3450386	13.84356667	neg
13.84_436.6920m/z	436.6919542	13.83571667	neg
13.84_512.8277m/z	512.827706	13.84356667	neg
13.84_622.6671n	603.6492922	13.84356667	neg
13.86_116.9252m/z	116.9252304	13.86183333	neg
13.86_399.7825m/z	399.7825118	13.86183333	neg
13.86_423.7388m/z	423.738769	13.86183333	neg
13.86_448.7836m/z	448.7836139	13.86183333	neg
13.88_104.9538m/z	104.9538495	13.87873333	neg
13.88_259.8646m/z	259.8646171	13.87873333	neg
13.88_426.8014m/z	426.8014195	13.87873333	neg
13.89_440.7511m/z	440.7511167	13.88881667	neg
13.90_563.6569m/z	563.6569052	13.89845	neg
13.91_358.7699m/z	358.7698637	13.90683333	neg
13.91_369.8191m/z	369.8190848	13.90683333	neg
13.93_149.9945m/z	149.9944878	13.93011667	neg
13.93_314.7849m/z	314.7849498	13.93011667	neg
13.94_125.9289m/z	125.928858	13.93851667	neg
13.94_161.9137m/z	161.9136592	13.93851667	neg
13.94_200.8589m/z	200.8589083	13.93851667	neg
13.94_416.7044m/z	416.7043782	13.93851667	neg
13.94_576.6096m/z	576.6095953	13.93851667	neg
13.95_167.8366m/z	167.8366363	13.9521	neg
13.95_506.7418m/z	506.7418099	13.9521	neg
13.96_218.9862m/z	218.986196	13.9622	neg
13.97_206.8978m/z	206.897757	13.97056667	neg
13.97_228.9559m/z	228.9558897	13.97056667	neg
13.97_229.9010m/z	229.9010368	13.97056667	neg
13.97_469.7674m/z	469.7673867	13.97056667	neg
13.98_169.8339m/z	169.833884	13.98415	neg
13.98_440.7514m/z	440.7513967	13.98415	neg
13.98_452.7770m/z	452.7769604	13.98415	neg
13.99_342.8312n	341.8239111	13.9942	neg
13.99_373.7639m/z	373.7639131	13.9942	neg
13.99_446.7411m/z	446.7410598	13.9942	neg
14.01_374.8106m/z	374.8106123	14.00603333	neg
14.02_155.8656m/z	155.8656328	14.01566667	neg
14.02_157.9550m/z	157.9550155	14.02363333	neg
14.02_222.8409m/z	222.8408672	14.02363333	neg
14.02_234.8199m/z	234.8199133	14.02363333	neg
14.02_363.8060m/z	363.8060066	14.02363333	neg
14.02_479.7471m/z	479.7471135	14.01566667	neg
14.02_740.5251m/z	740.5251284	14.02363333	neg
14.02_741.5043m/z	741.5042603	14.01566667	neg
14.04_199.8510m/z	199.8510086	14.04215	neg
14.04_244.9082m/z	244.9081568	14.04215	neg
14.06_511.7789m/z	511.7789066	14.06406667	neg
14.08_153.8687m/z	153.8686645	14.08458333	neg
14.08_162.9824m/z	162.9824278	14.08458333	neg
14.08_421.7646m/z	421.7646499	14.08458333	neg
14.08_561.6821m/z	561.6820862	14.07546667	neg
14.08_563.6568m/z	563.6568703	14.07546667	neg
14.10_214.8271m/z	214.82711	14.09616667	neg
14.10_594.6411m/z	594.6411128	14.09616667	neg
14.12_146.9967m/z	146.9966766	14.11821667	neg
14.12_212.9109m/z	212.9109269	14.11821667	neg
14.15_141.9238m/z	141.923775	14.1452	neg
14.15_297.9567m/z	297.956738	14.15365	neg
14.15_299.7763m/z	299.7763248	14.15365	neg
14.15_385.7667m/z	385.766675	14.15365	neg
14.20_287.8840m/z	287.8840245	14.20485	neg
14.21_130.9442m/z	130.9441931	14.2133	neg
14.21_381.2317m/z	381.2317069	14.2133	neg
14.21_399.7016m/z	399.7016011	14.2133	neg
14.21_479.7471m/z	479.7471209	14.2133	neg
14.23_417.2106m/z	417.2106486	14.2269	neg
14.25_209.0043m/z	209.0043388	14.24543333	neg
14.25_296.7942m/z	296.7942345	14.25393333	neg

0.001403199	207.8201839	396.0974839	157.346315	419.8669811	0.001403199	449.5763594	228.3107681	278.3364796	
576588.9609	614292.3905	626642.9711	588470.569	707500.0151	642983.6223	697425.7557	650581.5631	655296.4109	
82043.74072	82875.4198	81723.27478	82476.99337	80953.14659	85679.3964	91240.042	79935.17015	90362.97627	
539.4262994	616.0412095	538.6503246	522.5804645	742.6417415	480.732262	508.4618406	555.3148136	470.3317338	
0.001403199	86.85622767	212.2476835	72.70257179	35.46240454	0.001403199	93.75291923	0.001403199	35.27254027	
191433.0165	195824.3926	196974.8204	193953.3952	217728.6322	208683.4724	218894.5083	200661.6121	212628.6708	
1907.657078	1345.044208	781.3946715	924.4492312	803.7728529	787.8086522	667.3587691	857.9554481	543.401035	
1520383.27	1552660.664	1545781.806	1567787.513	1693300.36	1645569.125	1749524.132	1564909.931	1665342.425	
4797.633809	3116.654115	4564.966134	3255.298122	3485.656358	4405.58589	3731.252221	6589.334306	3019.952161	
263365.4694	277571.7484	290438.4978	271309.5376	325608.4137	303915.7745	317899.1672	290143.7066	303701.8231	
1967.45594	2146.511403	1524.826586	1381.073525	1803.320816	3189.365518	2963.789831	2622.876356	1944.869807	
38719.48857	38591.90852	41084.31925	35310.53707	46874.03938	44895.9187	45727.67243	41813.8787	43335.95947	
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493.080613	1080.862678	522.2476094	373.6556002	561.1152453	245.9711565	1001.273997	892.1281367	331.5512581	
137187.309	151046.2073	152114.8905	149427.9278	167339.4711	148443.9893	170447.7496	150311.0249	159710.8166	
82655.85835	86317.73346	82736.71707	84184.24785	89548.3585	89492.03205	91436.64181	84657.83266	91548.31527	
867.1818368	993.6610351	442.1858975	819.8445034	668.8997991	0.001403199	623.0432833	1057.020391	810.2166332	
7185.878334	6458.324361	7060.994792	7238.423851	5223.586027	6684.608155	7693.797396	5199.979554	4627.079651	
67415.2375	68513.46894	67778.79396	70039.10286	72703.40613	71532.79886	74952.42707	70182.39672	66495.65448	
1719868.294	1706526.704	1701579.343	1676017.712	1785356.923	1740504.503	1891479.143	1732597.895	1773701.183	
707.0183005	1050.174242	327.5668761	900.9592412	527.6980777	772.0757029	975.8706202	933.3949197	1121.336813	
606585.2042	628900.5248	630458.0444	618283.7563	697611.364	656109.9044	718032.136	655450.5999	680718.8266	
1774.832011	1760.411354	1250.405609	1149.361109	1408.927305	1249.467631	1678.754172	1584.72436	1641.839687	
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42861.43645	42529.70003	39925.28488	39498.1881	42886.33679	40786.75707	46461.7877	44984.35549	42949.58405	
197898.1138	195281.466	196187.5842	192770.9376	213499.1941	209790.5381	222011.5786	206163.47	208967.5811	
25593.92341	24734.41796	25847.90671	22020.05228	23807.9843	22797.00914	29077.81355	24929.40143	25910.31705	
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13250.42719	14684.04145	14302.55452	13962.37414	14169.82369	13029.34348	15660.56116	13316.60194	12902.35268	
29342.66708	29665.94571	29614.07894	30868.85095	33108.58183	33567.53801	34168.42428	31366.01898	30887.28168	
156150.2408	167135.6759	166206.2208	157233.5535	184927.938	180596.0273	189886.3653	174260.9121	182778.8678	
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17648.63212	16943.65706	16690.07996	18158.81789	16611.74971	18138.35687	17444.45355	15165.85401	18430.90067	
503485.0654	509057.8602	493965.5614	505232.6132	539147.7266	536245.4057	564021.6464	507005.2309	539122.5607	
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260.1928791	591.1376218	321.9999892	245.957268	314.1686004	200.4390338	216.1928162	493.2191238	362.5281214	
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2355.937918	3262.934879	3205.322139	3097.987	1943.874736	3068.216724	3305.913232	3050.223503	2723.257657	
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95382.53544	96569.03023	93245.91758	88697.83679	100122.066	100184.6921	105449.1492	97613.29494	103270.4897	
170237.1683	167853.0698	156100.6682	158972.3356	169410.8139	167466.2716	177963.3195	162085.4441	172490.8961	
819.2312129	408.4321398	635.3667476	1252.763993	799.9169487	533.0822222	1109.160092	481.3068917	291.351721	
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32226.38652	32200.29489	30761.63223	30490.76466	32098.41008	30667.0369	36790.80723	33042.76251	32486.92774	
607.3139482	896.3051588	725.3787135	736.2859817	978.4487574	767.1330736	819.6052849	879.7274437	704.4509723	
672.1005107	490.6970689	1033.013939	649.618993	1138.737157	499.5267329	731.3351748	1030.344342	1019.543135	
96926.52316	97245.51532	93022.2099	91345.2099	101922.5324	101251.0554	108736.6599	97359.65961	103501.1359	
930.5578705	1240.898872	1665.454218	988.8834664	205.9561683	446.9944533	1278.52557	1192.507519	1605.107861	
6443.135714	6291.295552	5636.242543	4416.056141	5553.216378	5315.39047	6155.332535	6291.840403	5952.215634	
637.3093571	597.798554	754.7999205	695.1647608	384.9012884	924.6218736	755.1302293	434.3249632	163.9108095	
342.2776765	439.1628114	0.001403199	363.1741	652.2649583	0.001403199	0.001403199	446.3252029	823.8998697	
563317.5546	558561.6012	540891.3436	545623.6803	579884.2337	579036.1004	615371.8786	550407.841	589998.6614	
0.001403199	141.2159527	167.4037625	0.001403199	120.6709362	264.5516041	0.001403199	0.001403199	129.2942615	
1361.368035	1234.400866	1182.656142	1037.820824	679.0480739	1007.307312	1550.08634	1254.424118	722.0438288	
1307.830749	1243.683521	1006.807274	1687.298781	1718.846888	2341.9196	1705.472425	1785.23216	1686.226054	
1202.837867	1207.652874	1237.301573	805.3312103	1206.179979	899.8182251	1100.770478	882.0796032	1520.753335	
14368.162	14331.3561	12754.35856	12456.03164	14293.0313	13594.59864	15006.90575	13766.01223	14074.08898	
83321.44435	85962.07554	83904.68457	86629.34055	93236.99468	89826.76071	96823.14594	85295.25323	91207.20147	
7491.102789	7651.442264	6884.111668	5213.925872	7733.700726	7248.368621	8293.447332	8946.77191	7972.425589	
2775.747876	2046.448104	2602.499038	2498.733259	2276.156093	2583.579657	2229.966563	2090.336632	1892.67982	
2478.096244	2195.566462	2962.76981	1733.295527	2065.575703	2571.042817	592.0751703	1967.865318	2030.536348	
5154.133908	2923.420391	4449.875253	849.1240625	741.4546688	1042.753974	4270.067388	2511.871033	1827.262411	
1451.27512	1396.396462	1022.716103	486.1426471	1124.556818	999.16216	1797.211759	3410.855084	1728.968628	
182187.9322	194321.0747	201120.8933	176588.742	217411.5052	200199.5753	230949.7423	207659.8204	212584.042	
38115.23937	40184.56095	38678.59669	36235.82652	40124.30426	37314.31857	43448.67549	38758.01096	40518.62015	
2833.962312	2172.052921	2901.7201	2935.557457	1978.4905	3216.993827	3468.426933	1974.8377	2597.602446	
4770.113642	4495.811017	4937.492661	3987.884069	4912.660104	4648.042785	5025.156074	5015.644358	5681.913241	
522323.4143	519250.467	530131.2692	532064.5035	573628.6546	577863.453	598546.5575	539708.0845	576653.1818	
613.479246	994.6637822	292.032081	1568.100963	598.8236714	420.3573371	1030.538532	947.8216011	1365.454941	
3147.977477	2274.086487	1178.232893	2722.080639	2467.417544	2839.61868	2111.520052	1802.632605	2683.141735	
2319.269684	2035.201113	1398.132266	2651.74218	2061.107964	2407.755069	1817.318921	1104.317698	2322.748643	
2777.72456	1866.445941	2395.849073	2764.806182	2419.204386	2482.727828	2763.290731	2671.644421	2479.095636	
603.8536203	505.6377037	1213.799747	843.5213028	1144.927022	1052.438532	1864.709535	1634.003506	1038.39997	
390.5690627	463.1658541	531.3022705	366.5021303	356.3891408	399.1251998	752.1932744	654.933404	400.3636176	
157246.2197	156780.6548	162591.5	167431.4313	188988.4914	192251.3993	184891.5031	174116.6344	186076.727	
25883.24186	25497.38409	25274.02609	25007.49212	26802.38555	26541.69135	28278.00603	27073.45081	27324.06133	
734.2433592	677.1614183	485.0866375	303.3700112	477.5509436	843.2289307	932.3632453	663.6689199	809.949528	
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117.5631049	171.4701586	63.27575281	410.8581971	80.49306723	185.3913517	380.2548407	139.5626984	109.7567013	
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42474.5371	16183.25891	17330.63254	13447.82832	17782.98343	17569.55404	17428.61152	39353.42406	18432.06955	
20332.46721	20599.53588	23822.69871	17737.54056	26039.26506	19382.39376	24544.87361	22709.61357	24443.87278	
1626.769194	1590.810023	1675.764229	1184.886671	1875.654217	1431.908568	1675.57204	2498.670289	2042.645228	
3042.21501	3151.646325	1731.1844	1787.479462	2711.484698	2488.854851	2079.183701	2794.001968	3450.250258	
584.9251258	449.7255988	535.3661055	692.9706322	389.6619011	607.5917512	357.0279239	808.4315522	393.1936804	
1452.883571	920.895215	1281.01467	1427.185171	1611.073598	983.4388297	1139.02368	1549.092445	2256.844857	

14.25_374.8106m/z	374.8105693	14.25393333	neg
14.25_494.7889m/z	494.7889058	14.24543333	neg
14.25_602.5855m/z	602.5855464	14.25393333	neg
14.26_265.1479m/z	265.1479182	14.26236667	neg
14.26_321.2106m/z	321.2105962	14.26236667	neg
14.26_425.2580m/z	425.257968	14.26236667	neg
14.28_433.3451m/z	433.3451461	14.28438333	neg
14.28_472.7616m/z	472.7615979	14.28438333	neg
14.31_554.7208m/z	554.7208192	14.30818333	neg
14.33_100.9257m/z	100.9257489	14.3287	neg
14.37_296.7941m/z	296.7940974	14.37456667	neg
14.40_270.8620m/z	270.8620053	14.39986667	neg
14.42_158.9755m/z	158.9754974	14.4204	neg
14.45_280.8982m/z	280.8982491	14.45468333	neg
14.45_740.5243m/z	740.5242694	14.45468333	neg
14.46_116.9229m/z	116.9229054	14.46495	neg
14.46_135.9709m/z	135.9709131	14.46495	neg
14.46_213.9639m/z	213.9638969	14.46495	neg
14.46_293.1794m/z	293.1794282	14.46495	neg
14.46_309.1743m/z	309.1743222	14.46495	neg
14.46_311.1688m/z	311.1687921	14.46495	neg
14.46_337.2057m/z	337.2056876	14.46495	neg
14.49_209.0043m/z	209.0043194	14.48676667	neg
14.49_347.2341m/z	347.2340962	14.48676667	neg
14.49_374.8106m/z	374.8106057	14.48676667	neg
14.51_877.0286m/z	877.0285956	14.51281667	neg
14.52_797.0409m/z	797.0409146	14.52215	neg
14.52_914.0247m/z	914.0247389	14.52215	neg
14.53_197.8566m/z	197.8565884	14.52905	neg
14.54_270.8620m/z	270.8619862	14.54401667	neg
14.54_297.1530m/z	297.1529771	14.54401667	neg
14.54_811.0179m/z	811.0179499	14.53538333	neg
14.58_691.0170m/z	691.0170236	14.57938333	neg
14.58_787.0123m/z	787.0122713	14.57938333	neg
14.59_353.2004m/z	353.2004245	14.58646667	neg
14.60_100.9257m/z	100.9256943	14.60391667	neg
14.60_347.2339m/z	347.2338985	14.59525	neg
14.61_797.0410m/z	797.0410336	14.61425	neg
14.62_655.1593m/z	655.159265	14.62056667	neg
14.63_559.1569m/z	559.1568924	14.63088333	neg
14.65_209.0043m/z	209.0042966	14.6516	neg
14.65_379.2521m/z	379.2520794	14.6516	neg
14.65_657.5055m/z	657.5055201	14.6516	neg
14.66_368.2418m/z	368.2418379	14.6619	neg
14.66_419.2393m/z	419.2392578	14.6619	neg
14.66_589.5179m/z	589.5178601	14.6619	neg
14.67_158.9754m/z	158.9754474	14.67045	neg
14.67_899.0505m/z	899.0504951	14.67045	neg
14.67_916.0408m/z	916.0407864	14.67045	neg
14.67_970.9793m/z	970.9793446	14.67045	neg
14.68_228.9557m/z	228.9556951	14.68256667	neg
14.68_381.2318m/z	381.2318065	14.68256667	neg
14.69_247.9600m/z	247.9599696	14.68933333	neg
14.69_789.0290m/z	789.02896	14.68933333	neg
14.69_799.0570m/z	799.0570474	14.68933333	neg
14.70_166.0441m/z	166.0440887	14.69558333	neg
14.70_208.0138m/z	208.0138045	14.69558333	neg
14.70_223.0284m/z	223.0283708	14.69558333	neg
14.70_240.0671n	239.0598266	14.69558333	neg
14.70_297.0472m/z	297.047159	14.69558333	neg
14.70_793.1679m/z	793.1678966	14.69558333	neg
14.70_797.0412m/z	797.0411651	14.69558333	neg
14.70_803.1968m/z	803.1968195	14.69558333	neg
14.70_820.1869m/z	820.1868876	14.69558333	neg
14.71_129.9363m/z	129.9363213	14.71336667	neg
14.72_102.9568m/z	102.9568255	14.72186667	neg
14.76_218.8581m/z	218.8581274	14.7582	neg
14.77_274.8125m/z	274.8124806	14.7654	neg
14.79_132.9002m/z	132.90023	14.79188333	neg
14.79_134.8947m/z	134.8946794	14.79188333	neg
14.79_136.8917m/z	136.8916602	14.79188333	neg
14.79_212.9992m/z	212.9992097	14.79188333	neg
14.79_321.2109m/z	321.2108673	14.79188333	neg
14.80_173.9261m/z	173.9261425	14.79928333	neg
14.87_999.0441m/z	999.0440884	14.86661667	neg
14.91_1099.2716m/z	1099.271637	14.9138	neg
14.91_141.0208m/z	141.0207756	14.9138	neg
15.00_193.9425m/z	193.9425377	15.00176667	neg
15.02_867.1871m/z	867.1870713	15.02455	neg
15.02_869.1853m/z	869.1853372	15.02455	neg
15.02_894.2062m/z	894.2061707	15.02455	neg
15.03_141.0208m/z	141.0207844	15.03281667	neg
15.05_116.9215m/z	116.9214724	15.04768333	neg
15.05_223.0284m/z	223.028438	15.05453333	neg
15.05_241.0633m/z	241.0632843	15.05453333	neg
15.05_246.9053m/z	246.9052538	15.05453333	neg
15.05_313.0787m/z	313.0786566	15.05453333	neg
15.05_877.2155m/z	877.2155441	15.05453333	neg
15.06_193.9425m/z	193.9425099	15.0628	neg
15.08_285.0653m/z	285.0653095	15.07821667	neg
15.09_802.9497m/z	802.9496773	15.08646667	neg
15.09_881.9867n	862.9688192	15.08646667	neg
15.09_965.9765m/z	965.9765183	15.08646667	neg
15.10_822.9564m/z	822.956366	15.09626667	neg
15.10_842.9625m/z	842.9624559	15.09626667	neg
15.10_928.9805m/z	928.980545	15.09626667	neg
15.12_213.9639m/z	213.9639288	15.1201	neg
15.17_1137.9640m/z	1137.964023	15.16735	neg
15.17_193.9425m/z	193.9425176	15.16735	neg
15.17_298.9573m/z	298.9572503	15.16735	neg
15.25_1043.0508m/z	1043.050816	15.24691667	neg
15.25_982.9690m/z	982.9689834	15.25375	neg
15.31_314.0780m/z	314.0780223	15.30628333	neg
15.31_951.2344m/z	951.2344207	15.30628333	neg
15.31_968.2242m/z	968.2242179	15.30628333	neg
15.36_1045.0656m/z	1045.065591	15.35553333	neg
15.41_298.9573m/z	298.9573487	15.40808333	neg
15.45_201.9970m/z	201.9970374	15.45366667	neg
15.46_225.0130m/z	225.0129798	15.4605	neg
15.49_1025.2531m/z	1025.253105	15.49083333	neg

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2203.232495	1360.028829	1838.269194	2179.273213	2053.76433	1841.323142	1680.7476	2615.525705	2363.093438	
815.6988681	1153.731512	173.777542	396.1546728	351.9638845	772.2759667	436.3615796	451.3645237	213.7231835	
158151.0782	156467.8153	152684.1264	135419.0466	154461.8854	146387.7114	176407.1891	168532.9456	167903.4361	
13560.67168	10102.9902	12800.96596	8494.417066	9129.695047	10936.90356	10340.36082	12818.23799	12104.22751	
26110.18468	9408.677903	10387.58514	6715.711451	10423.54517	11012.02723	10067.00788	22869.78544	10918.13158	
3130.925496	2013.629232	2015.411313	2118.155122	3144.908083	2593.199435	2632.289751	3530.80883	5020.421201	
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2724.761101	1729.082634	1855.90515	2342.934322	2559.02448	1736.449836	2252.616727	1591.906417	3163.510688	
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532.532609	624.5108051	732.5361669	502.0989038	532.3530995	502.9779386	906.0528355	581.5736566	453.5236604	
491.9017054	718.3758525	714.188198	488.4565036	737.5004928	739.263116	834.3911977	1457.041114	472.4153611	
54133.06758	57877.06336	46754.06406	32724.37821	40593.34082	43656.92056	55216.66762	46142.98048	48674.18171	
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34104.12509	33400.09899	33707.77883	28791.65917	33564.54572	31789.83521	38857.91619	33583.00105	34666.73591	
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45468.95411	45446.5103	46183.33605	40551.08366	46280.04826	44496.34414	54538.64207	51726.51695	53903.49188	
172389.213	170398.3149	162873.2336	145845.9776	168167.711	163549.6919	195056.7309	186465.8825	183335.7255	
33212.66559	32116.48191	30934.16747	27932.57045	33308.49488	31269.45307	38007.48167	36581.33549	37552.86124	
1043.565456	1384.638678	974.4211234	902.6575655	795.1950521	1127.650237	1415.687867	1236.202398	782.3083227	
964.7679236	982.191058	843.6523323	454.4741468	624.5705331	1069.731151	1521.627876	1066.934825	684.514691	
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5031.786351	4708.104517	4529.508774	3463.574556	4202.721987	2993.20207	5285.474786	2773.626689	3759.590502	
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3500.512531	3153.110808	2136.86495	3769.153887	3777.201566	3210.90627	2648.946659	2635.374084	2961.10445	
3988.95378	3793.680671	3880.305773	3134.365971	4250.675741	2962.32983	3737.151948	3527.597622	4724.491427	
2225.603449	2919.393803	3125.696153	1810.715284	2273.524719	1762.439704	3409.741866	2461.539735	3242.568344	
7643.920363	8402.695528	7820.505506	6852.768892	8168.588708	7541.876015	9281.883486	9387.13992	10159.44656	
80.819115	59.5258251	80.03987947	103.2603269	126.9637259	131.9361519	96.27778651	80.82853567	111.7028215	
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4299.602727	4372.646929	4229.470296	3415.674157	4208.498796	3165.160492	4417.07236	4450.505625	4397.945457	
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1849.640434	1475.823281	2347.132977	1578.77163	1306.685206	1004.689297	1561.630251	1104.551956	1127.107352	
8183.504167	6198.128795	6205.811674	4627.763292	5703.140319	5570.215287	6292.56952	5495.879093	5255.065734	
24045.56888	20477.12353	21353.20403	16527.06625	20625.72802	18862.91605	22070.77843	18558.91853	20677.58354	
5312.446497	3283.811101	4122.637663	2192.820902	3075.247981	3019.419694	3799.667324	2724.187962	3374.604431	
1343.827827	1167.04513	1290.043107	1277.291259	1333.275384	1355.851313	1462.699657	1516.528738	1234.065917	
63429.16661	61413.73679	54230.96283	55958.55025	59400.9975	53527.92969	67336.14636	60128.80346	61231.54349	
3136.215331	6095.462229	3875.323197	4668.022549	4480.136521	4491.600752	5381.149951	5150.356738	4911.000219	
1366.182041	3496.673505	1865.089028	2660.654808	3307.924721	2926.11083	2515.253105	3430.259094		
1141.448621	1014.176303	995.2188784	1077.900601	1532.914068	1527.638554	1399.207851	1582.914939	1277.444889	
9119.958975	10235.25677	9319.049818	8965.851288	10062.45925	9748.533973	11671.1861	12070.13111	12099.70246	
492.8640125	640.2470201	618.9892534	443.974645	993.2777284	921.174808	807.1426292	893.0818672	785.0730881	
808.6272993	1813.363176	2145.985071	1483.429924	2204.015551	1274.974316	1605.076178	2102.595865	2066.80918	
16822.78701	18716.62295	15980.63979	17604.72681	20179.15205	17694.62607	20458.76434	17204.62709	16491.61293	
6726.50921	0.001403199	0.001403199	612.2221363	2.244947096	0.059444494	0.084999941	0.002806398	0.001403199	
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550695.1584	13132.67908	8754.553555	180808.1853	20760.53588	11148.29441	6548.42365	8536.224833	6083.868788	
16293.60792	1398.564397	1399.652647	1100.082269	933.834713	478.4868016	600.6201137	947.5414982	498.1055337	
789179.3729	804.0656791	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	
4761.424971	5259.149646	3924.256536	5555.845577	4261.214655	4815.138345	6358.473816	6029.399827	4801.666091	
3316557.985	17545.07936	2520.409422	1037.188691	2214.105212	1370.166405	3076.880772	1020.475448	1497.70373	
454718.4945	320.9016785	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	
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89.61160462	235.6871269	223.5666795	180.6374933	185.7125248	169.9702736	288.1316491	201.8932925	152.178851	
38.14682037	115.1753015	153.9134613	0.67724992	212.1704285	72.4499834	131.1055897	163.6450117	117.6753414	
1639.290877	3265.56991	3342.943013	2438.481724	3117.905742	3409.72963	4011.584759	2741.596441	3513.695698	
53930.97524	53707.20639	54092.78909	52999.75564	57018.23068	55060.59327	62327.93394	56906.22578	58819.82913	
1270760.326	1256799.935	1252822.705	1236896.997	1330222.143	1282359.833	1443108.56	1318581.961	1363984.05	
427911.6405	423663.5365	422015.1341	415130.8446	446619.6243	428855.1434	484565.4791	443730.7595	459419.0661	
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11.22734129	292827.2761	658.2123253	12.85745535	13.48694855	10.33274905	19.08913139	25.75987667	37.41401555	
405.8891871	367.6907629	381.9539483	398.4371334	388.4709124	313.9481912	493.2078917	325.4900064	366.3163465	
5285.266467	6302.618857	5537.42924	6998.345413	6112.382821	5533.893347	6718.217354	6763.288003	6883.853901	
61038.18199	337366.2695	32659.99482	122465.8185	4801.41917	23864.6792	120336.7897	11078.04669	22568.83197	
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4314.094441	4459.494877	4212.005741	3242.281353	3434.339173	3183.513436	4471.614214	4569.766035	4461.322645	
70808.47558	461500.4189	31669.86537	153748.8291	39546.10306	28039.03092	24017.46471	23677.34805	24238.97646	
3951.521617	3278617.651	27287.65008	1893.671459	3117.244184	2849.796449	8643.426813	4333.450447	5849.94335	
231.1556793	253.901138	326.7668627	194.8349982	251.0384662	252.5118631	289.2319088	273.0281471	139.0264453	
352.259818	4403.95713	207.6213803	775.500302	102.2821146	58.9356568	77.47282692	10.46766233	47.33377366	
1873.544011	566.7318364	1305.171346	1629.642988	1613.972648	1092.45836	1736.106971	1652.729683	1572.103946	
38750.19861	28395.01787	33384.13872	31347.85547	40172.69982	29442.43549	38013.49159	38829.52401	41055.69172	
2673.224212	1427.975138	2035.696571	1696.30124	2117.234038	2100.126321	2439.158346	2740.94212	2680.343849	
10452.53397	7120.088943	9163.74261	9489.662239	10924.15336	8651.3128	10717.69378	11050.09756	12247.00706	
39058.98523	29966.64374	33960.60348	32264.44175	39976.67952	29969.81647	38120.89894	39495.75303	42184.54407	
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354.5449649	365.5191689	426.5173586	271.1432407	388.5389331	239.9418343	485.7659262	360.9480787	554.1224334	
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604.0938841	649.9447742	793.2758437	672.2739617	620.2948051	557.6814275	617.2563203	819.9330101	862.8417266	
902.3014898	700.2041446	1087.160564	794.7330439	872.5237329	1118.549797	599.5488644	1199.725313	1152.848174	
21635.38479	19303.71963	18817.46354	15894.63601	17389.81588	12608.44194	16641.02473	28397.07888	19141.80033	
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7765.846066	12279.80968	3992.772173	15433.96043	15161.87294	5041.859178	117366.8146	4481.860735	4515.343987	
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159.3292261	89.71782896	69.00436665	42.108201	89.42800591	92.58729946	131212.885	974.1127927	11.04746709	
6218.585005	5694.592142	5469.636799	5762.996276	4427.405856	3889.430253	5744.095826	7977.396951	5647.509451	
1391.292723	1303.825288	1233.081554	1121.243366	1172.654756	1588.817573	1459.832598	1260.730087	1466.802843	
866.8523717	937.9690244	846.6610605	988.3566412	985.6120846	1303.89071	1275.319498	1046.667925	1125.688048	
22428.003	21541.79028	23047.7494	23553.09618	26295.4725	25862.811	25606.54752	25094.48872	26744.74056	
0.001403199	127.1147893	0.001403199	0.001403199	169038.4603	11233.62112	15.49816063	59.99475804	59.17372462	

| | | |

2.17_477.8653m/z	477.8653305	2.172	neg
2.17_530.7924m/z	530.7923914	2.172	neg
2.18_229.9931m/z	229.9930954	2.180683333	neg
2.18_295.9848m/z	295.9847644	2.180683333	neg
2.18_312.9751m/z	312.9751309	2.180683333	neg
2.18_545.8539m/z	545.853911	2.180683333	neg
2.19_363.9724m/z	363.9723801	2.194566667	neg
2.19_364.0878m/z	364.087808	2.194566667	neg
2.19_376.0385n	421.036825	2.194566667	neg
2.19_431.9594m/z	431.9593895	2.194566667	neg
2.19_432.0752m/z	432.0751733	2.194566667	neg
2.19_489.0242m/z	489.0242236	2.194566667	neg
2.20_234.9814m/z	234.9813756	2.203283333	neg
2.20_245.0102m/z	245.0102031	2.203283333	neg
2.20_262.0003m/z	262.0003331	2.203283333	neg
2.20_276.9477m/z	276.9477089	2.203283333	neg
2.20_296.9721m/z	296.9721191	2.203283333	neg
2.20_308.0510n	353.049317	2.203283333	neg
2.20_312.9979m/z	312.9978954	2.203283333	neg
2.20_344.9349m/z	344.93491	2.203283333	neg
2.20_380.9856m/z	380.985641	2.203283333	neg
2.20_448.9727m/z	448.9727316	2.203283333	neg
2.20_500.0630m/z	500.0629651	2.203283333	neg
2.20_516.9600m/z	516.9599753	2.203283333	neg
2.20_584.9476m/z	584.9476488	2.203283333	neg
2.22_124.0404m/z	124.0403635	2.215433333	neg
2.22_152.9046m/z	152.9046088	2.215433333	neg
2.22_217.9891m/z	217.9891285	2.215433333	neg
2.22_412.9215m/z	412.9215326	2.215433333	neg
2.22_435.9110n	870.8029184	2.215433333	neg
2.22_516.8375m/z	516.8375338	2.215433333	neg
2.22_526.7931m/z	526.7930703	2.215433333	neg
2.22_577.7904m/z	577.7904262	2.215433333	neg
2.22_704.8159m/z	704.8158543	2.215433333	neg
2.22_724.8008m/z	724.8008003	2.215433333	neg
2.23_355.8596m/z	355.8595509	2.227683333	neg
2.23_370.9576m/z	370.9576161	2.227683333	neg
2.24_148.9732m/z	148.9732064	2.236416667	neg
2.24_357.0831m/z	357.0831398	2.236416667	neg
2.24_456.9108m/z	456.9107713	2.236416667	neg
2.24_509.8030m/z	509.8029961	2.236416667	neg
2.24_584.8260m/z	584.8260442	2.236416667	neg
2.24_676.7966m/z	676.7966037	2.236416667	neg
2.25_264.0913m/z	264.0912515	2.248516667	neg
2.25_281.0256m/z	281.0256194	2.248516667	neg
2.25_322.8312m/z	322.8312343	2.248516667	neg
2.25_462.1234m/z	462.1234008	2.248516667	neg
2.25_524.8982m/z	524.8982109	2.248516667	neg
2.25_569.8507m/z	569.8507364	2.248516667	neg
2.25_812.7705m/z	812.7705511	2.248516667	neg
2.26_105.9359m/z	105.9358583	2.26065	neg
2.26_303.0836m/z	303.0836344	2.26065	neg
2.26_394.1357m/z	394.1356537	2.26065	neg
2.26_606.9582m/z	606.9581929	2.26065	neg
2.27_149.4750m/z	149.4750316	2.27405	neg
2.27_388.9234m/z	388.923373	2.27405	neg
2.27_470.9830m/z	470.9830247	2.27405	neg
2.27_538.9706m/z	538.9705633	2.27405	neg
2.27_639.9107m/z	639.9107475	2.27405	neg
2.28_148.0525n	295.0936149	2.2828	neg
2.28_184.8898m/z	184.8898133	2.2828	neg
2.28_299.9734m/z	299.9733955	2.2828	neg
2.28_358.0057m/z	358.0056912	2.2828	neg
2.28_377.9897m/z	377.9897315	2.2828	neg
2.28_425.9930m/z	425.9930159	2.2828	neg
2.28_435.9484m/z	435.948403	2.2828	neg
2.28_436.0217m/z	436.0216733	2.2828	neg
2.28_445.9771m/z	445.9771395	2.2828	neg
2.28_513.9645m/z	513.9645252	2.2828	neg
2.28_571.9235m/z	571.9235133	2.2828	neg
2.28_581.9522m/z	581.9521922	2.2828	neg
2.28_629.9558m/z	629.9557842	2.2828	neg
2.28_659.8950m/z	659.8949895	2.2828	neg
2.28_707.9717m/z	707.971653	2.2828	neg
2.28_717.9272m/z	717.9272571	2.2828	neg
2.28_785.9144m/z	785.9144478	2.2828	neg
2.29_191.9463m/z	191.9462839	2.294983333	neg
2.29_210.0384m/z	210.0384215	2.294983333	neg
2.29_249.0493m/z	249.0493227	2.294983333	neg
2.29_320.9358m/z	320.9357644	2.294983333	neg
2.29_367.9609m/z	367.960865	2.294983333	neg
2.29_493.9805m/z	493.9804547	2.294983333	neg
2.29_503.9362m/z	503.9362059	2.294983333	neg
2.29_571.9966m/z	571.9966305	2.294983333	neg
2.29_591.9072m/z	591.9072008	2.294983333	neg
2.29_639.9842m/z	639.9841919	2.294983333	neg
2.29_649.9398m/z	649.9397641	2.294983333	neg
2.29_775.9593m/z	775.9592896	2.294983333	neg
2.30_222.0304m/z	222.0304136	2.303733333	neg
2.30_328.0677m/z	328.0676885	2.303733333	neg
2.31_286.9845m/z	286.9844826	2.3142	neg
2.31_414.9460m/z	414.946047	2.3142	neg
2.31_428.9618m/z	428.9618164	2.3142	neg
2.32_352.1154m/z	352.1153612	2.322933333	neg
2.32_360.9745m/z	360.9744939	2.322933333	neg
2.33_191.0351m/z	191.0350539	2.331716667	neg
2.33_286.9498m/z	286.9498012	2.331716667	neg
2.33_367.0344m/z	367.0343545	2.331716667	neg
2.35_209.0069m/z	209.0068882	2.34905	neg
2.35_224.9994m/z	224.9994106	2.34905	neg
2.35_241.9207m/z	241.9207025	2.34905	neg
2.35_276.9943m/z	276.9943054	2.34905	neg
2.35_292.9870m/z	292.9870297	2.34905	neg
2.35_344.9818m/z	344.9817638	2.34905	neg
2.35_412.9693m/z	412.9693324	2.34905	neg
2.35_490.9126m/z	490.9126386	2.34905	neg
2.36_175.0144m/z	175.0144085	2.36465	neg
2.36_177.0115m/z	177.0114956	2.36465	neg
2.36_185.0432m/z	185.043189	2.36465	neg
2.36_202.0335m/z	202.0334807	2.36465	neg

2747.547646	2265.631413	2484.009357	3196.580308	2785.301305	2441.00252	2324.185344	2730.858197	3222.083909	
5347.288819	4241.65227	4351.122245	4249.533289	4162.358143	4120.046396	4898.359048	3954.368368	4985.526592	
1882.57921	1640.046478	2033.953717	0.001403199	23.12196625	35.33379344	1500.655172	1631.403564	1550.550116	
9161.950168	8148.867456	9392.085194	543.5804791	613.6480661	575.1005283	8213.607553	9154.395647	8756.145561	
1765.483549	1052.20402	1695.380238	41.90415434	0.001403199	0.001403199	866.3706987	1145.723452	1670.646457	
5204.311576	5063.76719	4991.924113	5819.060704	5560.487326	5640.89178	6136.277013	5644.102417	5545.341333	
2361.019893	1921.699958	2574.75756	50.89192594	0.001403199	0.001403199	1394.386506	2097.131904	2018.807752	
5774.575613	4571.540494	6170.134138	6373.49215	5640.776577	5674.783572	4794.085108	5205.805652	5082.883249	
1722.474629	1631.6703	1950.962245	101.9553712	74.16306123	106.6457143	4267.234246	4807.905297	4641.514111	
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2697.474898	2111.796409	3033.798565	3228.140246	2890.864625	3279.307298	1871.124157	2923.276172	2408.420747	
873.906656	892.3144109	1120.157316	149.1593794	74.89821783	67.3905942	3153.492228	3208.561227	2445.557824	
1951.736177	1624.782715	1964.114245	2663.313931	2432.776536	2465.222943	1966.465617	2084.00223	1908.555539	
14282.96012	13135.71562	14873.71695	19991.31628	18696.02558	19667.37229	14529.5318	16186.32714	14280.8959	
2692.042417	2389.113811	2835.608068	4057.373245	3826.440967	3775.541817	2727.788419	3061.771617	3067.491715	
2175.501767	1743.759571	2104.243268	2442.379609	2401.856496	2335.36224	1804.408248	2244.696654	1880.934333	
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3842.147608	3580.572525	4098.902457	453.2066427	237.6285761	398.1332109	10597.07459	11264.52307	10587.64085	
5634.744227	5379.044245	6199.336301	8082.935439	7636.734643	8103.201853	6433.100332	6692.979976	5795.520336	
1253.831713	1225.960782	1355.603262	1225.852444	1410.225062	1222.946026	795.4907309	1193.195811	809.5222874	
4623.104129	4314.190322	5184.814295	6122.079638	6400.034219	6604.020117	4418.282804	5559.86118	4773.16361	
4423.600492	4461.578334	4647.935972	6049.384974	5853.888448	5940.085181	4425.282785	4900.60944	4016.985769	
1490.848071	1241.049126	1481.046503	1938.644345	1776.451022	1582.243039	1022.748592	1450.178824	1502.624085	
3054.592873	3021.353393	3056.193851	4189.248532	3622.68207	3949.818904	2673.978652	3000.76112	2705.011736	
1898.463857	1740.263805	2072.319059	3055.203335	3032.544275	3254.034683	2023.125462	2348.032253	1999.005107	
268.1131616	302.6655599	466.5262065	311.6603867	385.5628784	368.0708915	242.2862837	337.3556454	335.0642695	
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44646.30484	48844.47608	56753.192	3162.942083	3017.129461	3116.401685	31713.66035	38109.36601	34005.81806	
1647.026223	786.6501643	1463.036849	1899.491991	1605.312162	1332.090898	946.5008354	1317.630035	1320.460141	
13133.30477	11792.85201	13171.02176	15501.60904	16584.06747	15824.78075	15333.77741	13510.27879	14189.77934	
3867.968075	4558.061578	4660.420279	6276.415909	5913.269748	6647.642441	6588.35723	6736.417121	6500.622608	
2622.18613	2320.107264	2169.702281	2956.15547	2538.746866	2495.605805	3048.180863	2071.430362	2328.235921	
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3270.7366	3823.313226	4268.765184	3973.056023	5767.240206	5068.500919	4629.469331	4527.887721	6399.15052	
16987.36731	14151.28813	14971.79356	16271.56835	17714.69299	16931.84903	20864.10081	13850.7336	17356.69051	
1755.007474	1206.846558	1626.43273	1237.260656	1296.116788	1148.515358	1110.600545	1028.748537	1102.181523	
2395.238715	2010.14269	2705.423645	2863.064345	2903.670804	3428.668199	2880.015884	2508.916945	2383.706149	
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94035.91822	81388.56939	73630.26712	79591.62245	81499.79023	78625.35389	95931.6066	73255.60422	78754.48911	
1915.996931	1504.210599	1892.020204	2962.145872	2514.428375	2335.926888	1591.761674	1881.146421	2387.590212	
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156.2386914	149.509305	129.3650523	190.187344	133.2982112	238.0492587	221.3607837	164.902187	168.2164582	
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1014.109663	1005.917913	872.1621911	1574.348023	1393.87284	1587.795475	1375.196514	1293.590228	1404.171116	
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1730.99665	1664.471586	1373.186907	755.8393423	752.9477364	798.637541	1025.456343	1066.6779	1105.198911	
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2616.884184	2240.852956	2056.335803	2298.577242	2771.506482	2201.19932	2064.691352	2221.120315	2401.68684	
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343.735524	340.853987	311.441917	445.7219539	479.4839713	412.9107281	302.3426938	492.341215	481.7965199	
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2686.900855	2632.019524	1927.229463	2462.381712	2888.119547	2670.227152	2653.619384	2964.896105	2464.371841	
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2387.736586	1936.936263	1952.215602	414.3936896	293.3469244	578.6429082	196.313397	207.3720378	240.6375682	
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25944.628	25646.2895	27936.66091	46666.87917	47866.52569	45812.57412	35586.15385	40045.09104	39695.08212	
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2.36_206.9518m/z	206.9517958	2.36465	neg
2.36_257.1008m/z	257.1008413	2.36465	neg
2.36_259.9625m/z	259.9625232	2.36465	neg
2.36_261.9782m/z	261.9782205	2.36465	neg
2.36_285.9754n	284.9680879	2.36465	neg
2.36_321.0182m/z	321.0182186	2.36465	neg
2.36_326.9746m/z	326.9745828	2.36465	neg
2.36_352.9556m/z	352.955622	2.36465	neg
2.36_389.0058m/z	389.0058419	2.36465	neg
2.36_421.9504n	420.9431149	2.36465	neg
2.36_446.9645m/z	446.96455	2.36465	neg
2.36_463.9250m/z	463.9249582	2.36465	neg
2.36_488.9306m/z	488.930634	2.36465	neg
2.36_514.9518m/z	514.9517821	2.36465	neg
2.36_524.9807m/z	524.9806696	2.36465	neg
2.36_531.9126m/z	531.9126408	2.36465	neg
2.36_548.9443m/z	548.9442942	2.36465	neg
2.36_556.9181m/z	556.9181186	2.36465	neg
2.36_728.9430m/z	728.9430335	2.36465	neg
2.38_174.0854m/z	174.0853596	2.380333333	neg
2.38_190.9822m/z	190.9822463	2.380333333	neg
2.38_192.0085n	237.0052283	2.380333333	neg
2.38_241.0695m/z	241.069548	2.380333333	neg
2.38_251.9495m/z	251.9495081	2.380333333	neg
2.38_256.9739m/z	256.973895	2.380333333	neg
2.38_273.9641m/z	273.9640789	2.380333333	neg
2.38_279.9631n	324.9613308	2.380333333	neg
2.38_309.0569m/z	309.0569455	2.380333333	neg
2.38_310.9895m/z	310.9894999	2.380333333	neg
2.38_346.9433m/z	346.943341	2.380333333	neg
2.38_356.8988m/z	356.8987603	2.380333333	neg
2.38_377.0446m/z	377.0445807	2.380333333	neg
2.38_378.9769m/z	378.9769166	2.380333333	neg
2.38_395.9375m/z	395.9375099	2.380333333	neg
2.38_438.1246m/z	438.1246104	2.380333333	neg
2.38_660.9558m/z	660.9558259	2.380333333	neg
2.39_264.8819m/z	264.8818888	2.390833333	neg
2.39_276.0548m/z	276.0548463	2.390833333	neg
2.39_344.0424m/z	344.042381	2.390833333	neg
2.39_392.9488m/z	392.9488352	2.390833333	neg
2.39_460.9367m/z	460.9366503	2.390833333	neg
2.40_280.0417m/z	280.041658	2.399566667	neg
2.42_212.0542m/z	212.0541795	2.415216667	neg
2.42_423.0774m/z	423.0774346	2.415216667	neg
2.43_407.8822m/z	407.8822141	2.429083333	neg
2.44_326.9035m/z	326.9035013	2.441233333	neg
2.44_384.8624m/z	384.8623698	2.441233333	neg
2.44_411.8813m/z	411.8812538	2.441233333	neg
2.44_462.8055m/z	462.8054574	2.441233333	neg
2.44_516.8378m/z	516.8378095	2.441233333	neg
2.45_365.8883m/z	365.8883086	2.451266667	neg
2.45_452.8499m/z	452.8498514	2.451266667	neg
2.45_462.8786m/z	462.8785866	2.451266667	neg
2.45_520.8370m/z	520.8370302	2.451266667	neg
2.45_598.8536m/z	598.8536283	2.451266667	neg
2.45_625.7989m/z	625.7989473	2.451266667	neg
2.45_673.8017m/z	673.8016974	2.451266667	neg
2.45_792.7876m/z	792.7876243	2.451266667	neg
2.46_344.9429m/z	344.9429312	2.460016667	neg
2.46_394.8908m/z	394.8908235	2.460016667	neg
2.46_479.8686m/z	479.8686256	2.460016667	neg
2.46_598.7798m/z	598.7798159	2.460016667	neg
2.46_647.7941m/z	647.7940838	2.460016667	neg
2.47_343.9061m/z	343.9061322	2.468783333	neg
2.48_232.9442m/z	232.944291	2.479216667	neg
2.48_264.0912m/z	264.0912247	2.479216667	neg
2.48_319.0025m/z	319.0024998	2.479216667	neg
2.48_350.9398m/z	350.9398353	2.479216667	neg
2.48_376.9611m/z	376.9611281	2.479216667	neg
2.48_444.8368m/z	444.8368177	2.479216667	neg
2.48_454.8476m/z	454.847556	2.479216667	neg
2.48_454.9776m/z	454.9775907	2.479216667	neg
2.48_522.9649m/z	522.9648615	2.479216667	neg
2.49_172.9987m/z	172.9987173	2.488016667	neg
2.49_183.0275m/z	183.0274956	2.488016667	neg
2.49_196.8944m/z	196.8943716	2.488016667	neg
2.49_200.0178m/z	200.0177636	2.488016667	neg
2.49_204.9362m/z	204.9362266	2.488016667	neg
2.49_251.0150m/z	251.0150416	2.488016667	neg
2.49_386.9901m/z	386.9900989	2.488016667	neg
2.49_666.7685m/z	666.7684509	2.488016667	neg
2.50_288.1455m/z	288.1454771	2.49675	neg
2.50_704.8158m/z	704.8157665	2.49675	neg
2.50_724.8011m/z	724.801128	2.49675	neg
2.50_730.8290m/z	730.8290409	2.49675	neg
2.51_339.9118m/z	339.9118002	2.510633333	neg
2.51_547.8562m/z	547.8561617	2.510633333	neg
2.51_798.8160m/z	798.8159837	2.510633333	neg
2.52_382.8675m/z	382.8675073	2.5212	neg
2.52_530.8660m/z	530.8659561	2.5212	neg
2.52_812.7715m/z	812.7715274	2.5212	neg
2.53_343.8938m/z	343.8937829	2.531716667	neg
2.54_198.9364m/z	198.9363998	2.5421	neg
2.54_216.1242m/z	216.124175	2.5421	neg
2.54_341.0468m/z	341.046769	2.5421	neg
2.54_352.0765m/z	352.0764879	2.5421	neg
2.54_409.0342m/z	409.0342078	2.5421	neg
2.55_334.9117m/z	334.9117223	2.552616667	neg
2.55_407.8823m/z	407.8823379	2.552616667	neg
2.56_734.8287m/z	734.8287155	2.56315	neg
2.58_433.0366m/z	433.036605	2.57535	neg
2.58_501.0242m/z	501.0241688	2.57535	neg
2.59_208.9928m/z	208.9927979	2.594616667	neg
2.59_220.0229m/z	220.0228709	2.594616667	neg
2.59_220.0650m/z	220.0649968	2.58585	neg
2.59_264.9556m/z	264.955602	2.594616667	neg
2.59_274.9845m/z	274.9844779	2.594616667	neg
2.59_356.0400m/z	356.040034	2.58585	neg
2.59_364.9537m/z	364.9536832	2.594616667	neg
2.59_366.0564n	365.049131	2.58585	neg

1352.905491	1331.56386	1285.707023	2269.272466	2320.79795	1804.370361	1552.887257	1861.248692	1822.990571
723.8757213	728.4922852	854.0983955	2466.72719	2345.68795	2068.738974	1176.361623	1809.330984	1841.486963
1486.661376	1476.304477	1586.611724	2662.670196	2966.29694	2563.488135	2157.144058	2442.914332	2333.307504
2433.281245	2134.196143	2381.38529	3744.059669	3644.07587	3425.663667	3041.122001	3266.410384	3321.047012
3366.389946	3156.959872	2893.195111	5039.938142	4938.342401	4629.262972	3609.852521	4726.041377	4658.99155
10994.95934	10584.84116	11212.14758	19807.74728	19806.25029	19395.85659	14398.53528	16278.02119	16291.10569
171.5398251	296.0461969	265.9504423	760.0482654	755.1684103	710.1663009	310.6281497	614.6236514	655.240325
5164.255831	4766.633813	5001.838647	7764.578728	8255.649961	7788.805812	6814.330166	7361.251024	6967.713178
9083.709278	9805.506279	10282.3937	17119.21826	17788.45606	18115.46439	13416.77472	14504.36943	15176.27728
6698.585145	6118.244841	6509.547597	10318.73268	10636.17574	9933.478656	8253.127473	9114.00064	9261.088668
1602.268254	1507.081357	1405.703219	2544.47231	2952.614748	2559.645407	1449.762488	2174.872879	2419.272321
1329.680501	1363.540605	1403.604874	2579.74078	2293.833192	2534.053678	1676.095812	1866.385196	2055.409679
2036.676596	2135.798202	2311.023495	4245.600611	4056.382307	3253.187608	2782.412998	3393.517627	3574.545201
660.469836	946.2074601	1244.763797	2114.693395	2055.876933	2120.242682	1305.32108	1624.579544	1533.727597
5583.293146	5151.43901	5850.403856	10202.38254	10497.59272	9969.552346	7129.226582	7830.573985	7999.603556
663.5316541	943.135801	888.7937644	1872.138269	2026.95455	1808.816418	852.1188049	2025.047049	1613.33763
2488.302989	2217.099245	2338.951253	1099.884744	1248.825501	493.655169	158.8185097	635.0803947	417.1235996
1228.203231	1228.167412	934.3922812	2686.650019	2742.08788	2545.787812	1771.711933	2463.913375	2388.26423
1498.153998	1397.9642	1119.759558	3050.555587	3879.427808	3241.749865	2040.630088	2840.57306	2685.617818
408.8632771	335.0767405	395.8908192	559.2169006	573.6479393	588.2706779	408.7797539	478.5060444	521.8052979
869.0250093	722.4070125	836.1743959	16.60514055	58.33791605	57.0499449	2956.390716	3447.960551	3280.862774
1533.798578	1528.367496	1418.789237	2945.306644	3103.103546	2436.127614	1874.312022	2482.997056	2367.695492
2943.201383	2515.616848	3037.61142	4261.494012	4261.938245	4104.771429	3182.614331	3618.541736	3461.01233
1123.021115	1084.962949	1037.902808	1642.19615	1753.337726	1485.057021	1027.614602	1649.976585	1459.36768
4532.953331	4764.249375	5046.728686	776.3617332	704.1194163	803.247689	15700.84	17748.97844	17546.03207
180.8777089	147.1483906	238.474177	0.001403199	0.001403199	0.001403199	840.3552244	1288.034797	765.6015268
1318.114234	1725.477125	1672.647309	55.96939455	247.4219471	130.2294533	4647.208162	6869.112351	5382.579269
1258.506531	1408.271628	1650.465619	2211.746557	2566.1666	2114.120695	1803.324487	2337.344869	1849.025121
1472.978023	1322.427988	1534.82327	2419.976919	2509.734898	2658.280463	1708.714724	1931.071092	2187.283084
157.737043	204.692829	111.2310462	0.001403199	0.001403199	0.001403199	999.0303833	1810.177376	801.1700262
403.9320961	358.6896689	531.5267494	96.78145055	146.6047203	47.71226001	1488.532205	1623.696672	1372.084862
718.1834008	712.5074348	667.5860134	1296.169499	1298.440281	1064.873424	806.5323638	1095.843414	1129.806016
1353.391407	1315.872009	1277.301721	2575.09424	2857.791295	2531.925643	2179.14411	2345.562147	2226.043401
1440.653813	1412.980565	1410.046605	2581.066355	2591.376523	2575.161959	1912.502329	2279.705291	2400.965728
269.5930035	492.7543351	160.6894202	387.7827017	360.2584021	381.0636639	469.0910593	350.6751294	121.8274944
3082.455179	3133.117902	3514.423045	5912.204855	6404.575435	6244.765096	4717.128349	5712.41505	5270.83334
742.1842567	541.2216539	698.2719197	971.6608957	1085.500872	989.9361654	708.5689777	676.2719125	387.8036617
5896.592647	6392.85629	6800.286904	3026.697958	2709.502618	2877.669438	2349.93097	3009.118495	2753.398785
2928.487589	2917.169507	3196.615464	1283.991279	1560.102455	1393.447708	1345.094087	1249.897329	1339.917525
1287.637391	1418.388505	1523.261198	63.32020843	298.657714	155.0987108	4330.752881	4991.166293	4512.084678
537.1680593	509.7703443	435.6436204	90.659157	53.34909671	44.43712775	2123.786385	2789.327544	1924.326685
641.0495108	855.2236368	962.4331484	1066.113792	1102.77088	1001.27355	793.6696651	1342.219631	776.7320561
2425.938064	2700.019063	3142.989425	3490.084171	3189.017245	2824.075888	3307.465741	3443.947371	2531.967278
1391.681542	1734.826814	1741.708931	2144.440313	2446.463588	2007.193657	1202.280261	1580.054512	1250.697231
1449.395128	1848.474342	2303.906812	2316.172887	1910.292346	1717.410676	2174.003047	1948.143031	1797.160387
1827941.941	1589173.738	1479941.884	1598327.32	1686398.606	1626135.936	1853470.624	1521364.621	1607786.705
660763.1792	576961.8456	533930.7634	570734.9832	602754.6342	579694.9536	677669.3074	549151.0952	583613.6356
291406.1275	250014.6789	238861.5492	252897.4807	268545.5719	261254.5888	297153.6799	240398.4201	254957.0355
3298.822196	3454.047267	2655.097474	2209.359525	2510.168151	1953.323985	2460.314785	3467.047939	2321.603337
11957.85344	10994.32209	10459.99859	14333.67945	13843.15472	13700.61782	13997.25487	12956.41122	13953.70476
88183.73897	73316.64882	69934.36064	73476.44085	80210.2187	72362.88111	80372.94404	69319.81424	72521.82488
341527.438	300220.1979	279248.6135	296338.3115	316608.8324	304902.8616	355050.2292	288070.5943	305203.1532
1665970.299	1456242.663	1342867.04	1448452.198	1546624.507	1475647.993	1701907.982	1369715.981	1454455.673
295925.4227	262142.2178	239799.3528	252737.2671	272657.1362	262698.5204	304730.5223	247781.305	261050.4046
1107253.067	973205.6861	895522.8521	979754.1028	1045837.622	997000.0374	1143864.737	917835.814	962017.3678
1415.0007	1802.226401	1765.27466	1460.543051	1301.216152	1364.080316	2237.349952	1222.304396	915.1115251
21320.21221	19996.09256	18492.83891	20020.61609	21210.44528	20624.10564	21340.8353	18757.87879	17339.57553
5919.07317	5058.354501	6078.403737	5619.386801	5304.989592	4293.982197	5006.935707	4569.694892	3776.061833
1162.580308	1353.684721	1321.992269	1381.438834	1120.25691	1191.68238	1455.684167	1199.725516	873.719869
3382753.448	2927063.645	2713057.668	3913125.08	3123696.24	2993507.91	3437910.444	2781453.86	2935302.014
123027.3166	109657.2036	103810.0313	112060.7477	118352.2471	111911.7046	127382.4335	105111.5102	107666.3942
2527.394953	2064.720989	2608.387871	2257.213002	1617.068039	1530.283963	2122.130177	1465.729271	1373.173402
2790.320121	3151.745718	3085.284725	2351.072174	1805.809364	2138.068365	2717.036539	1937.736902	2107.736577
1784.193901	1760.683381	2024.433612	1915.629046	1579.603007	1384.9132	1569.236677	1232.068981	1498.649276
2759.578894	2817.974605	2972.803543	3966.77	4618.341573	4445.743599	3022.923664	2743.731655	3138.941325
977.8513421	1108.243378	1041.923371	1454.601097	1200.085946	1270.328634	1650.677184	1715.212464	1387.658421
3748.437977	4064.859707	4243.378827	6083.869559	4941.76919	5433.827059	4794.28993	4425.264658	4364.198324
1206.048083	923.4046516	1133.908235	1607.755963	1331.170885	1415.830223	1017.497283	1445.570662	1151.685252
804.8716277	1019.879514	811.6681036	1236.967522	1047.135221	1188.735316	876.6398452	750.1871261	758.496817
2466.825279	1971.793595	2144.337984	2276.552588	1702.034839	1097.696002	2342.507407	1947.354659	2034.593528
49811.13045	42825.30612	41900.24809	41994.89578	48159.00746	44191.9822	51186.48798	41327.1078	41574.69953
2739.396413	2637.980556	3510.35718	4370.996927	4157.039427	3979.573569	3134.292185	3397.144691	3162.305249
2403.062515	2285.894947	2778.569285	3425.249941	2867.120842	2954.636192	2508.818714	2726.211075	2262.587109
1332.999246	1428.81059	1488.356268	2039.407475	1745.203302	1786.415087	1673.128615	1571.483723	1620.862991
5261.301809	5670.912429	5989.864942	8086.633241	7578.499581	7612.233228	6417.246859	6758.397057	6431.204922
246.3961872	231.5134414	247.0545416	409.9200641	223.7674415	222.4658841	284.795374	177.0994225	211.0098833
1170.580671	1276.198612	1233.1612	1923.636197	1535.636496	1803.56887	1441.685714	1488.714279	1563.745931
235.0648544	225.5195557	219.7832122	288.2899443	182.2830214	212.8158653	243.0421702	159.8972343	168.5118551
1940.723974	2113.289796	2620.875324	3426.775804	3099.478006	3114.396416	2596.24396	2693.467267	2571.347036
3728.989284	4022.052531	4382.050314	5891.838393	5168.769139	5340.495261	4908.157094	4374.547344	4928.247305
1812.446772	1713.568787	1973.810265	1789.539652	1089.438552	1170.188871	2371.032089	1550.321152	1491.982082
821.3474836	863.8782919	853.6181946	1731.787507	1555.072852	1665.820373	951.6355744	961.1247576	911.8555221
7138.067355	5915.914491	6400.058413	5940.815017	6998.588624	6798.350946	8730.235545	6558.087175	7225.781998
33352.69195	3129.158974	27246.06011	28410.16936	28828.63127	28105.60438	35552.46825	25947.80534	30588.4561
51493.2635	49272.16708	47394.29195	64847.93319	68329.73193	68583.67712	61361.61115	54421.10456	58242.80558
1767.856404	1236.8337	1707.569416	1300.464829	1019.043821	1155.246861	1704.719802	1001.28504	1133.441775
176303.0957	153382.3189	141199.5026	158891.1454	172127.6651	164642.9127	184706.1928	145246.1252	155483.4684
13018.1604	12296.26025	12786.65239	17571.3483	18217.09241	17659.11375	18521.28875	13909.89536	16570.65
8087.785275	8076.236538	6325.288097	7051.505518	6887.008291	5772.812875	6867.869031	6315.152656	5371.072134
1293636.333	1135439.681	1040832.781	1135573.054	1206388.185	1149413.72	1329005.308	1079941.294	1129474.661
15396.19163	13875.52627	13598.16502	11001.97174	11204.41264	10831.20606	13860.62104	11183.97105	11650.33498
50724.35966	44566.50889	43602.37631	45025.89476	47748.20813	44810.73658	51380.56429	43185.69809	42389.95977
1023.899657	1088.836314	1061.361598	890.8396741	1051.108596	1205.211493	1228.094318	769.1117014	1401.13573
550.7293789	748.2383924	650.3924411	678.6047548	668.2123026	693.5873129	720.2488624	635.6088791	808.1570338
1177.379851	1260.058917	1268.332967	1458.981025	1515.313094	1566.620815	826.5292623	1012.061738	1253.866252
5126.398272	6033.703366	6392.576465	7589.707231	7237.703268	7031.99063	5223.152682	6203.702299	6811.631926
1198.312424	1596.758881	2078.574501	1846.051091	1696.670552	1731.088889	1244.096575	1409.319677	1421.984772
817.4328553	1127.567155	661.7225968	688.8410929	723.9784	1006.409446	645.2882493	529.2776503	1020.933796
4601.073915	4414.485352	4536.610945	5877.225875	7070.360636	6417.15207	5549.297574	5174.812445	5779.122962
520652.5311	464098.0318	421999.6711	464316.9	506246.7163	484554.7014	547932.8447	427630.6745	459342.2019
11328.38843	12137.53566	13772.99498	2055.828066	2009.452872	2191.357632	8894.970993	9819.798128	10120.18237
6384.633118	7361.050794	7705.815671	825.2180558	765.0112143	930.7474967	4620.38193	5707.02199	5811.658824
3540.883676	4149.928046	4213.259986	1433.022015	1576.338673	1544.216997	1729.210674	1864.223577	1857.813772
1053.736797	1192.4945	984.0110038	1548.66043	1668.027932	1552.326593	696.4367417	937.0293879	920.5040756
3753.053174	4023.227965	4475.108123	10143.63317	9914.548763	9518.555064	10199.98442	11548.02388	11718.0243
1037.671928	1129.803113	1046.433111	554.3988046	509.3882005	519.2742847	491.2135793	576.8140569	616.5642343
11529.12327	12548.65239	13943.4841	5834.683974	5534.558666	5588.567242	6124.391453	6698.074838	6483.847948
762.1470456	847.0203122	889.520276	2031.612749	2634.640576	2414.196572	2424.718522	2471.493596	2638.925135
1722.786366	1764.150131	1918.673628	739.0900909	907.2331284	856.8003863	833.8708528	803.4260273	935.3905715
19422.3251	21067.41058	23705.31857	3348.4014	3188.947749	3555.865058	14613.74989	17078.78814	16787.58266

2.59_478.9472m/z	478.9471578	2.594616667	neg
2.59_546.9345m/z	546.9344963	2.594616667	neg
2.59_569.0116m/z	569.0116435	2.58585	neg
2.59_751.8182m/z	751.8181672	2.594616667	neg
2.61_178.9044m/z	178.9043613	2.6102	neg
2.61_204.9613m/z	204.9612508	2.6102	neg
2.61_206.9970m/z	206.9969621	2.6102	neg
2.61_294.0846m/z	294.0846187	2.6102	neg
2.61_342.9719m/z	342.9719001	2.6102	neg
2.61_596.8567m/z	596.8566622	2.6102	neg
2.61_683.8305m/z	683.8304817	2.6102	neg
2.61_802.8161m/z	802.8160596	2.6102	neg
2.62_185.0431m/z	185.0430714	2.622366667	neg
2.62_226.9661m/z	226.9661074	2.622366667	neg
2.62_301.0001m/z	301.000148	2.622366667	neg
2.62_316.8747m/z	316.8747382	2.622366667	neg
2.62_317.9902m/z	317.9901781	2.622366667	neg
2.62_341.8902m/z	341.8902289	2.622366667	neg
2.62_410.9595m/z	410.9595359	2.622366667	neg
2.62_740.7845m/z	740.7845024	2.622366667	neg
2.63_234.0442m/z	234.0442503	2.634083333	neg
2.63_290.9714m/z	290.9713518	2.634083333	neg
2.63_355.8596m/z	355.8595638	2.634083333	neg
2.63_504.9628m/z	504.9627531	2.634083333	neg
2.63_666.8413m/z	666.8413218	2.634083333	neg
2.64_530.7926m/z	530.7926296	2.642816667	neg
2.64_545.8539m/z	545.853922	2.642816667	neg
2.64_588.8247m/z	588.8247063	2.642816667	neg
2.64_656.8126m/z	656.8125582	2.642816667	neg
2.65_264.9344m/z	264.9344157	2.651566667	neg
2.66_190.8885m/z	190.8885086	2.661	neg
2.66_439.8890m/z	439.8890382	2.661	neg
2.66_704.8157m/z	704.8157318	2.661	neg
2.66_870.8034m/z	870.8033868	2.661	neg
2.67_160.0697m/z	160.0697006	2.6698	neg
2.67_403.8496m/z	403.8495886	2.6698	neg
2.68_254.0284m/z	254.0283909	2.680233333	neg
2.68_318.8715m/z	318.8715462	2.680233333	neg
2.68_423.0774m/z	423.0773653	2.680233333	neg
2.68_491.0648m/z	491.0648447	2.680233333	neg
2.70_258.0076m/z	258.0076098	2.70125	neg
2.71_199.0226m/z	199.022552	2.709983333	neg
2.71_221.0045m/z	221.0045189	2.709983333	neg
2.71_288.9921m/z	288.9920558	2.709983333	neg
2.71_356.9796m/z	356.9796312	2.709983333	neg
2.72_229.0694m/z	229.0694067	2.72215	neg
2.72_292.9870m/z	292.9870042	2.72215	neg
2.72_304.0127m/z	304.0127298	2.72215	neg
2.72_360.9745m/z	360.9744834	2.72215	neg
2.72_362.0449m/z	362.0449179	2.72215	neg
2.72_428.9618m/z	428.961781	2.72215	neg
2.72_430.0323m/z	430.0322667	2.72215	neg
2.72_433.0321m/z	433.0321017	2.72215	neg
2.73_216.0410m/z	216.0409966	2.734316667	neg
2.73_218.0380m/z	218.0380236	2.734316667	neg
2.73_226.0699m/z	226.0698788	2.734316667	neg
2.73_243.0599m/z	243.059909	2.734316667	neg
2.73_372.0001m/z	372.0001414	2.734316667	neg
2.73_439.9878m/z	439.9878339	2.734316667	neg
2.73_496.9493m/z	496.9493405	2.734316667	neg
2.73_498.0200m/z	498.0199935	2.734316667	neg
2.73_507.9750m/z	507.9750375	2.734316667	neg
2.73_812.7717m/z	812.7717234	2.734316667	neg
2.74_213.0382m/z	213.0382046	2.743066667	neg
2.74_284.0286m/z	284.028619	2.743066667	neg
2.76_274.0029m/z	274.0029449	2.75705	neg
2.76_294.9539m/z	294.9539065	2.75705	neg
2.76_295.9849m/z	295.9848723	2.75705	neg
2.77_314.8795m/z	314.879522	2.7675	neg
2.79_429.0506m/z	429.0505937	2.790116667	neg
2.79_530.7926m/z	530.7926102	2.790116667	neg
2.81_324.8880m/z	324.8880448	2.8089	neg
2.81_577.7905m/z	577.7905402	2.8089	neg
2.81_647.7945m/z	647.7944819	2.8089	neg
2.82_232.9443m/z	232.9443369	2.817666667	neg
2.83_424.9672m/z	424.9671549	2.826466667	neg
2.84_175.0145m/z	175.0144556	2.83525	neg
2.84_185.0432m/z	185.043166	2.83525	neg
2.84_199.0225m/z	199.0225414	2.83525	neg
2.84_216.9807m/z	216.980656	2.83525	neg
2.84_221.0046m/z	221.004578	2.83525	neg
2.84_253.0307m/z	253.0306643	2.83525	neg
2.84_288.9920m/z	288.992045	2.83525	neg
2.84_321.0179m/z	321.0178525	2.83525	neg
2.84_356.9796m/z	356.9795532	2.83525	neg
2.84_456.9932m/z	456.9932409	2.83525	neg
2.85_389.0057m/z	389.0057366	2.852583333	neg
2.86_220.0348n	265.0330704	2.864816667	neg
2.86_280.0301m/z	280.0300859	2.864816667	neg
2.86_331.0276m/z	331.0275627	2.864816667	neg
2.86_467.0023m/z	467.0023201	2.864816667	neg
2.88_196.0558m/z	196.0558277	2.877083333	neg
2.89_287.0152m/z	287.0152082	2.8859	neg
2.89_407.8825m/z	407.8825395	2.894666667	neg
2.89_598.7806m/z	598.7805695	2.894666667	neg
2.91_570.8371m/z	570.837116	2.9068	neg
2.91_792.7879m/z	792.7879445	2.9068	neg
2.92_178.9043m/z	178.9043377	2.9156	neg
2.92_225.9890m/z	225.9890118	2.9156	neg
2.92_304.0053m/z	304.0053435	2.9156	neg
2.92_371.9927m/z	371.9926952	2.9156	neg
2.92_439.9802m/z	439.9802237	2.9156	neg
2.92_507.9675m/z	507.9674501	2.9156	neg
2.92_590.8207m/z	590.820654	2.9156	neg
2.93_275.9184m/z	275.9183822	2.934866667	neg
2.93_362.9421m/z	362.9421174	2.934866667	neg
2.93_382.8676m/z	382.8675878	2.926066667	neg
2.93_539.9052m/z	539.9052011	2.934866571	neg
2.94_392.8760m/z	392.8760344	2.94365	neg
2.94_615.8432m/z	615.843171	2.94365	neg

3282.074522	3350.399395	3675.819088	1586.585238	1877.424182	1543.823561	1475.602079	1634.993286	1961.210217
2160.757595	2577.715433	2345.720502	1044.127328	929.6412272	817.653881	848.5500077	1041.662118	1440.510097
2848.3441	3481.473175	3707.289223	344.9383463	366.7376915	560.4488177	2656.235988	2028.259546	2525.024956
5735.145866	6143.82701	4600.192906	5808.991853	5578.311211	5222.748261	5862.581919	4774.462786	4919.315487
1385.790102	1212.374482	1169.897901	1286.52709	1330.047549	1218.767407	1328.947967	1019.957629	1346.01281
865.9880205	854.5889526	868.7305234	511.5673533	457.9387329	398.9307002	1012.903929	952.9335803	933.1304302
94556.35832	99516.24161	109228.664	45131.10846	44549.04915	43770.11279	48492.82338	51223.32142	51749.37533
1063.469825	1053.070535	1187.065873	1123.835716	1343.129683	1190.82367	1148.692887	1228.628871	1237.545215
6542.47738	7135.995217	7377.553364	3086.728822	2915.73025	3210.900578	3188.870779	3391.387561	3613.638633
65132.81067	60013.29459	55436.61972	63041.08285	71553.7951	67167.69671	74173.53446	58012.90792	63062.72849
53703.18537	47356.7464	46320.19819	47577.1517	56284.08196	49461.3766	59976.77125	44259.92739	46325.13572
209001.4367	182650.1262	174534.5747	187444.9578	200453.4447	188877.9835	214423.9337	171903.5464	180940.9883
152.1059799	162.9088815	190.8554969	365.3742464	495.1188628	294.4516594	287.0240092	256.2673196	296.0809291
361.6605079	314.2497913	358.5535129	541.4202198	573.736883	458.2907279	430.8550768	297.3169746	474.2337617
7045.445185	7774.296472	7690.810207	306.5066287	360.3520228	378.0148852	10220.05362	10810.04416	10850.34841
284496.0892	247442.5025	232268.3113	248557.2483	261777.7455	250970.2727	293889.2509	241391.6109	252943.9922
676.723119	608.4450023	614.283931	38.67420852	0.001403199	0.001403199	804.8596551	875.8728828	857.0857241
3433.715318	3606.761906	3535.21384	4025.061027	4449.111171	4468.072378	3695.464073	3483.743591	3705.11572
3399.025826	4258.296554	3965.864993	1699.806713	1860.411474	1741.344167	1912.88412	2005.076451	1915.204038
21261.22363	15995.95848	15711.71659	16681.59118	18314.458	17759.06551	18102.2078	15818.46105	17556.90802
780.9505159	669.4006607	688.0399681	1888.069984	1880.16919	1722.734961	1152.298137	1133.141104	1156.972119
5287.37366	5677.094337	5289.242296	3445.50519	3561.180154	3668.730047	5425.084365	4571.004135	5346.627241
1741.550278	1288.287224	1009.422371	1316.698639	1444.966681	1376.117645	1482.778926	1195.706291	1251.252528
1094.153178	1329.882788	1037.229229	0.001403199	0.001403199	0.001403199	1598.948223	1853.934738	1547.010553
781531.9748	689661.6791	642272.0183	699821.0752	756212.2125	722707.5836	813612.4236	653220.5077	697362.9009
3580.722231	3055.704882	2430.441313	4205.1012	2568.61313	2639.159724	3568.643666	2513.433853	2365.74386
3950.550685	3632.864666	3451.14108	4170.266231	3585.001094	3352.47143	3897.541771	2985.605361	4010.668524
310196.5515	272028.9422	252585.0132	266964.6397	290392.1309	271660.171	319689.5218	256140.553	272766.095
180041.5731	167871.1201	154070.3316	164710.9874	176888.2362	169619.0659	192397.7035	155797.6966	168909.0395
1222.479732	1142.491838	1007.223766	1466.12118	1196.924517	1187.357027	1222.5774	1146.223671	1063.716455
1683.294017	1681.746485	1842.77214	2000.134577	2037.534471	2174.281175	2039.178378	1593.141033	1838.313154
4592.756756	3742.277143	3143.626806	3950.58935	3238.754102	2755.283384	3494.675163	3167.531461	3394.522608
4014.372659	2705.878683	3418.335641	4143.628611	4159.582101	3333.46894	3934.94261	2500.847069	3374.30548
45753.91959	42621.43593	38160.96435	39058.22871	41344.71812	42038.85971	47422.31826	39185.92415	39621.01488
60.38485797	84.94247262	116.9804802	178.517439	163.4600309	136.1433723	128.1776639	101.153406	129.492739
1651.971343	1087.021304	1144.621434	1370.584098	1360.883648	922.7153528	1405.811503	1181.358269	925.8558391
1325.283134	1411.469455	1448.517467	2323.559741	2047.250671	1850.205163	1729.416662	1843.358476	1702.578904
6464.578234	5479.390781	5525.675253	6076.752615	6217.931621	5703.193229	6272.468599	5223.352278	6245.52489
6100.344502	6140.146313	5376.254117	8626.1785	8268.929711	8259.346757	6604.753195	6650.953329	6883.892499
2829.413627	2554.663464	2507.256124	4666.442081	3843.490164	4194.007445	2771.634993	2949.077317	2806.717671
2209.670167	2345.851147	2174.383698	2420.590713	2109.398944	2313.821058	2576.109191	2759.92356	3126.938671
1444.744881	1363.726959	1628.37276	1446.14887	1401.647762	1565.894879	1236.54229	1369.685175	1465.747829
3746.5788	4057.062514	3704.462259	3766.390577	3518.885105	3604.253373	3137.559966	3416.920805	3806.686963
2665.244202	2765.776334	2906.676451	3049.664249	2926.17668	2824.634546	2307.336321	2417.620858	2523.736475
1719.757268	1676.544653	1784.66254	2157.482538	2232.430131	1974.290957	1299.084858	1473.908031	1573.137068
6526.839	6828.069023	6543.674047	7806.852441	8199.61736	8470.926483	6531.863101	7081.764987	7539.862781
4593.511265	4923.72831	3895.142602	4452.678855	4142.714847	4426.347686	5152.703502	4842.764052	5231.678771
3010.914572	2840.922197	2915.796326	2534.930933	2528.503036	2729.200037	3346.186663	3672.44373	3937.263039
4209.359692	4102.133072	3899.913115	3586.734317	3807.502278	3726.594428	4206.07984	4223.080572	4788.934834
5285.770089	5866.775269	6163.54963	3600.482392	6018.152253	5743.171378	6896.164583	6374.858016	7713.247512
1708.849321	1990.705355	1934.594148	2029.662666	2454.81493	2049.538034	1939.786324	1723.364128	1884.569101
4651.536431	4794.816151	4906.454821	4580.487449	4678.529418	4254.177072	5268.090392	6098.113726	6352.455588
1663.329916	1653.703921	1686.799736	2018.433074	2335.928106	2147.880325	1780.39302	2039.98419	1857.180669
1289.000671	1411.541381	1471.406705	1360.20568	1261.767136	1255.232777	1709.105762	1716.349938	1866.737901
270.4714078	403.1142632	438.9995271	322.6921659	338.3688894	395.3429535	436.0757903	480.4647388	511.2043538
18387.93836	19625.66685	19453.17831	18138.87668	18511.2376	18568.47713	22074.9535	24538.85682	24757.79718
565.4346323	601.8975014	578.4903956	685.2629274	713.186506	648.2424159	800.520797	906.0034104	777.8471914
2248.442594	2222.25219	2030.072204	1594.823952	1992.973253	1771.789212	2338.4428	2651.550578	2722.588679
2132.352616	1937.465891	1953.856616	1892.83525	1842.198093	1652.031225	2350.239911	2663.913309	2500.780143
1707.993306	1529.448848	1882.408203	1886.847419	1997.299561	1628.667696	2000.274519	1942.264327	1932.974518
3800.700341	3800.786603	3648.250515	3791.101405	4150.042683	3549.415084	4654.753758	4977.115367	4852.695889
2731.549081	2862.793227	2518.639325	2414.26815	2244.636044	2201.853099	3204.185782	3310.054296	3464.447344
6988.548534	7594.355283	4946.043409	4684.146453	5249.288681	4837.874413	6497.973003	5632.952347	5115.53507
982.1982035	1046.651856	969.942843	1142.929043	1251.863343	1239.460034	1088.476432	1179.187321	1194.153001
534.8026028	604.7472211	497.9012737	586.5792004	632.8172241	617.137721	777.2660685	800.2301006	753.193192
9108.78371	9855.584715	10556.53503	909.8691435	806.9846294	821.9285491	5418.220378	6005.133589	5511.228806
614.5719757	530.5378043	481.585614	454.7927268	586.3992382	619.7582154	733.9577425	561.5525702	619.8703209
1806.99791	1914.414649	1495.506817	0.001403199	0.001403199	27.89197712	1037.77326	1059.041715	1214.038877
521.9431741	359.9624956	448.1350729	388.9675538	777.8042149	581.8606426	502.2296272	424.5743363	395.2895768
1992.969762	2553.538723	2076.466888	1909.607204	1988.321605	2225.492464	1627.855208	2638.519641	2654.866354
4169.072602	4211.807152	2967.685384	1882.224357	2282.058588	2526.212286	3489.902036	2876.605906	3398.436728
62973.28598	55109.06175	52404.88044	56428.62656	58831.50409	56811.18588	64880.8032	52371.30451	56192.96186
14062.95876	13095.14526	11726.16337	11118.64028	12987.19414	11857.73188	13930.36008	11579.82091	12870.99363
2207.265703	2524.2276	2019.367803	1668.918511	1346.079294	1563.906638	1327.005304	1834.503839	2234.295601
1338.932588	1515.161144	1132.791242	1717.851297	1969.952144	1946.082058	1429.736211	1401.689776	1490.724086
1524.665792	1092.765915	1890.149865	1661.469448	1688.541316	1556.645562	1378.412338	1815.643337	1410.522551
375.800627	333.9591551	507.5253013	648.0722071	614.1224854	614.3000106	403.9927167	474.0714721	431.5053666
5505.991594	5846.528788	6529.099752	10601.65152	10427.28084	9689.848816	7099.166435	7418.49525	6875.67363
1885.062615	1750.887953	1873.079512	2224.922663	2076.166026	1965.683361	1611.489712	1992.938527	1857.85194
725.1170761	684.5517699	784.8861989	912.0938286	818.3433867	885.4474569	646.493687	818.4897743	827.9277768
1648.02522	1453.225673	1760.570066	1885.867845	1822.528084	1706.331325	1477.15566	1775.032795	1653.414371
1734.984827	2010.316334	2053.011149	3459.068942	3170.698934	2982.336611	1869.005797	2148.007382	2051.702261
4513.721678	4400.784915	4778.271242	5176.250004	5366.933234	5180.959334	4665.688027	5054.513499	4839.858836
3318.264996	3236.085952	3897.575446	5161.895855	5766.473279	5429.196874	3677.939064	4460.966351	3882.17193
3459.806277	3263.895733	3446.292113	3823.678579	4011.504878	3817.387673	3312.631657	3722.145313	3484.456949
1724.551945	1947.889518	2295.737051	3858.210443	3405.238394	3567.856652	2217.848676	2679.518497	2283.75671
2687.159576	3272.340251	2969.220026	5095.485221	4990.979556	4766.026496	3361.098147	3497.690852	3128.982695
2994.132739	3070.121784	3647.810027	0.001403199	0.001403199	0.001403199	1720.631382	1695.606541	1533.996402
3498.946979	3472.960838	3852.392659	5645.157299	5030.615904	5402.261098	4582.575428	4606.972442	4384.349035
4567.958574	4588.738847	5186.651587	7743.572926	7432.983014	6932.790062	5925.51529	6328.537281	5552.777723
1771.662806	1638.846821	2297.505918	2639.119547	2289.621812	2621.933044	2230.490563	2335.903291	1591.584104
2617.796301	2709.165238	3006.539084	4097.593695	4106.475844	3893.462252	3203.577256	3412.807998	3081.429672
1167.315837	988.2122888	1287.26985	0.001403199	0.001403199	0.001403199	588.1609666	735.5543082	526.6630392
3548.203062	2575.060401	3809.579424	4525.623545	6344.548174	4966.472403	4620.010911	3325.285393	3378.488504
2561.162325	1829.893951	1908.542174	1587.06525	1399.336377	1456.304832	2645.551411	1767.752213	1519.161697
7157.600568	7724.32885	8649.064671	8660.612717	11377.48294	9584.762502	9368.583235	8290.08763	8976.601766
8444.454298	6961.93637	6620.987072	6463.984617	6115.057616	6511.013814	8884.216257	6756.287961	7194.132249
496.8140498	403.2684881	396.7713527	484.508289	358.6614876	401.2082798	608.5793237	441.9517626	378.1896346
2136.206571	2068.973965	2311.066487	1574.938707	1368.187381	1681.680966	1565.555369	1594.518463	1316.036638
6749.590615	6278.1087	7260.659596	5073.557565	4485.361292	5261.587731	4693.051674	5417.739251	4650.947517
7493.493849	7040.686807	7908.406195	5275.608052	5474.748746	5626.348605	5146.615057	5284.720733	5091.066993
5494.755122	5525.478641	6102.915686	4404.415453	4166.400413	4430.014058	4018.291827	3877.160602	3437.702429
2572.47425	2063.252787	3023.299379	2236.322133	1884.73266	2155.59309	2072.836824	2167.644161	1891.338618
6491.217971	4558.274213	5473.043274	5363.175996	5430.804071	5846.743533	7683.643992	5215.330735	5139.194699
713.0357981	438.4426073	580.2743873	667.6565584	628.692486	733.4797093	734.6070649	573.4023727	518.5061545
2223.867285	1963.870072	2555.686917	2474.078795	2598.888372	2501.349878	3223.044586	2409.959124	2270.114287
7444.087923	5567.349648	5309.554836	4193.768355	5714.642302	5537.432097	5847.525697	4302.831022	4705.26973
1352.355526	1476.438703	2278.727867	1406.025468	2272.106053	2060.26408	1540.000571	1621.593956	1563.673579
92905.29625	80795.26333	74926.68116	80902.96405	87214.17437	83722.85927	94024.4113	75910.85996	81493.3914
77040.12005	65207.37821	63636.98052	67541.20112	75920.15324	74103.09112	81214.70264	62657.68818	67040.99435

2.94_664.8294m/z	664.8294237	2.94365	neg
2.96_514.8933m/z	514.8932797	2.962916667	neg
2.97_414.9464m/z	414.9463779	2.971633333	neg
2.97_812.7717m/z	812.7717286	2.971633333	neg
2.98_154.9188m/z	154.9188374	2.982066667	neg
2.98_428.9615m/z	428.9615309	2.982066667	neg
2.98_704.8159m/z	704.815936	2.982066667	neg
2.98_870.8035m/z	870.803474	2.982066667	neg
3.00_249.0381m/z	249.0380806	3.004583333	neg
3.00_331.9227m/z	331.9226822	3.004583333	neg
3.00_347.0863m/z	347.0862933	3.004583333	neg
3.00_403.8496m/z	403.8496418	2.995933333	neg
3.02_317.0255m/z	317.0255379	3.02	neg
3.02_483.0611m/z	483.0610713	3.02	neg
3.04_218.9881m/z	218.9880959	3.041866667	neg
3.04_218.9969m/z	218.9969493	3.041866667	neg
3.04_241.9862n	286.9844456	3.041866667	neg
3.04_276.9555m/z	276.9554671	3.041866667	neg
3.04_300.9344m/z	300.9343864	3.041866667	neg
3.04_303.9746m/z	303.9746263	3.041866667	neg
3.04_309.9738n	308.966476	3.041866667	neg
3.04_319.9290n	364.9272761	3.041866667	neg
3.04_360.9286m/z	360.9285757	3.041866667	neg
3.04_366.9248m/z	366.9248206	3.041866667	neg
3.04_368.9219m/z	368.9219124	3.041866667	neg
3.04_376.8801m/z	376.8801456	3.041866667	neg
3.04_377.9612n	376.9538824	3.041866667	neg
3.04_386.9092m/z	386.9092307	3.041866667	neg
3.04_428.9153m/z	428.9152549	3.041866667	neg
3.04_434.9123m/z	434.9123368	3.041866667	neg
3.04_444.9413m/z	444.9413579	3.041866667	neg
3.04_454.8967m/z	454.8967282	3.041866667	neg
3.04_460.9833m/z	460.9833151	3.041866667	neg
3.04_461.9316m/z	461.9315824	3.041866667	neg
3.04_497.8787m/z	497.8786861	3.041866667	neg
3.04_512.9287m/z	512.9286716	3.041866667	neg
3.04_522.8842m/z	522.8842482	3.041866667	neg
3.04_528.9708m/z	528.9707956	3.041866667	neg
3.04_529.9190m/z	529.9189612	3.041866667	neg
3.04_565.8664m/z	565.8663891	3.041866667	neg
3.04_580.9161m/z	580.9160838	3.041866667	neg
3.04_638.8753m/z	638.8752652	3.041866667	neg
3.04_648.9038m/z	648.9037587	3.041866667	neg
3.04_658.8600m/z	658.860025	3.041866667	neg
3.04_726.8469m/z	726.8469375	3.041866667	neg
3.06_203.9733m/z	203.9732608	3.05735	neg
3.06_293.9424m/z	293.9424102	3.05735	neg
3.06_299.9448n	298.9374955	3.05735	neg
3.06_326.9637n	371.9619968	3.05735	neg
3.06_338.9466m/z	338.946571	3.05735	neg
3.06_344.0496m/z	344.0496256	3.05735	neg
3.06_379.9144m/z	379.914447	3.05735	neg
3.06_393.9439m/z	393.94388	3.05735	neg
3.06_403.9113m/z	403.9112873	3.05735	neg
3.06_412.0371m/z	412.0370653	3.05735	neg
3.06_429.8910m/z	429.8909743	3.05735	neg
3.06_460.0900m/z	460.0900419	3.05735	neg
3.06_502.9000m/z	502.8999585	3.05735	neg
3.06_512.8562m/z	512.8561631	3.05735	neg
3.06_550.9524m/z	550.9523635	3.05735	neg
3.06_570.8872m/z	570.8871536	3.05735	neg
3.06_590.8721m/z	590.8720776	3.05735	neg
3.06_626.0283m/z	626.0282855	3.05735	neg
3.06_654.8697m/z	654.8696501	3.05735	neg
3.06_716.8905m/z	716.8904594	3.05735	neg
3.07_203.0022m/z	203.0021656	3.067683333	neg
3.07_276.0620m/z	276.0620276	3.067683333	neg
3.07_412.9306m/z	412.9306174	3.067683333	neg
3.07_444.8681m/z	444.8680861	3.067683333	neg
3.07_490.0535m/z	490.0535277	3.067683333	neg
3.07_558.0409m/z	558.0409001	3.067683333	neg
3.08_402.9002m/z	402.9002278	3.076266667	neg
3.09_722.8573m/z	722.8573137	3.0884	neg
3.10_208.0651m/z	208.0650774	3.10055	neg
3.10_254.9581m/z	254.958141	3.10055	neg
3.10_331.9225m/z	331.9224907	3.10055	neg
3.11_578.7953m/z	578.7953126	3.112733333	neg
3.12_259.9624m/z	259.9624177	3.123216667	neg
3.12_322.9458m/z	322.9457608	3.123216667	neg
3.12_352.9555m/z	352.9555447	3.123216667	neg
3.12_456.9932m/z	456.9932099	3.123216667	neg
3.12_660.9557m/z	660.9557167	3.123216667	neg
3.13_175.0144m/z	175.014389	3.131933333	neg
3.13_185.0432m/z	185.0431556	3.131933333	neg
3.13_202.0334m/z	202.0334227	3.131933333	neg
3.13_211.0225m/z	211.0224867	3.131933333	neg
3.13_253.0307m/z	253.0306852	3.131933333	neg
3.13_254.0647m/z	254.0647088	3.131933333	neg
3.13_321.0181m/z	321.0181479	3.131933333	neg
3.13_389.0058m/z	389.0057526	3.131933333	neg
3.13_524.9804m/z	524.9804317	3.131933333	neg
3.13_592.9681m/z	592.9680616	3.131933333	neg
3.14_232.9443m/z	232.9442737	3.142483333	neg
3.14_282.9893m/z	282.9892972	3.142483333	neg
3.14_284.9682m/z	284.9682442	3.142483333	neg
3.14_322.0521m/z	322.0521409	3.142483333	neg
3.14_420.9430m/z	420.9430106	3.142483333	neg
3.14_448.8502m/z	448.8502336	3.142483333	neg
3.16_381.8681m/z	381.8680631	3.16405	neg
3.16_407.8825m/z	407.882509	3.16405	neg
3.17_146.9466m/z	146.9465755	3.17455	neg
3.17_226.9662m/z	226.966191	3.17455	neg
3.17_246.8853m/z	246.8853112	3.17455	neg
3.19_121.9440m/z	121.9440365	3.186766667	neg
3.19_870.8031m/z	870.8031132	3.186766667	neg
3.20_428.9617m/z	428.9617341	3.1972	neg
3.20_570.8371m/z	570.8370796	3.1972	neg
3.21_224.9993m/z	224.9992929	3.209383333	neg
3.21_512.8230m/z	512.8229541	3.209383333	neg
3.21_704.8157m/z	704.8157251	3.209383333	neg

2938.382824	2952.406939	2418.088394	2901.669598	4076.416494	3509.607853	2686.782682	2106.623283	2903.597502	
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3760.507132	3112.488606	3578.163066	4558.421897	6216.777129	5614.464056	4533.839761	4083.024976	3811.874193	
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466.9881722	462.4391809	354.9350308	456.7409017	811.8077943	550.7136029	501.9786977	446.9226603	460.0303948	
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18407.26479	14828.53154	15191.55046	15657.2267	21215.28022	18868.60985	18454.78054	15710.05208	13386.23312	
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624.8527428	589.4089782	672.5305334	312.8812375	261.4849419	339.713278	500.7524539	593.1402533	415.4315065	
1316.321965	1177.384606	1357.379067	1348.616194	1630.250982	1536.264114	1134.929068	1965.21896	987.6169549	
719.3261811	823.7252145	847.9237442	0.001403199	0.001403199	0.001403199	356.7922177	766.9371039	211.4523803	
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155657.4174	156135.1103	173114.6965	14897.05066	15178.21911	14318.7476	135726.335	139512.5761	134038.3237	
25233.82341	24148.09296	26719.33574	8293.197866	8397.936545	8181.521868	23210.8151	22840.29268	22066.09243	
2678.253888	2607.563729	3071.867827	522.8972494	519.4422761	551.3376465	2431.094699	2675.366403	2413.251196	
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3393.411205	3458.395753	4203.307406	495.6867901	441.5304073	870.2632904	2838.318271	3543.785009	3098.478557	
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2705.169348	2516.936613	2924.10983	8.676636696	0.001403199	67.55958676	2520.329669	2377.473552	2112.695073	
2298.398134	1951.464279	2341.494059	0.001403199	22.35814579	0.001403199	1489.78754	1903.462236	1498.740798	
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4432.829103	4292.758858	4956.560556	0.001403199	128.9999902	175.8108948	3898.814377	3665.03019	3783.144636	
2423.667997	2442.511157	3151.205028	0.001403199	87.01418914	0.001403199	2357.438907	2373.341995	1910.480795	
37865.36739	37309.5616	40849.31745	2510.202155	2759.538899	2156.621008	33380.77269	33121.5024	32994.34715	
22651.92463	22973.99738	25497.97157	185.5473485	162.4260282	0.001403199	18045.88428	17747.35	16909.83936	
2733.865157	3081.181627	3831.486651	0.001403199	0.001403199	0.001403199	1416.090814	2465.55829	1940.196284	
2942.435168	2800.3775	3439.297986	0.001403199	0.001403199	0.001403199	2352.370425	2916.537747	2416.28421	
2336.56184	1819.462507	2812.575234	0.001403199	0.001403199	0.001403199	1998.077616	1642.677258	1605.861424	
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674.944398	749.2238102	716.9597475	0.001403199	20.39344196	0.001403199	692.8919629	706.029108	697.6353832	
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7720.941492	8636.697006	8879.466291	0.001403199	0.001403199	112.0278184	7852.766504	7838.152247	7882.42801	
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5503.771897	5552.393134	5974.797949	5268.32826	4665.929403	4542.244957	5212.403974	5747.678003	5604.64418	
5640.192253	6335.19588	6666.465363	9750.869381	8965.039766	8194.518991	7150.157201	9336.403075	7061.614869	
5482.662999	5665.289495	6587.809362	8939.161448	8242.923557	7980.000263	6509.53529	7162.861709	7476.518675	
3577.714456	4000.029994	4453.504374	6088.179888	5702.243911	5185.401873	4235.218109	5261.444041	4690.817891	
2907.317838	3446.210104	2735.661538	3487.967231	3704.808789	3250.704243	2893.922093	4447.004982	3936.432221	
722.2524842	718.4944336	782.7868825	1057.030579	1094.591573	926.0436276	836.2579644	817.2223131	1146.088129	
985.2380079	1290.167128	1026.273446	1433.229469	1243.677611	1176.700294	1210.251737	1216.914272	1361.875332	
862.3734591	847.4458408	1285.059252	933.6540477	925.6477976	714.8451903	1160.337888	1219.909166	1235.569135	
3060.268897	2977.674853	3454.25481	2924.083733	2776.281206	2618.568833	3101.279863	3393.696756	3626.344527	
1309.534118	1445.546922	1499.125513	913.7109656	1199.836293	1297.359924	1476.857823	1573.877762	2074.625406	
3540.859884	4374.437893	4206.163556	6278.842429	4994.258121	5940.648834	5049.817734	4349.606818	5433.763842	
4582.924018	3718.108449	4520.97863	5612.523476	5727.360939	4685.239767	4396.693036	4331.755278	4700.262264	
3067.683141	2605.319557	3036.157433	3806.828095	3555.077186	3198.772894	3142.86375	2827.442365	3729.894906	
1261.108784	1142.561361	1206.218533	1513.286247	1275.122124	1391.618505	1425.147093	1290.587759	1454.604314	
689.8000477	1002.7567	666.6332367	738.3650798	736.308938	615.3871698	872.4375838	841.6950075	1082.451683	
511.5676732	599.839804	468.0371923	655.6122618	644.3992626	666.1796024	588.7026888	600.5476761	597.7640146	
655.6132432	639.1704391	566.8648257	671.3597111	599.2864317	694.0082475	649.1263948	616.5150728	783.870619	
20190.45345	16202.57648	18578.8473	21905.54739	20660.65547	19835.03169	22366.03216	18785.21857	20080.29299	
1464.80456	1417.871607	1045.788039	1519.239113	1153.739399	1693.64435	1288.344971	1346.574234	1169.172566	
6164.482035	5578.799908	5949.197137	8644.078495	7615.397193	8265.320217	8816.54459	6312.97325	6589.246801	
656.1402598	649.5524425	567.9151788	666.7146692	623.0572355	616.6328473	563.8302378	583.4834785	537.2514474	
701.8874891	270.8798415	455.9873792	542.1554953	406.0858564	204.6751937	459.4948492	124.5983805	219.5171601	
11737.48466	10469.08003	9607.777886	14531.87623	15511.18172	15718.58639	12029.63184	10454.07093	12271.90555	

3.22_245.1143m/z	245.1143076	3.215616667	neg
3.22_277.0387m/z	277.0387384	3.22435	neg
3.22_346.9585m/z	346.9585084	3.215616667	neg
3.22_474.0362n	519.0345933	3.215616667	neg
3.24_541.0164m/z	541.0164373	3.23635	neg
3.25_296.1364m/z	296.1363849	3.248283333	neg
3.26_446.9673m/z	446.9672825	3.260183333	neg
3.26_468.9491m/z	468.9490896	3.260183333	neg
3.28_207.9890m/z	207.989038	3.280233333	neg
3.28_240.9443m/z	240.9442825	3.280233333	neg
3.28_262.9399m/z	262.9399015	3.280233333	neg
3.28_285.9291n	284.9218163	3.280233333	neg
3.28_288.9338m/z	288.9337977	3.280233333	neg
3.28_302.9792m/z	302.9791948	3.280233333	neg
3.28_304.9050m/z	304.9049853	3.280233333	neg
3.28_317.9403n	362.9385099	3.280233333	neg
3.28_321.9086m/z	321.9085988	3.280233333	neg
3.28_346.9128m/z	346.9127606	3.280233333	neg
3.28_369.8994m/z	369.8993726	3.280233333	neg
3.28_379.9285m/z	379.9284981	3.280233333	neg
3.28_415.8756m/z	415.8755973	3.280233333	neg
3.28_422.8943m/z	422.8943143	3.280233333	neg
3.28_430.8518m/z	430.8517773	3.280233333	neg
3.28_432.9518m/z	432.9517848	3.280233333	neg
3.28_440.8804m/z	440.8803904	3.280233333	neg
3.28_480.1077m/z	480.1077378	3.280233333	neg
3.28_508.8676m/z	508.867628	3.280233333	neg
3.28_576.8557m/z	576.8556859	3.280233333	neg
3.28_712.8302m/z	712.8302368	3.280233333	neg
3.29_279.9329n	324.9311335	3.293883333	neg
3.29_283.9535n	566.9002598	3.293883333	neg
3.29_286.9188m/z	286.9187947	3.293883333	neg
3.29_289.9590m/z	289.9589761	3.293883333	neg
3.29_294.8772m/z	294.8771845	3.293883333	neg
3.29_295.9579n	294.9506383	3.293883333	neg
3.29_311.9410m/z	311.9410456	3.293883333	neg
3.29_338.9401m/z	338.9401369	3.293883333	neg
3.29_342.8804m/z	342.8804333	3.293883333	neg
3.29_352.9094m/z	352.9094154	3.293883333	neg
3.29_354.9064m/z	354.9064393	3.293883333	neg
3.29_362.8648m/z	362.8647731	3.293883333	neg
3.29_372.8932m/z	372.8932198	3.293883333	neg
3.29_385.9276n	430.925835	3.293883333	neg
3.29_406.9276m/z	406.9275618	3.293883333	neg
3.29_414.8998m/z	414.8997941	3.293883333	neg
3.29_420.8969m/z	420.8969471	3.293883333	neg
3.29_447.9161m/z	447.916101	3.293883333	neg
3.29_456.0277m/z	456.0277955	3.293883333	neg
3.29_476.9158m/z	476.915808	3.293883333	neg
3.29_483.8630m/z	483.863022	3.293883333	neg
3.29_488.8843m/z	488.8843093	3.293883333	neg
3.29_498.8395m/z	498.8394638	3.293883333	neg
3.29_498.9134m/z	498.9133976	3.293883333	neg
3.29_544.9032m/z	544.9032026	3.293883333	neg
3.29_556.8716m/z	556.8716197	3.293883333	neg
3.29_612.8903m/z	612.8903076	3.293883333	neg
3.29_624.8592m/z	624.8592299	3.293883333	neg
3.29_644.8431m/z	644.8431318	3.293883333	neg
3.29_702.8757m/z	702.8757026	3.293883333	neg
3.31_302.9108m/z	302.9107969	3.305783333	neg
3.31_490.8812m/z	490.8811623	3.305783333	neg
3.31_515.9028m/z	515.9028331	3.305783333	neg
3.31_551.8505m/z	551.8505428	3.305783333	neg
3.34_227.9974m/z	227.997419	3.3365	neg
3.34_249.0074m/z	249.0073549	3.3365	neg
3.34_321.0706m/z	321.0705835	3.3365	neg
3.35_472.0701m/z	472.0700525	3.350266667	neg
3.35_608.0451m/z	608.0450905	3.350266667	neg
3.36_389.0582m/z	389.0582169	3.362333333	neg
3.36_509.8027m/z	509.8027328	3.362333333	neg
3.36_579.8062m/z	579.8061522	3.362333333	neg
3.37_271.9072m/z	271.9071747	3.371	neg
3.37_374.8335m/z	374.833455	3.3751	neg
3.37_870.8036m/z	870.8036468	3.3751	neg
3.38_138.9069m/z	138.9068881	3.384783333	neg
3.40_264.9912m/z	264.9911761	3.40385	neg
3.40_285.9760n	284.9687723	3.40385	neg
3.40_342.9273m/z	342.9273208	3.40385	neg
3.40_352.9563m/z	352.9563094	3.395166667	neg
3.40_420.9438m/z	420.9437675	3.395166667	neg
3.40_488.9315m/z	488.9314949	3.40385	neg
3.40_556.9188m/z	556.9188016	3.395166667	neg
3.42_227.0650m/z	227.0650282	3.417666667	neg
3.42_278.0705m/z	278.0704701	3.417666667	neg
3.42_300.0525m/z	300.0525115	3.417666667	neg
3.42_350.9285m/z	350.9284567	3.417666667	neg
3.42_418.9162m/z	418.9161572	3.417666667	neg
3.44_165.0169m/z	165.0168577	3.440016667	neg
3.44_217.0350n	262.0333142	3.440016667	neg
3.44_252.0046m/z	252.0045888	3.440016667	neg
3.44_254.0017m/z	254.001721	3.440016667	neg
3.44_279.0235m/z	279.0235147	3.440016667	neg
3.44_285.0226n	330.0209402	3.440016667	neg
3.44_319.9921m/z	319.9920576	3.440016667	neg
3.44_353.0101n	398.0083001	3.440016667	neg
3.44_361.0311m/z	361.0311423	3.440016667	neg
3.44_362.9657n	407.9637002	3.440016667	neg
3.44_387.9796m/z	387.9796276	3.440016667	neg
3.44_422.0166m/z	422.0166389	3.440016667	neg
3.44_439.0473m/z	439.0473157	3.440016667	neg
3.44_488.9848n	533.9832993	3.440016667	neg
3.44_523.9544m/z	523.9544029	3.440016667	neg
3.46_167.0326m/z	167.0325587	3.455516667	neg
3.46_222.9756m/z	222.9756342	3.455516667	neg
3.46_233.0044m/z	233.0044448	3.455516667	neg
3.46_294.9782n	339.9762362	3.455516667	neg
3.46_300.9920m/z	300.9919847	3.455516667	neg
3.46_306.0233m/z	306.0233131	3.455516667	neg
3.46_313.9956m/z	313.9956228	3.455516667	neg
3.46_368.9794m/z	368.979381	3.455516667	neg

780.0925341	804.5364548	722.8112147	1342.875402	1142.120558	1263.778608	737.7340039	903.80578	788.5803669
1455.226176	1775.446005	1415.880643	1008.138447	848.8032108	958.598051	1226.77653	1690.234234	1459.156363
6462.378292	6189.347261	6723.521581	8330.434361	8115.884243	8405.679976	7823.120247	7531.377144	7778.360949
6746.423132	6833.727396	6473.022562	0.001403199	0.001403199	124.0215382	3390.881408	4532.883495	3663.240432
3378.009925	3276.277709	3161.169277	66.39640956	121.905395	0.001403199	1735.369138	2682.912487	1968.346855
1964.315664	1788.312186	1507.845784	746.7092493	716.1360663	601.5674345	336.1573556	188.1210625	255.3866076
4417.881167	4329.469835	4322.065057	226.3309146	280.9584722	73.17915017	2062.730895	2555.623276	2140.759991
1168.516337	1370.419707	1077.937084	0.001403199	0.001403199	0.001403199	913.6464114	824.274682	294.2059251
787.1692007	739.6172234	722.4791926	64.79901552	36.95886528	64.66589889	793.44203	622.8599234	705.8770874
827.9131467	589.1476942	594.385602	39.6232302	0.001403199	25.82920939	450.6382269	525.6265965	459.8992321
18748.87649	19286.82424	19611.75359	6034.951647	5948.8142	6025.979736	17381.20717	18292.73296	17563.86858
15614.55821	16182.43629	15096.52434	2634.967011	2989.116332	2737.160563	13904.06877	14132.79009	13955.65952
755.6581207	664.7817389	1166.425982	1180.640553	887.7738991	964.0906215	1219.646666	962.7103653	1103.543531
302.1863271	508.7413163	168.6902291	11.07447261	1.650193882	2.303717489	165.436724	225.1612778	433.8412484
32378.38718	30720.42579	29725.4786	15360.68198	15423.82096	16537.63873	29043.23084	28242.08447	28473.10958
22891.2123	230185.4777	227192.6749	43492.63703	42839.32021	43521.01901	197484.4744	209651.8412	204779.9431
1503.310754	1150.285364	689.4953843	0.001403199	0.001403199	0.001403199	403.7644286	640.6530933	206.9043015
7269.93916	7689.242212	8438.558937	1168.580562	976.6581009	1218.938357	6267.759672	7400.505482	7002.543262
696.0151896	984.7799402	948.6722107	0.001403199	0.001403199	0.001403199	192.1005503	614.9663467	396.291587
13576.99082	14355.00786	12897.75208	2156.742229	1783.169703	1728.183679	11645.07531	11141.44839	11448.00409
3861.636283	3308.528593	2815.976283	420.4531788	257.911972	515.2408813	3115.455147	2768.313923	3262.636681
4500.801852	3578.418781	3923.020074	741.0374412	629.6716646	569.8129591	3236.586345	3734.144519	3944.810347
4533.731409	3996.459322	4345.232883	575.2189932	750.1451402	549.9138127	2973.17612	3903.069359	3763.094334
35208.33607	36709.25435	40436.86491	271.1294603	376.7146289	238.3819739	19502.53868	26973.38385	24945.71153
54118.60288	50270.70777	45665.32234	14374.55143	14142.42341	14988.98517	43947.712	41757.68194	42252.81309
786.8497538	453.5753369	851.3998834	1386.616613	3538.617002	3972.568626	2139.951032	1533.029976	2038.525888
39569.96805	35481.59809	32876.80123	11238.84926	11093.00934	11789.43425	31740.87217	30016.94644	29615.34849
19604.00558	17523.02205	16571.39295	5936.859284	5828.985954	6376.70134	14865.8932	15073.21602	14632.48562
4014.833163	4252.248919	3011.722984	1756.657707	2799.320076	1599.94931	3413.498044	3472.05641	3583.030086
5752.621744	5097.855252	5561.792388	223.1370997	555.0719744	314.9737785	5054.537733	4964.464499	5082.216479
52175.18486	52379.46366	52357.24481	17251.50011	16307.88673	17068.0898	47220.5442	48370.50311	
4524.526475	4665.469098	4236.44859	557.6087328	384.6279349	457.8184103	3963.687995	4096.328018	3453.747948
10284.94239	10671.16323	10892.64869	1730.852146	1517.964443	1723.076696	8453.282369	9400.318464	9503.515599
2395.682568	1783.353391	1880.938559	440.5377902	523.4150803	516.9688012	1516.111005	1556.942352	1548.003503
210767.7172	218343.711	213596.4024	36319.43488	35162.58057	34090.81772	182335.3511	196664.0301	191236.8898
10451.94859	9860.273788	9784.461774	1415.686681	1560.75266	1738.773068	8907.338549	10087.40271	9477.843935
4558.644209	3827.378284	4154.120392	477.4386101	464.1941596	403.0157101	3395.732975	3767.038184	3765.675639
1070.222991	1198.772718	1359.209375	165.3488458	120.5294715	106.9730687	1360.12427	1295.971721	1187.665914
35407.0112	36028.03245	35732.74413	5592.786835	4891.043033	5584.735212	29817.29069	32715.05929	31124.01508
10207.52643	10388.85511	10263.38836	1271.662625	1418.9712	1205.146015	9695.782883	10151.57761	9729.507665
1958.201146	993.5712132	1397.879592	11.02549213	47.09838966	105.2980961	946.4917717	806.2356121	1006.456609
24729.23608	22249.45712	21456.92165	6867.423867	6186.178764	6125.045041	18431.62044	19455.19962	19176.63017
109349.0053	113876.6165	109634.6943	22140.46589	22105.55649	22314.50098	98750.03965	103615.9241	102013.001
3063.211394	3482.079895	3020.350598	358.2517636	217.6791359	258.7464695	3043.505504	2919.333302	2872.900174
1503.140082	1416.690069	1343.782125	214.8026997	154.4219052	309.858633	1277.684245	1356.011613	1178.853501
16729.77863	18946.53384	17559.25104	2575.46982	2622.035889	2890.723603	15508.90864	16404.16157	16811.42304
9857.611704	10022.03797	9519.089955	1075.177533	1399.236463	1165.627866	8412.589484	8630.659084	8164.010917
3651.871817	2716.077738	4145.185163	5.735861762	4.405453782	3.463384583	1368.404252	2264.388551	1967.530316
10997.31072	11760.06934	11834.20097	102.7580709	87.6536921	0.001403199	5958.791025	8805.582763	8179.077487
5333.802973	5721.203091	6122.501663	832.009994	679.7030807	817.2515301	5421.113022	5579.079123	5042.968193
13093.96608	13453.28532	12783.21819	1437.116194	1662.024555	1834.877628	10503.42084	11726.06275	11577.59117
5443.099478	4458.700646	3955.993402	604.0089306	528.5518599	270.7435836	4100.791356	3773.032509	3540.746702
76115.32625	79289.04622	75320.08507	15392.23467	13858.54205	14679.15503	68612.82768	69008.10437	70203.28405
9132.464845	9896.410706	10011.81073	0.001403199	0.001403199	92.57087392	4527.579575	6843.793574	5803.774573
9546.018835	8401.777048	8573.821742	1285.454149	995.288856	1013.709035	7911.039217	7938.657626	7343.295315
4372.845286	4443.158277	5101.000545	0.001403199	0.001403199	0.001403199	2964.625351	4076.939758	3761.783314
5441.518175	5251.361895	5441.893145	716.5307517	496.1490814	375.2971123	4633.686693	4456.020671	4333.412365
12901.03227	11397.66683	8930.172965	3813.148562	4013.060733	4833.984128	10036.68228	8718.082461	8202.123952
8758.581401	8877.584051	7910.702152	1493.263005	705.6098341	881.6206115	7215.392675	6980.981323	7913.452989
1508.660932	1014.803005	956.0132233	933.3904771	980.441895	1015.060265	1112.699238	966.1262893	805.4584375
3235.418251	2802.193897	2672.464643	299.2000115	368.0445489	454.0464919	2944.795893	3034.820041	3201.232785
7531.14622	7568.902269	7859.867219	860.8056585	1311.986664	1033.058865	6389.722555	6115.74295	6752.589985
3641.355703	2941.366548	3945.375305	586.2949562	583.8751493	479.8724592	2153.953322	3239.011681	3150.19013
10240.90206	11094.66934	10796.35354	698.5946354	587.4982105	630.3419533	9455.582269	10905.80654	9744.505732
3408.351231	3567.042434	3493.31952	1325.678783	1353.643491	1239.844186	3119.673876	3433.514683	2796.793963
3112.359196	3211.607717	2881.205537	4851.572366	5251.336243	4676.079699	3206.225155	3883.200251	3280.918147
4632.692708	4973.998858	5016.427884	6967.855613	6412.490765	6651.923994	4724.44024	6170.609347	4854.374927
1662.270438	1146.482197	1386.980735	1486.370776	1902.563234	1735.847536	982.3153106	1166.741486	814.9737951
1311.071306	1227.674941	1112.166036	1967.357	1913.679884	1954.368548	1368.108261	1494.658997	1487.667591
2709.756451	2789.398633	2191.788712	2473.074008	3429.707729	2887.997342	2948.673679	2812.118832	2345.674007
1729.255356	1866.398562	792.912593	1277.895315	1372.670289	1242.402892	1576.298425	917.437973	1141.946077
933.9472696	1245.244267	777.2011964	1168.549219	1318.256618	1343.915586	1280.398655	918.8347125	916.9878897
5313.418782	5570.228239	4782.189012	5146.676564	5467.772045	5389.009945	6220.746124	5288.648228	5556.675929
5248.704178	5682.083008	4434.677512	5195.328876	6990.695645	6080.691283	5794.004995	4460.015963	4444.740107
223.3655892	247.4313345	119.5257761	174.2779542	182.2213653	223.8689498	197.853928	111.7675028	149.2050043
386.9092595	560.47163	328.1329226	646.5771952	723.1078225	400.8073528	201.7333161	422.2092628	178.1472821
26919.5365	30235.8111	26920.2157	33899.51709	32498.92847	32667.24211	25126.4737	27476.12237	25266.06305
860.5117042	903.55412	719.6998779	1193.139136	1147.657716	1117.144906	718.0019198	864.2660783	487.3535657
16361.27171	18815.79202	17282.02838	21098.87002	20982.52465	20445.24555	15499.91825	17099.79788	15816.12501
10552.29902	10771.82756	10282.9421	12740.2952	12505.44641	12429.15347	9449.978974	9355.551496	9200.473326
3356.242924	4200.009439	3514.136418	4700.741447	4607.76719	4346.167912	2982.611632	3351.215854	2618.714096
2028.154787	2642.912256	2113.731604	2838.334584	2837.851937	2977.332466	1919.336024	2017.220239	1222.451879
877.3056478	930.5615543	907.7452573	1521.949246	1571.640304	1414.236017	1314.889016	1528.633056	1181.947601
1028.631915	1099.528496	1029.710221	1641.228178	8491.817958	8403.452992	4790.196937	4602.960117	4397.615618
115.9040143	65.37768638	53.7918258	1697.193591	1504.686815	1364.849472	757.2108434	728.209837	608.203083
618.4332197	540.4843894	520.0541062	1026.727195	1170.851601	1042.723944	827.4292384	1061.111458	461.7864915
1712.494713	2013.284835	2221.713675	3276.702153	2828.240156	2698.04388	3614.322591	3299.019849	2885.170095
1129.064371	1472.447019	1360.366329	2320.472496	2227.360599	2187.710034	1636.208828	1541.34646	1630.470307
76746.78329	88385.31236	89417.27561	50096.93703	48087.49006	49673.03737	88442.57699	91090.48447	81395.45272
8927.09867	10107.34566	10781.83178	5727.714199	5495.521749	5417.4669	9916.547771	9610.234172	9420.628468
2562.668453	3047.877094	3371.846095	1575.620144	1630.832262	1651.989897	3137.985733	2708.915586	2704.663301
6181.923777	7621.268862	7513.191117	4188.675776	4055.993425	4337.407154	7569.401875	7048.5736	6335.594933
41680.20754	47750.11486	47862.98907	27414.91288	25932.70208	26809.3769	47781.04142	42267.2583	42685.72288
4996.625461	5471.900776	5627.906531	3144.176382	2992.88004	3227.19092	5433.768339	5352.85984	5212.806604
31903.3546	36553.97749	37391.55002	21096.60531	20703.57685	21073.33287	37635.90036	34745.44724	34384.42389
1480.943767	1559.730601	1515.602347	620.8455464	630.0757403	435.6209847	880.2889992	822.5879898	507.6150719
5108.430858	4847.099881	5456.224102	2313.229353	2317.482323	2060.667546	5136.840378	4462.049096	3799.805473
5555.064228	6711.450477	6652.476359	3461.614885	3420.434459	3476.95479	6340.951193	6025.474671	5968.442046
4893.766894	6449.146301	6560.012375	59.56135519	138.0575012	179.9854676	3571.768133	3719.465783	3585.318573
8406.457283	8901.583287	8144.32688	3941.821908	3820.595692	4191.923302	4702.712422	4690.675446	4158.796633
15820.96518	19955.50705	19020.58056	11292.17071	11614.79359	12454.91093	21190.87101	18771.64925	17555.01162
2881.980412	2580.668585	3392.207395	1704.521903	1907.462753	1639.700482	3348.298963	3641.59022	2764.552127
1052.116218	1235.38227	1229.35895	2033.178312	1884.496107	1947.809947	1594.067431	1534.794645	1511.561637
314.4706448	311.5092622	376.770675	733.1083002	646.8040151	810.1357467	458.3788607	451.3477364	398.0726732
2908.286866	3283.237148	3684.064729	5967.176451	5693.238976	5782.839552	4561.650665	4236.806555	4096.03209
4662.383527	5131.325231	5740.394768	2705.514014	2024.535341	2418.2739	4910.689667	4833.258857	4158.984201
2551.194426	3232.604158	3258.60433	5470.738262	5158.189266	5370.121674	4165.401475	4064.23866	3754.700157
1559.234514	1880.035079	1888.136718	1171.131722	948.7907874	1116.318628	1724.020296	1808.908216	1574.435183
1755.582566	2045.347114	2265.252688	1019.040593	988.5633397	1177.365633	2203.549524	2182.437582	1725.656266
1739.651428	2215.916341	2419.444619	4657.421409	4487.920903	4505.811877	3023.951867	3288.82651	2708.338004

3.46_373.8278m/z	373.8277511	3.455516667	neg
3.46_393.1406m/z	393.1405662	3.455516667	neg
3.46_414.9986m/z	414.998644	3.455516667	neg
3.46_420.9975n	465.9957705	3.455516667	neg
3.46_429.9456m/z	429.9456096	3.455516667	neg
3.46_436.9666m/z	436.9666898	3.455516667	neg
3.46_455.9672m/z	455.9671507	3.455516667	neg
3.46_472.9275m/z	472.9274727	3.455516667	neg
3.46_498.9406n	543.9385571	3.455516667	neg
3.46_555.9647m/z	555.9646709	3.455516667	neg
3.46_601.971m/z	601.971043	3.455516667	neg
3.46_659.9298m/z	659.9297805	3.455516667	neg
3.46_669.9586m/z	669.958643	3.455516667	neg
3.46_737.9462m/z	737.9461659	3.455516667	neg
3.47_357.0837m/z	357.0836797	3.47105	neg
3.47_482.9862m/z	482.9861593	3.47105	neg
3.48_233.0126m/z	233.0125914	3.484883333	neg
3.48_368.0745m/z	368.0744919	3.484883333	neg
3.48_436.0620m/z	436.062045	3.484883333	neg
3.48_446.0908m/z	446.0907902	3.484883333	neg
3.48_457.1579m/z	457.1579495	3.484883333	neg
3.48_650.0533m/z	650.0533388	3.484883333	neg
3.48_718.0411m/z	718.0410617	3.484883333	neg
3.50_322.0545m/z	322.054518	3.498716667	neg
3.50_567.9050m/z	567.9049881	3.498716667	neg
3.51_242.0130m/z	242.0130181	3.509133333	neg
3.51_342.1310m/z	342.1310151	3.509133333	neg
3.52_211.0588m/z	211.058821	3.52125	neg
3.52_224.9630m/z	224.9630285	3.52125	neg
3.52_279.0463m/z	279.0462992	3.52125	neg
3.52_347.0339m/z	347.0339487	3.52125	neg
3.52_442.8203m/z	442.8203332	3.52125	neg
3.53_441.8155m/z	441.8154981	3.529966667	neg
3.53_590.8207m/z	590.8206649	3.529966667	neg
3.53_663.8472m/z	663.8472202	3.529966667	neg
3.53_683.8305m/z	683.8304877	3.529966667	neg
3.54_308.8643m/z	308.86429	3.540433333	neg
3.54_360.9744m/z	360.9744344	3.540433333	neg
3.54_484.2418m/z	484.2417639	3.540433333	neg
3.54_662.8418m/z	662.8417673	3.540433333	neg
3.55_270.0959m/z	270.095914	3.549183333	neg
3.55_321.0650m/z	321.065008	3.549183333	neg
3.55_366.0832m/z	366.0831624	3.549183333	neg
3.55_389.0946m/z	389.0946453	3.549183333	neg
3.56_144.9433m/z	144.9432952	3.564783333	neg
3.56_216.9813m/z	216.9813073	3.564783333	neg
3.56_246.0806m/z	246.0806305	3.564783333	neg
3.56_246.1217n	245.1143433	3.564783333	neg
3.56_277.0307m/z	277.0307368	3.564783333	neg
3.56_335.0840m/z	335.0839611	3.564783333	neg
3.56_403.0713m/z	403.0712799	3.564783333	neg
3.56_537.8268m/z	537.8267931	3.564783333	neg
3.58_248.9872m/z	248.9871732	3.584083333	neg
3.58_268.9739m/z	268.9738503	3.584083333	neg
3.58_330.0597m/z	330.0597016	3.5753	neg
3.58_360.1416m/z	360.1415706	3.584083333	neg
3.58_381.8680m/z	381.8679533	3.5753	neg
3.58_393.1405m/z	393.1405246	3.584083333	neg
3.58_428.9616m/z	428.9616245	3.5753	neg
3.58_434.2146m/z	434.2145633	3.584083333	neg
3.58_444.0525m/z	444.0525177	3.584083333	neg
3.58_482.9333m/z	482.9332951	3.584083333	neg
3.58_514.8931m/z	514.8930852	3.584083333	neg
3.60_201.0770m/z	201.0770159	3.601516667	neg
3.60_210.9835m/z	210.9835205	3.601516667	neg
3.60_224.9993m/z	224.9993218	3.601516667	neg
3.60_570.8371m/z	570.837118	3.601516667	neg
3.60_704.8157m/z	704.8156686	3.601516667	neg
3.61_233.0126m/z	233.0125861	3.611966667	neg
3.61_258.0077m/z	258.0076857	3.611966667	neg
3.61_336.1124m/z	336.1123523	3.611966667	neg
3.61_346.9585m/z	346.9585257	3.611966667	neg
3.61_350.9283m/z	350.9282859	3.611966667	neg
3.61_388.9233m/z	388.9233332	3.611966667	neg
3.61_446.9062m/z	446.9062266	3.611966667	neg
3.61_456.9108m/z	456.9108486	3.611966667	neg
3.61_477.8655m/z	477.8655462	3.611966667	neg
3.61_724.8020m/z	724.8020442	3.611966667	neg
3.62_146.946m/z	146.946603	3.624166667	neg
3.62_171.0201m/z	171.0200815	3.624166667	neg
3.62_272.1042m/z	272.1042105	3.624166667	neg
3.62_320.9357m/z	320.9357478	3.624166667	neg
3.62_654.8700m/z	654.8699648	3.624166667	neg
3.62_722.8575m/z	722.8574844	3.624166667	neg
3.63_241.0694m/z	241.0694499	3.630433333	neg
3.63_270.0079m/z	270.007866	3.630433333	neg
3.63_278.1068m/z	278.1067636	3.630433333	neg
3.63_291.0183m/z	291.0182567	3.630433333	neg
3.63_328.0676m/z	328.0676301	3.630433333	neg
3.63_350.0495m/z	350.0494883	3.630433333	neg
3.63_418.0372m/z	418.0372499	3.630433333	neg
3.63_604.8717m/z	604.8717132	3.630433333	neg
3.64_189.9898m/z	189.9897823	3.640916667	neg
3.64_190.9823m/z	190.9822889	3.640916667	neg
3.64_210.9683m/z	210.9682843	3.640916667	neg
3.64_256.9739m/z	256.9738799	3.640916667	neg
3.64_278.9558m/z	278.955778	3.640916667	neg
3.64_346.9434m/z	346.9433649	3.640916667	neg
3.64_414.9311m/z	414.9310579	3.640916667	neg
3.64_420.9436m/z	420.9436084	3.640916667	neg
3.64_482.9186m/z	482.9185923	3.640916667	neg
3.64_524.8983m/z	524.8982581	3.640916667	neg
3.65_148.9732m/z	148.9732057	3.64965	neg
3.65_149.4750m/z	149.4750332	3.64965	neg
3.65_307.8561m/z	307.8560601	3.64965	neg
3.65_336.9149m/z	336.9149352	3.64965	neg
3.65_397.0731m/z	397.0730855	3.64965	neg
3.65_424.8865m/z	424.8864873	3.64965	neg
3.66_277.032m/z	277.032878	3.6635	neg
3.66_282.9894m/z	282.9894102	3.6635	neg

748.7030994	823.4658741	697.8527678	1050.936843	925.7908836	913.7175212	1120.422928	1152.926391	884.0676138				
341.0119546	578.0295476	437.7083456	609.629096	726.956007	695.7592545	1093.170433	1223.558254	1249.891406				
1821.453011	1781.754948	2067.958092	1149.386361	1103.998853	871.977623	1795.982133	1884.940073	1614.633323				
22958.24911	28457.26719	28102.90231	15785.32513	15630.31583	16451.54843	28530.10781	25752.4137	24635.1097				
4082.61014	4092.277463	3935.053247	1961.766019	1687.220497	2149.113853	3900.928673	3697.918941	3197.270354				
1477.626608	1688.940698	1852.934941	3512.815768	3314.118121	3689.999577	2397.878394	2842.055973	1864.902147				
5272.157948	5240.326045	5238.530977	3019.223477	3289.313971	2931.584273	5472.663676	5650.436394	4343.523766				
1075.151308	1477.774412	1390.793109	359.3286923	387.7724381	346.6651896	947.962691	1292.628087	1248.240003				
5480.34568	5225.404206	5775.713363	2646.084204	2595.358224	2640.851193	5140.841347	4827.953971	4183.146437				
2407.076754	2145.573107	2657.071437	1659.642514	1580.820344	1593.223131	2609.870478	2851.790142	2493.837562				
10560.22636	11985.52213	12676.27401	7582.580287	7376.472194	7209.597407	12221.94016	11362.8587	11109.32228				
1988.71338	1873.218437	2335.398317	1401.346025	1223.503813	885.5488291	2492.784836	2368.84081	1886.405175				
8974.420742	9861.421341	10060.95198	5578.177217	5523.026719	6406.516897	10263.61713	9832.998544	9111.332504				
7019.011571	6950.993335	7183.063237	3915.210759	4014.746265	4087.031188	7244.602529	6979.914813	5965.30077				
1051.970005	1399.960153	1485.189436	1332.323997	1163.295801	1308.264204	1603.626606	1293.299252	1811.991407				
1985.298928	1904.004816	2052.404878	1155.634233	1013.316368	1212.092529	2012.129531	1777.231341	1469.380657				
2067.408069	2432.130141	2707.082922	1841.108042	1730.537994	1681.280783	2121.480713	2345.911617	2254.644054				
1557.499366	1981.231786	2334.222644	3279.150822	2511.863563	2797.205963	2610.643313	2382.059936	2256.304007				
1237.043808	1424.43597	1429.89696	1791.846404	1522.077995	1753.556613	1412.272557	1410.423775	1509.926886				
10312.29705	11435.89937	12892.70687	15877.3167	13590.79342	14158.25958	13642.14575	12675.77833	12422.80495				
1137.899896	1472.323604	1569.622179	2427.645615	2097.036447	1807.129752	1407.707988	1598.018117	2093.304395				
2588.667052	3069.278528	3250.425275	5586.579026	4559.754156	5128.692509	3838.788864	4162.543566	3787.701628				
1922.324185	3061.684442	2307.752429	3735.388308	3232.096885	2986.343003	2487.783254	1969.3774	2552.021746				
2276.311583	2464.057776	2499.736407	386.9005984	249.1180207	366.9891333	1809.531308	2141.545251	1831.613036				
760.8751962	615.8864432	724.1691342	259.6463911	211.174993	286.0114582	118.3143412	813.0075436	424.6055442				
841.9959937	930.9923865	1019.012799	714.1561189	649.3417052	653.4408205	1135.114798	1286.650299	1155.674869				
669.7970567	553.6476622	797.8198805	596.6219334	727.9012526	787.673389	622.6508649	579.6212872	758.4496366				
2168.443735	2276.547374	2239.698062	2849.020645	2974.709504	2925.011004	1766.134354	2099.303211	1892.337641				
1331.102756	1455.20642	1321.336009	1102.58732	1444.545531	1302.416357	1784.379878	1327.299591	1717.396048				
1657.465998	1823.372974	1762.00691	2207.512756	2357.570534	2137.887697	1298.416134	1542.227492	1514.729903				
1137.981959	1074.281306	1308.682353	566.5303784	1297.657362	1169.368892	949.6932053	1003.031226	1018.578398				
1440.300488	1597.145139	1340.571151	1141.176479	1097.542272	1206.262765	1549.965771	1467.557234	1182.074951				
1282.963331	1504.593306	1004.041691	969.3446137	823.4860861	1118.813555	1568.011006	1203.02811	874.2841263				
2331.179526	2312.301829	2813.291448	1724.434857	1881.420029	1278.042556	2644.361284	1987.502174	2021.080314				
4828.015166	6081.709405	4996.450385	5126.769929	5563.990237	5263.613242	7312.92644	5421.450865	5353.298075				
3129.881193	3938.291345	3474.433997	2777.94544	3269.23727	3298.960559	4366.978972	3446.978973	3431.533972				
1956.908205	1575.369289	1291.793902	1037.713297	1265.209001	1312.174248	1406.657649	1367.867758	1193.461523				
2732.082543	3305.410666	2970.471253	2776.815369	2980.489469	3017.695402	3993.800643	3278.79504	3054.085578				
1122.09707	1005.621119	835.6393481	1178.224902	1259.869006	1304.510803	1121.698775	1193.108338	1251.863269				
2162.432955	2418.181113	2635.014799	3138.831581	3281.504941	2976.189522	3352.074033	2962.044731	2896.739788				
504.769414	470.9102271	446.5338907	275.4064957	298.7615485	296.6865222	269.1782963	214.4020622	244.9977823				
6118.363113	7040.44001	6314.214296	370.7367539	355.7191734	386.1438318	4388.459828	4689.077142	4617.305528				
723.119475	1065.665097	843.6174644	1009.316198	992.0304679	835.1745408	800.19988	630.2260628	640.0375326				
1841.060091	2214.056541	2058.380522	1038.402138	1201.39919	1194.007256	789.0753154	708.6903553	667.769033				
813.5866871	706.5536866	642.7802593	679.3445575	745.9411394	634.3469914	698.3811866	575.1815007	637.7871737				
1412.796285	1585.078936	1449.551887	385.948604	346.7598199	399.4580091	523.5755833	738.8258384	703.040356				
4391.372745	4811.550584	4708.842986	6233.875296	6294.621016	5731.671957	4930.802979	5170.348195	4557.101089				
11729.98117	13324.32502	12705.48596	17257.55309	18140.00169	16683.62751	13042.3664	14186.41935	14024.92097				
364.9184285	547.6203626	504.5232424	883.0948443	874.9176182	709.572979	545.0268021	638.0220942	634.4655434				
3240.314186	3867.933597	3582.527895	5132.983364	5307.036789	5174.618263	4313.415513	4893.754147	4042.195733				
1347.771303	1642.047186	1408.565452	2261.331941	2560.273644	2483.1886	1708.08445	2165.023795	1764.740267				
5173.886832	3382.681576	3481.463952	3651.734967	4267.689836	4070.613912	5065.639953	3368.754272	3825.688556				
167.5933142	246.9815386	227.8757728	244.1724372	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199				
5550.91817	6432.452442	6196.086475	5668.338737	5600.626363	5824.804886	4257.273266	4793.028893	4668.559929				
340.026752	477.5959402	804.6894059	226.6378813	249.1662398	266.8253131	676.3337726	703.5051811	555.9514438				
1516.786662	1881.707799	1655.846428	1553.636471	1608.485105	1789.608942	1536.524721	1831.37525	1616.265496				
2210.62883	2559.137064	2296.434756	2826.203777	2862.868923	2518.859943	2566.103783	2004.269978	2691.649383				
577.7380974	667.3120135	906.2492864	678.0686034	531.0810629	577.1236388	1370.135693	1363.311348	1322.286755				
2448.262047	2935.723114	2533.62829	2366.701678	2597.456847	3063.453668	2604.978268	2492.841876	2818.524243				
314.934198	411.1043684	493.4711486	572.0954123	482.1176566	407.1149169	515.5679234	415.3805466	376.5814416				
1474.286653	2066.132645	1707.356258	0.001403199	0.001403199	0.001403199	1306.214014	1701.746683	1596.290331				
1774.437079	2767.997267	1864.784413	1681.960371	2322.412898	2394.350394	2125.745558	2464.264443	2743.522453				
16096.17888	16917.71677	16386.9977	14891.18356	17054.80584	15409.73867	19131.77594	17926.54334	16664.52913				
345.2258341	411.7620892	383.3058741	270.2505226	267.1342275	374.6236873	290.7244646	367.1940433	424.8737755				
481.0112522	477.3091617	363.7851528	519.3288666	546.9771857	664.9814047	666.8184663	604.0145123	617.0776252				
1330.15197	1419.361065	1394.807401	1201.924733	1531.650098	1483.658791	1613.242257	1326.849968	1561.963494				
8071.075246	7487.62732	7718.11595	8002.714956	10494.20415	9248.24956	9278.662	7895.874878	8312.490224				
8852.966127	8194.654968	7371.952257	9168.785741	9628.174052	10007.73653	11069.69308	7825.101467	9358.95779				
2627.189181	2757.970887	2565.021249	669.2970983	742.1365907	746.749995	1282.089187	1590.245109	1555.369053				
857.3980038	934.6756176	763.0641583	820.1523194	886.897681	985.5253666	854.1887275	1014.463267	1143.219694				
352.8281631	511.780175	463.8248903	753.4882611	501.9988035	704.5024508	243.2964895	159.6375751	236.2908496				
8774.52385	8678.128702	8423.245406	10851.57827	12469.14417	11484.90946	11372.00717	9884.758318	10362.01333				
2487.25192	2362.781202	2261.532444	2647.059207	3574.271618	3414.119386	2770.357073	2632.730373	2549.275195				
45077.45208	48414.47607	48834.07345	2285.906651	2252.890421	2103.535092	33264.12354	33762.53365	34425.65322				
11970.25357	11554.3591	10153.65358	12353.29493	13690.09767	12454.36688	13359.64766	11161.90602	11989.51704				
16294.96649	17158.89398	15449.68573	316.5113577	791.2527378	314.5547497	11251.7932	13039.70407	12049.36258				
4401.52942	3738.402336	3028.440428	4541.500705	5480.420078	5188.162619	4174.1714	3606.855825	4699.284154				
10955.08241	11411.23638	10371.78361	8378.547842	11185.153	10844.59808	12150.06523	10621.25827	10883.72198				
520.0348075	453.1967431	419.3434243	460.4805551	482.3299876	468.9632016	589.5209031						
618.6862586	618.1389476	393.6546629	580.4527624	745.382731	726.4024509	568.1170251	511.9752555	651.3621414				
743.3062596	652.3161141	519.7559718	466.2922507	515.2867691	460.2223813	731.0453237	617.2773521	964.5496123				
120911.6409	129260.4093	128441.5233	8939.867856	8006.633298	7910.201754	85099.91823	89682.93995	89537.57643				
7855.420454	7925.138549	7084.883725	7808.261444	9752.672072	9259.760256	8984.739536	7782.922964	8051.860825				
4762.532191	4374.193434	3783.833505	5884.539246	6010.788866	5122.062067	4732.459412	4791.532333					
410.1758726	388.2273105	424.0526572	487.3164488	609.4779282	560.0728923	261.7438853	281.066555	330.9881076				
651.3528576	708.0659847	571.8366278	380.1095914	397.9862517	497.2907767	485.2918048	388.3671811	536.890852				
269.0481422	274.1063106	353.9695985	294.2355408	602.300767	514.3316351	312.7616125	207.5287758	331.3952714				
1019.718524	1028.153437	929.7205307	630.1692475	723.6275357	608.2261201	1061.778519	787.4482307	899.4659622				
5758.48967	5767.067477	5481.887295	12254.15375	12360.09636	12147.26625	7514.565245	7414.76805	8426.677004				
2483.519353	2608.950456	2303.266964	5154.656201	4995.46786	4772.029648	3339.314687	2929.784076	3380.124252				
1143.218129	897.0958503	1003.274175	2375.17667	2425.190472	2497.123108	1385.173833	967.9788094	1341.21875				
12870.735	12306.36653	10572.68308	13570.26582	15255.88649	13111.52657	15618.24703	12658.7042	14114.88072				
9019.011153	9925.84026	9428.516584	3079.984937	3005.656445	2561.589234	5899.832385	6145.89417	6588.070923				
5062.32498	5211.303197	5171.172408	1686.154884	1752.292141	1542.393672	3417.871405	3521.831603	3624.745692				
962.8833732	844.4326878	763.6772718	256.9427864	250.219245	241.9846158	679.2059895	365.04528	552.9625976				
3457.701835	3910.230616	3536.871323	1211.507448	1044.540046	934.9916677	2353.648543	2406.057349	2974.758078				
7604.922126	8715.460677	7802.950854	2511.033992	2516.316327	1907.125124	5114.458701	4657.730285	5509.226615				
8180.891069	8875.140076	8456.313013	1856.805413	2034.180623	1810.303145	4842.362588	4921.822818	5942.880668				
4293.849356	4628.764141	4597.915203	767.3419885	1023.733984	963.3784683	2916.034054	2629.886117	2879.748799				
1102.311228	1387.797986	1141.128204	914.512487	1095.586154	1130.782336	890.8613468	879.2197723	887.9672506				
2670.255534	2485.32531	2899.226198	1542.024811	1948.632621	1500.655015	2468.548251	1390.712979	1709.211097				
3715.550616	2850.947261	3273.462242	0.001403199	115.4206331	89.20731854	1772.154843	1972.846227	2228.814155				
83310.23794	87299.83302	88977.25227	7423.907647	7057.951968	6738.875039	60168.30065	63851.42957	63919.67544				
3533.333737	3957.837257	3734.487955	156.8725373	176.2098723	102.6250454	2234.917044	2625.13869	2763.717074				
1120.884164	610.8173958	609.1841595	736.5488568	1014.917845	657.2001422	823.432965	606.7737961	728.6145034				
1077.869302	648.0610074	1106.235753	158.9197754	0.001403199	237.1966648	578.9826029	434.0226261	464.1332669				
891.1218842	914.3065413	898.0596615	1394.127804	1524.704289	1303.926429	761.9671356	976.4908532	1065.028966				
1435.338459	1072.18912	736.5164333	89.41785659	235.3223337	0.001403199	609.5523658	107.7882805	467.4755404				
667.9575997	700.6426832	742.0433494	1192.211175	1050.723496	661.0712933	912.5594602	560.1091347	793.6389715				
729.7008999	623.4142093	503.3416059	590.5388846	491.56281	481.4224328	843.4570571	433.5032671	392.4809253				

3.66_314.9795m/z	314.9794865	3.6635	neg
3.66_336.9614m/z	336.9614392	3.6635	neg
3.66_404.9488m/z	404.9488141	3.6635	neg
3.66_472.9363m/z	472.9362739	3.6635	neg
3.66_540.9238m/z	540.9238357	3.6635	neg
3.69_167.0332m/z	167.0331715	3.685866667	neg
3.69_176.0386m/z	176.0386367	3.685866667	neg
3.69_196.0558m/z	196.0557599	3.685866667	neg
3.69_202.9658m/z	202.9657838	3.685866667	neg
3.69_235.0208m/z	235.0207554	3.685866667	neg
3.69_242.0131m/z	242.013064	3.685866667	neg
3.69_255.0081m/z	255.0081477	3.685866667	neg
3.69_276.0003n	320.9985708	3.685866667	neg
3.69_280.0301m/z	280.0300865	3.685866667	neg
3.69_286.0291n	331.0272621	3.685866667	neg
3.69_292.9507m/z	292.9507282	3.685866667	neg
3.69_303.0082m/z	303.0081622	3.685866667	neg
3.69_315.0021m/z	315.002092	3.685866667	neg
3.69_337.9887m/z	337.9886949	3.685866667	neg
3.69_340.9828m/z	340.9828176	3.685866667	neg
3.69_354.0167n	353.0093783	3.685866667	neg
3.69_363.9718n	408.9702625	3.685866667	neg
3.69_369.9994m/z	369.9994101	3.685866667	neg
3.69_398.9413m/z	398.941324	3.685866667	neg
3.69_404.9711m/z	404.9711285	3.685866667	neg
3.69_413.0942m/z	413.0942128	3.685866667	neg
3.69_422.0043n	467.0019971	3.685866667	neg
3.69_430.9523m/z	430.9522614	3.685866667	neg
3.69_456.9737m/z	456.9736645	3.685866667	neg
3.69_478.9557m/z	478.9557028	3.685866667	neg
3.69_481.0817m/z	481.0816742	3.685866667	neg
3.69_483.9925m/z	483.9924619	3.685866667	neg
3.69_489.9916n	488.9843058	3.685866667	neg
3.69_499.9476n	544.9453089	3.685866667	neg
3.69_505.9744m/z	505.9743918	3.685866667	neg
3.69_546.9432m/z	546.943219	3.685866667	neg
3.69_549.0695m/z	549.0695392	3.685866667	neg
3.69_556.9716m/z	556.9716283	3.685866667	neg
3.69_602.9776m/z	602.9775854	3.685866667	neg
3.69_624.9594m/z	624.9594831	3.685866667	neg
3.71_185.0430m/z	185.0429588	3.708366667	neg
3.71_199.0587m/z	199.0587325	3.708366667	neg
3.71_227.9974m/z	227.9974015	3.708366667	neg
3.71_229.9930m/z	229.9929989	3.708366667	neg
3.71_295.984m/z	295.984711	3.708366667	neg
3.71_317.9662m/z	317.9662193	3.708366667	neg
3.71_337.0239m/z	337.0238981	3.708366667	neg
3.71_350.0617n	395.0601198	3.708366667	neg
3.73_216.0878m/z	216.087772	3.730516667	neg
3.73_249.9791m/z	249.9791231	3.730516667	neg
3.73_274.0700m/z	274.0700216	3.730516667	neg
3.73_320.9665m/z	320.9665302	3.730516667	neg
3.73_327.0159m/z	327.0158849	3.730516667	neg
3.73_395.0030m/z	395.0029544	3.730516667	neg
3.73_401.0261m/z	401.0261479	3.730516667	neg
3.73_404.0136m/z	404.0136111	3.730516667	neg
3.73_423.0081m/z	423.0081385	3.730516667	neg
3.73_428.0447m/z	428.0446588	3.730516667	neg
3.73_433.0367m/z	433.0366645	3.730516667	neg
3.73_472.0000m/z	471.9999891	3.730516667	neg
3.73_502.0315n	501.0242697	3.730516667	neg
3.73_636.9990m/z	636.9989957	3.730516667	neg
3.73_704.9866m/z	704.9866499	3.730516667	neg
3.73_772.9738m/z	772.9738154	3.730516667	neg
3.75_288.0605m/z	288.0605094	3.747833333	neg
3.75_340.0052m/z	340.0052273	3.747833333	neg
3.75_349.0132m/z	349.0131986	3.747833333	neg
3.75_391.9951m/z	391.9950609	3.747833333	neg
3.75_397.0163m/z	397.0162597	3.747833333	neg
3.75_413.0027m/z	413.0026627	3.747833333	neg
3.75_438.9822m/z	438.9821787	3.747833333	neg
3.75_560.0104m/z	560.0104258	3.747833333	neg
3.75_565.1299m/z	565.1298819	3.747833333	neg
3.75_600.9791m/z	600.9791334	3.747833333	neg
3.75_627.9986m/z	627.9986392	3.747833333	neg
3.75_668.9668m/z	668.9668335	3.747833333	neg
3.75_688.9507m/z	688.9507003	3.747833333	neg
3.75_746.9827m/z	746.9827187	3.747833333	neg
3.75_756.9382m/z	756.9381757	3.747833333	neg
3.75_882.9571m/z	882.9570606	3.747833333	neg
3.77_186.9820m/z	186.9819786	3.770416667	neg
3.77_213.0382m/z	213.038212	3.770416667	neg
3.77_226.0721n	271.0701996	3.770416667	neg
3.77_246.0807m/z	246.0806798	3.770416667	neg
3.77_294.0596n	339.0575671	3.770416667	neg
3.77_314.0684m/z	314.0683934	3.770416667	neg
3.77_345.0171m/z	345.017148	3.770416667	neg
3.77_353.0868m/z	353.0867613	3.770416667	neg
3.77_382.0554m/z	382.0554073	3.770416667	neg
3.77_417.0007m/z	417.0006854	3.770416667	neg
3.77_459.9827m/z	459.9826634	3.770416667	neg
3.77_465.0037m/z	465.0036973	3.770416667	neg
3.77_475.0325m/z	475.0324714	3.770416667	neg
3.77_484.9880m/z	484.9880278	3.770416667	neg
3.77_492.0230m/z	492.0229918	3.770416667	neg
3.77_532.9913m/z	532.9913328	3.770416667	neg
3.77_543.0201m/z	543.020148	3.770416667	neg
3.77_611.0078m/z	611.0077572	3.770416667	neg
3.77_620.9632m/z	620.9631742	3.770416667	neg
3.77_670.9638m/z	670.9637748	3.770416667	neg
3.77_678.9950m/z	678.9950286	3.770416667	neg
3.77_736.9539m/z	736.9539309	3.770416667	neg
3.77_814.9700m/z	814.9700345	3.770416667	neg
3.78_170.9682m/z	170.9682331	3.779133333	neg
3.78_203.9973m/z	203.9972649	3.779133333	neg
3.78_216.9813m/z	216.9812649	3.779133333	neg
3.78_217.0351n	262.0333633	3.779133333	neg
3.78_287.0322m/z	287.0322153	3.779133333	neg
3.78_302.1360m/z	302.1359538	3.779133333	neg
3.80_224.9992m/z	224.9992331	3.801716667	neg

5286.904176	5633.161016	6119.756425	1772.458588	1804.849589	1461.368342	6355.462494	6921.941534	6909.733502
8778.89237	9942.726256	9894.187856	6151.508415	6002.338801	5652.042903	8699.241348	8947.337973	9642.383047
4631.657184	4590.806775	4813.838829	2139.607071	2212.55396	2036.717742	4456.938252	5038.981918	5495.07966
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1815.699121	2340.135609	1594.542531	1129.636299	1076.187502	777.7732628	1906.052238	1561.482945	1911.278848
2231.624686	2299.319728	2315.743705	2911.546642	3058.960251	2065.09028	2305.84747	2398.465672	2369.161039
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9184.125324	9717.390702	9664.312666	15103.90503	15840.61715	11904.54155	11907.78001	12605.77959	12737.46541
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3834.824028	3530.772858	3721.592509	5100.232269	4969.200342	3888.898411	3502.409677	3552.572617	3817.100157
4303.388284	4646.109687	4649.192431	2676.637847	2797.719136	1896.932016	4190.805328	4919.258154	5139.043582
1238.718804	1741.736534	1572.818816	2291.293624	2490.180318	1835.792092	1912.108774	1898.951333	2081.284162
2010.802742	2441.950223	2137.354038	3590.613966	3819.32403	2634.980623	2716.454951	2894.446289	2867.959521
7592.967607	9453.639492	8712.545553	13700.55666	14125.07868	10489.98205	11056.70914	11013.89471	11158.25448
20503.96695	22081.37882	21853.04297	34412.39293	34624.60899	25253.25739	26477.33099	27415.17319	27914.23592
1067.995523	768.8022285	887.2031306	1374.249336	1153.966142	645.5361185	1240.580233	675.1109028	1017.029323
2628.647648	2658.097549	2442.53497	3579.260997	3579.521624	2676.21395	2553.474558	2309.680135	2480.029492
1002.254951	984.0243926	866.7809274	2162.843879	1434.559211	1075.567814	1208.299585	827.2268963	1224.596683
256.7315652	387.8693354	424.8018556	678.0346831	681.5768843	235.5898051	314.0144434	269.3373231	405.7136364
2822.001367	2552.167653	2690.463225	4124.761337	3850.384026	2851.033279	3231.985414	3252.555989	3454.515303
20339.34859	21554.19018	20430.81066	34939.92771	35068.19097	25890.7781	26370.99648	27569.32223	26536.84101
6358.841729	5651.928764	5554.596234	8736.026094	8327.414624	6109.359876	7298.681441	6867.89873	6893.554144
1560.954102	2262.854686	1766.315789	3298.213768	3602.63473	2426.505464	2383.134339	2152.764092	2210.215243
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4276.799894	3696.449986	3715.817493	5833.724558	5352.415085	3800.367917	4648.781632	4577.493073	4411.382131
2341.486523	2243.30066	3133.606743	4000.556876	3741.550355	2891.375542	3590.324212	3185.064747	2874.655339
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725.2682076	883.4202223	908.1011623	1545.95723	1466.329491	1228.067619	1076.247037	874.5958018	1271.982641
1313.484355	1082.518412	1313.520447	1893.169835	1322.840388	759.5900003	1221.487067	1485957	968.1827917
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3042.696963	3720.788711	3730.227651	5639.945997	5566.706639	4232.213495	5162.020486	4754.295774	4553.343053
2136.435419	1413.723874	1834.105919	3665.421649	1985.246915	1308.345786	2253.035201	1151.810852	2285.594389
1802.407458	2104.289942	1907.769247	3328.531165	3030.222079	1910.743076	1964.400538	2280.413441	2889.239089
567.0404946	557.2222103	596.208049	1000.369756	1092.197139	642.6062456	993.1236011	608.451458	974.5402325
313.7273447	309.3530643	334.3554438	498.9701952	502.1638794	232.5352336	319.6037315	453.3090395	340.5251491
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318.0325377	291.1945063	328.143632	0.001403199	0.001403199	0.001403199	273.9944995	270.2346741	246.7227618
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3823.360575	4781.676422	3852.322021	975.6152858	826.8225972	923.987798	2753.497561	2852.309772	2926.766696
2977.785623	3008.495767	3098.752373	598.912768	779.4193912	734.838609	2087.180044	2190.461879	1738.853796
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3.80_243.0851m/z	243.0851126	3.801716667	neg																
3.80_252.0046m/z	252.0046438	3.801716667	neg																
3.80_254.0018m/z	254.0017937	3.801716667	neg																
3.80_270.0079m/z	270.0079465	3.801716667	neg																
3.80_277.0310m/z	277.0309776	3.801716667	neg																
3.80_279.0236m/z	279.0236084	3.801716667	neg																
3.80_291.9899m/z	291.9899234	3.801716667	neg																
3.80_300.1455m/z	300.1454814	3.801716667	neg																
3.80_319.9920m/z	319.9919752	3.801716667	neg																
3.80_324.9916m/z	324.9915787	3.801716667	neg																
3.80_335.0840m/z	335.0839952	3.801716667	neg																
3.80_344.9429m/z	344.9429387	3.801716667	neg																
3.80_347.0108m/z	347.0108404	3.801716667	neg																
3.80_347.0361m/z	347.036112	3.801716667	neg																
3.80_377.0724n	376.0651006	3.801716667	neg																
3.80_387.9795m/z	387.9795415	3.801716667	neg																
3.80_398.0085m/z	398.0085168	3.801716667	neg																
3.80_401.8526m/z	401.8526164	3.801716667	neg																
3.80_415.0494n	414.0421608	3.801716667	neg																
3.80_423.9985m/z	423.9984947	3.801716667	neg																
3.80_429.1383m/z	429.1382841	3.801716667	neg																
3.80_448.0591n	447.0518709	3.801716667	neg																
3.80_455.9668m/z	455.9667686	3.801716667	neg																
3.80_482.0295m/z	482.0295012	3.801716667	neg																
3.80_515.0391m/z	515.0390594	3.801716667	neg																
3.80_533.9832m/z	533.983176	3.801716667	neg																
3.80_550.0171m/z	550.0171314	3.801716667	neg																
3.80_618.0045m/z	618.0044728	3.801716667	neg																
3.80_685.9919m/z	685.9919377	3.801716667	neg																
3.82_197.9917m/z	197.9917283	3.82415	neg																
3.82_198.4934m/z	198.4934042	3.82415	neg																
3.82_231.9922m/z	231.9922214	3.82415	neg																
3.82_233.9881m/z	233.9880981	3.82415	neg																
3.82_257.1872m/z	257.1871506	3.82415	neg																
3.82_272.0236m/z	272.023582	3.82415	neg																
3.82_282.0477m/z	282.0476722	3.82415	neg																
3.82_327.9910m/z	327.991043	3.82415	neg																
3.82_350.0353m/z	350.0352922	3.82415	neg																
3.82_359.0891m/z	359.0890522	3.82415	neg																
3.82_380.0723n	379.0650392	3.82415	neg																
3.82_382.0315m/z	382.0314888	3.82415	neg																
3.82_417.0871m/z	417.0870874	3.82415	neg																
3.82_418.0229m/z	418.0228532	3.82415	neg																
3.82_591.9100m/z	591.90995	3.82415	neg																
3.85_163.0634n	162.0561447	3.84605	neg																
3.85_180.0609m/z	180.0608985	3.84605	neg																
3.85_199.0401n	198.0328456	3.84605	neg																
3.85_200.0299m/z	200.0299134	3.84605	neg																
3.85_255.9915m/z	255.9915406	3.84605	neg																
3.85_257.9884m/z	257.9884464	3.84605	neg																
3.85_258.0442m/z	258.0442122	3.84605	neg																
3.85_262.0756m/z	262.0756316	3.84605	neg																
3.85_264.0352m/z	264.0351693	3.84605	neg																
3.85_266.0203m/z	266.0202857	3.84605	neg																
3.85_268.0173m/z	268.0173329	3.84605	neg																
3.85_276.9559m/z	276.9558658	3.84605	neg																
3.85_278.9539m/z	278.9538861	3.84605	neg																
3.85_296.0309m/z	296.030851	3.84605	neg																
3.85_299.9690n	280.9512072	3.84605	neg																
3.85_305.0702m/z	305.0702429	3.84605	neg																
3.85_315.0325m/z	315.0325257	3.84605	neg																
3.85_323.9790m/z	323.9790193	3.84605	neg																
3.85_325.9759m/z	325.9759294	3.84605	neg																
3.85_329.0370m/z	329.0370315	3.84605	neg																
3.85_334.0078m/z	334.0078332	3.84605	neg																
3.85_335.9316m/z	335.9316307	3.84605	neg																
3.85_336.0049m/z	336.0048718	3.84605	neg																
3.85_343.9631m/z	343.9631485	3.84605	neg																
3.85_346.9675n	391.9664149	3.84605	neg																
3.85_350.9887n	700.9601727	3.84605	neg																
3.85_350.9980m/z	350.9979606	3.84605	neg																
3.85_368.9185m/z	368.9185437	3.84605	neg																
3.85_376.1980m/z	376.1980309	3.84605	neg																
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3.85_393.9632m/z	393.9632423	3.84605	neg																
3.85_401.9951m/z	401.9950799	3.84605	neg																
3.85_402.0756m/z	402.075578	3.84605	neg																
3.85_407.0963m/z	407.0962833	3.84605	neg																
3.85_407.9515m/z	407.9514514	3.84605	neg																
3.85_411.9508m/z	411.9507543	3.84605	neg																
3.85_414.9553n	459.953979	3.84605	neg																
3.85_418.9853m/z	418.98533	3.84605	neg																
3.85_419.0549m/z	419.0548547	3.84605	neg																
3.85_455.9353m/z	455.9352973	3.84605	neg																
3.85_457.0823m/z	457.0822654	3.84605	neg																
3.85_461.9509m/z	461.9508585	3.84605	neg																
3.85_469.9826m/z	469.982555	3.84605	neg																
3.85_471.9794m/z	471.9794352	3.84605	neg																
3.85_476.9149m/z	476.9148939	3.84605	neg																
3.85_476.9432m/z	476.9432252	3.84605	neg																
3.85_479.9382m/z	479.938169	3.84605	neg																
3.85_482.9429n	527.9413328	3.84605	neg																
3.85_486.9731m/z	486.9730828	3.84605	neg																
3.85_487.0425m/z	487.0424691	3.84605	neg																
3.85_488.9695m/z	488.9694609	3.84605	neg																
3.85_489.0395m/z	489.0394695	3.84605	neg																
3.85_494.9571n	539.9666146	3.84605	neg																
3.85_496.9981m/z	496.9980968	3.84605	neg																
3.85_500.0024n	498.99515	3.84605	neg																
3.85_529.9380m/z	529.9380387	3.84605	neg																
3.85_537.9701m/z	537.9701189	3.84605	neg																
3.85_539.8940m/z	539.8939794	3.84605	neg																
3.85_541.9947m/z	541.9947444	3.84605	neg																
3.85_544.9316m/z	544.931617	3.84605	neg																
3.85_546.9980m/z	546.9979653	3.84605	neg																
3.85_547.9258m/z	547.925783	3.84605	neg																
3.85_550.9306n	595.9291599	3.84605	neg																
3.85_554.9603m/z	554.9603246	3.84605	neg																
3.85_555.0298m/z	555.0297726	3.84605	neg																
3.85_567.9895n	612.9882683	3.84605	neg																

1637.328971	1939.031214	1830.559397	3160.889777	3031.541136	2879.738987	1664.718576	1704.710816	1883.673982											
1762.750602	1668.871291	1564.402679	135.4893498	161.7641533	74.15068036	949.4582335	931.6327885	943.3808884											
539.9020452	436.1238354	465.1677387	0.001403199	0.001403199	0.001403199	135.8061622	229.1104202	243.5805586											
3192.5974	3073.217732	3182.630217	3835.498381	3867.514168	3616.658522	3281.210991	3530.130266	3717.257592											
862.0506755	644.5365853	870.0538284	1349.026191	1154.366256	911.7199166	755.6592914	601.2559704	650.6110937											
1368.102887	933.7016848	1136.963909	140.2673721	86.84734964	76.83418863	603.9517891	616.6414871	562.8269119											
2121.307469	1937.453612	1878.766878	2075.159081	2178.055697	2157.505606	2328.119114	1988.218323	2299.245491											
932.4096006	867.5738015	926.8903669	518.5644873	526.7284854	876.0329579	803.5685075	889.687938	884.1884322											
1478.427831	1351.37783	1341.590138	50.72446491	118.2906743	33.92212928	683.9675871	673.0392151	675.6242146											
570.4856754	644.3106356	658.817558	616.69112	343.9498383	409.6473961	413.7590522	537.8327087	553.6606972											
591.402318	552.5648204	587.9190634	809.978879	827.4626566	967.3569242	549.860997	756.1863129	509.4862563											
1230.428084	1283.359103	852.2437389	1484.476385	1385.148424	1187.627686	1487.197907	907.1999969	1292.522437											
958.5001305	884.6173638	799.8981901	0.001403199	0.001403199	0.001403199	392.4015707	431.0851644	322.0530269											
1085.443738	1148.588842	1116.430693	1190.265082	1128.455747	899.78765	562.7419701	474.4198456	918.5801362											
1791.945065	1848.283236	1869.518754	809.4997633	572.2400542	602.0048507	1749.643348	1523.439581	1867.963857											
1224.477048	944.1552544	976.0671469	55.32065084	0.001403199	225.5180774	577.5841243	586.3717897	531.8926204											
7025.231151	5903.20043	6793.102762	455.1352671	458.2916016	1580.479401	4105.898273	3569.769211	4454.468531											
1094.87046	1010.85657	698.9380844	934.7286479	672.7096114	577.0594653	1102.42195	580.6156405	686.5839471											
15503.94293	15726.06326	15282.59299	1154.211707	1122.278457	1155.739296	13142.56827	13864.61853	13784.81381											
1302.722667	1248.098083	1004.846541	0.001403199	0.001403199	0.001403199	765.5736111	625.1180852	578.893075											
1216.538186	1101.218351	1169.342722	414.1352759	304.6989807	542.7392253	1437.550426	1160.29625	1230.931353											
2895.683973	2799.795748	3364.888929	2216.969144	2060.917574	2364.202228	1638.425077	1755.0835	1915.456546											
605.9603956	777.2907	765.5758812	0.001403199	0.001403199	0.001403199	280.597911	476.5493936	437.6103869											
8667.716018	8556.940633	9017.065112	426.5900026	638.7949682	586.2993963	8316.090477	8564.104362	7878.104419											
1541.820636	2029.100107	1660.126894	1436.081358	1564.683146	1476.867205	1109.542258	1140.000226	1079.928363											
2939.86351	2712.731629	2747.671986	191.1587179	84.06610314	346.3240344	1251.700706	1275.417236	1587.088008											
5181.416143	5512.025624	5172.627322	253.2737685	275.0613641	217.3706193	4935.171919	6014.256264	5812.778491											
2301.276816	1909.323825	1654.466815	0.001403199	123.9845599	0.001403199	2030.985173	2067.91616	1830.182553											
2659.993229	2866.255334	2239.355577	38.82535814	58.65270362	123.0083244	2203.652655	2518.600784	2872.38509											
1287.967709	1491.600631	1480.649537	583.2853188	555.8612391	504.4880312	1608.610142	1717.130801	1705.187134											
119.8395331	87.89621919	124.3347018	39.28810107	0.001403199	0.001403199	48.61633301	66.41220067	166.9220929											
3571.72999	3502.568589	3421.1441	6351.155932	5890.560911	5745.625176	4923.209465	5229.520512	5014.221885											
221.9368595	177.7503415	381.86974	172.0937366	139.0851916	136.3116505	211.7736997	292.2284336	200.4952561											
319.6804818	267.2264484	208.0922127	145.6289248	139.725867	303.2446754	353.5062636	201.6181259	330.3250974											
1406.403999	1329.414359	1409.367098	930.9706637	642.0888968	936.4947155	1147.289426	1248.499281	1247.272682											
9780.416473	10435.84272	11629.02383	1310.227879	1307.53138	12663.3545	15805.02205	16626.95318	16874.42402											
435.808444	434.3096135	503.0024597	580.8322135	536.1839224	286.2326616	507.1600995	532.2144599	565.2173541											
2793.402596	3089.410831	3487.278944	3991.301824	4068.460388	3274.281362	4699.980903	4956.826342	5296.662949											
852.7676856	966.3893012	955.0813568	1204.78435	949.3960091	723.0209339	732.93567	324.6972582	696.0786217											
6518.93682	7465.738578	7138.883856	4340.139332	4178.919032	4049.029699	3910.411063	3978.224506	3819.939565											
618.5912655	616.5256699	698.2009821	0.001403199	0.001403199	0.001403199	580.0498798	686.9934319	713.1462875											
1277.243706	1134.891921	993.6383666	1853.951726	1473.166955	1707.381723	1242.333207	1647.36736	1568.60686											
1382.13936	1257.907213	1495.580978	1767.132407	1891.839128	1629.894084	2083.650957	2253.780469	2223.682111											
262.9890768	623.8813216	282.5959609	657.215354	345.8923543	181.7738163	20.6866974	618.1160678	336.7083134											
900.7754574	943.1624757	960.1023949	930.5363143	1109.769428	1023.80914	1136.960111	1213.860128	1287.155413											
2587.961639	2831.11244	3131.479479	3273.833075	3397.6826	3232.038588	3261.604027	3553.873695	3329.057826											
69764.54199	71046.5704	77736.89579	78542.6893	93325.38025	86256.45442	96944.68762	91807.61916	96042.04095											
23082.91664	23342.45762	26054.34966	25566.34118	31281.04935	28092.10005	32315.21351	30187.09862	32434.11409											
4739.725667	4938.34841	4709.39019	4876.123414	5785.813564	5401.934731	6088.649006	5503.863374	6072.507001											
3799.970799	4381.477799	3855.006329	3664.129275	4263.931138	3900.236516	4925.451637	4700.910648	4984.278209											
599.4645773	598.1458809	701.4916337	6909.414657	6593.524211	6288.548657	656.8297847	627.7960381	862.6984254											
348.8130613	420.7547548	465.9410009	393.1091272	382.3146894	450.4200232	513.8189791	593.1660365	481.7661337											
10167.64293	10466.21181	11005.99908	11937.9093	12218.26176	12048.42827	11799.65718	13003.89499	13258.51832											
87983.23103	90789.87402	97995.00183	97826.28059	116526.1662	105400.6752	125146.4146	113451.3018	118725.737											
30201.53909	31120.25225	33489.51395	32472.9869	38965.62586	34227.43222	41317.90998	38261.6823	41246.5197											
16548.58569	15378.53506	14452.90043	14429.43094	15062.56955	14015.92382	15485.61584	13666.28421	14235.25738											
10267.91693	9445.616582	9232.048779	8257.555074	8440.003485	8221.481548	9425.632323	8330.836341	8691.626814											
209.7134824	310.5948035	163.3577779	331.5144062	315.3618965	334.206521	405.0393151	365.6311328	353.1162335											
3343.034309	3533.555383	3559.114035	1779.967793	1957.316006	2482.429967	2968.848878	2639.466985	2857.046959											
2287.953732	2529.461319	2850.516397	0.001403199	0.001403199	0.001403199	929.9728464	937.4284438	795.4435294											
7156.388886	7932.913221	7945.452351	8517.418409	8705.617847	8581.014991	8150.286218	9328.339475	9444.804155											
3241.10532	3609.140729	3787.833717	3513.650754	4046.579119	4030.352629	4688.228525	4521.655358	4126.467043											
2843.090359	2710.29407	2453.069549	2802.491665	3113.209929	2817.236203	3581.079528	3308.489846	3054.333528											
2299.064055	2246.990883	2261.773327	2483.319398	2552.656551	2344.667635	2433.389502	2726.226013	2827.189115											
45386.64973	45097.18195	49722.74469	49626.87587	58233.87905	54352.37948	62131.26885	59343.85585	58571.67389											
1286.664622	1157.745252	1080.861617	617.6101642	967.9198796	908.7001167	1350.405604	1036.816448	1278.353846											
14318.90952	14823.30266	16102.80993	15954.80995	18161.46496	17908.17078	19535.31903	17757.61296	18829.23101											
8706.550513	8008.732793	8201.45545	7579.734876	8257.151535	7108.761852	9564.908555	9214.469977	8821.035866											
11736.61095	10712.0223	11406.81836	10719.93553	11399.19278	10944.014	13101.04525	12132.87635	12763.19839											
1470.945998	1316.949958	1927.328076	1210.342899	1196.650865	1382.081978	2108.927624	2042.122482	1547.824137											
2923.338076	2710.760253	3109.350318	2259.742453	2593.731287	2750.121938	3317.909784	2692.958776	2857.400872											
515.6019817	671.2604279	441.6788077	241.6852756	806.5517161	536.0620386	698.0712958	415.3820399	609.3932746											
2746.100142	2871.497637	2615.635468	3428.781654	3248.33547	3571.410239	2948.117545	3394.510107	3384.557674											
654.4282659	628.0091382	584.5959003	1393.519956	1488.761497	1509.334489	1051.537242	1127.566359	798.8234538											
4107.370159	4437.901592	4549.78907	3810.614999	5440.295072	4493.117814	6000.844191	4814.606144	4767.395015											
36584.16861	37108.89485	38862.39095	39459.33375	46788.33208	43837.38845	48212.74005	45400.39852	46547.97774											
1094.376526	1184.034673	1464.075057	1122.017443	1585.107476	1432.07737	1318.367069	1682.480064	1890.256125											
253.3577851	114.6434821	210.7734207	0.001403199	130.8641573	158.6110224	655.4267548	917.528801	1051.567242											
648.310439	748.892846	577.2023832	1090.000501	1075.066353	830.5634108	1191.00087	1661.852389	950.180709											
6491.564549	5945.29656	5511.943526	5144.651793	5164.12579	4960.137835	6187.682754	5928.857051	5514.981585											
10432.80441	9095.861904	9606.351993	9484.05342	9448.247927	9784.600288	12202.57495	9376.83873	10417.51405											
4561.373346	4638.229035	4536.535657	4139.759411	4441.47359	4641.809684	5184.584492	4988.118024	5281.698785											
4333.192667	4757.325518	4413.862748	5702.253936	6829.935342	6279.454341	6479.122262	6563.521994	6237.781008											
861.8361347	884.0455008	1138.82397	1172.462526	1130.809886	1373.767494	1732.781426	1487.486084	1128.536682											
131.8046117	107.4038471	320.4727812	800.3820904	726.4925137	730.554238	357.2526294	217.3803403	366.3785289											
3721.915581	3809.589871	3873.441616	3930.323075	4661.102511	4206.85598	5289.138196	4258.432084	4799.670159											
28860.9431	29544.5224	29497.09406	29061.90635	34654.45503	33587.02909	35948.3325	31500.93076	34835.60634											
9550.281496	9050.564925	9693.779186	9895.14866	10416.63752	11137.83822	11371.33795	9871.624992	10409.23384											
1115.252405	933.4646065	935.1004406	308.2594477	558.90256	1012.659836	1335.325468	994.5177667	1118.544208											
431.6940543	798.0347522	671.9117904	436.0681725	1102.709466	724.0201352	878.3243123	783.5853381	654.0949086											
6739.721349	6261.381464	6429.978888	5636.678645	5659.540382	5899.272138	6964.812143	6458.483009	6392.401274											
9195.048317	8863.798641	7974.628862	8090.629552	8853.113837	9029.856326	11121.01721	7836.252333	8821.823198											
3606.358423	3776.416859	3597.858571	3597.030423	3986.024678	3903.073775	4655.766182	4249.37382	3859.511917											
6243.019536	7563.20391	7710.445363	7714.983142	9789.633812	8637.068497	9721.243638	9288.134173	8979.101926											
1005.346121	936.7601178	1169.523858	279.4549652	412.1501898	1140.770516	1203.92845	1072.791748	795.4522531											
4409.033087	5578.93896	5361.197982	5463.053928	7253.682715	6116.855233	6255.417231	7010.4801	7423.553119											
6495.733967	6982.880065	7184.151918	6812.317002	7215.797108	7819.268993	7707.947971	6981.49346	7463.669573											
1316.569098	1755.7611	1501.731403	1294.654796	1644.109881	1770.719147	2110.045417	1347.153809	2087.394184											
2156.514301	2729.352515	2723.263052	1807.104561	2837.769752	3074.685379	3127.849403	2423.644752	2869.019568											
3297.040005	3523.774118	3162.952342	2323.269896	2892.553811	2798.285328	4104.562827	3624.365853	3643.592726											
20545.07051	21795.6991	20844.58494	20758.46637	24820.80209	23416.29693	25694.65569	22515.75835	24640.56557											
820.3594032	740.4571024	641.6112001	779.4569805	494.8552664	607.8850601	802.2839724	570.7219437	690.662135											
893.7069994	728.2571516	741.2796924	951.591805	1186.468912	1326.750523	1126.859023	1174.023156	868.7126188											
1013.930052	539.9899296	916.6361749	955.8598401	782.9513498	582.2784389	681.3462436	881.2134323	95.43490296											
727.4477078	895.4052153	370.2497906	0.001403199	199.1146998	789.0515337	922.1643562	764.5334081	807.5180619											
7729.225087	6405.283468	6397.727787	5936.647934	5639.273748	5561.080777	7138.384444	6232.950914	6102.034409											
8075.634163	7040.846974	6680.741361	6840.673707	7276.556521	6944.494406	8512.922422	7004.256917	8463.647524											
3125.771997	2893.547302	2321.376488	3021.656719	3694.947962	3210.160549	2853.731159	2768.041051	3151.853848											
6641.756836	8806.781219	7677.34427	7096.109313	10196.10042	8759.079157	10940.85903	10252.42447	9909.768852											
2126.156917	3217.380638	2368.319434	1318.330115	1324.897566	2561.362491	3122.301122	2827.02005	3336.224647											

3.85_597.0534m/z	597.0534483	3.84605	neg
3.85_597.9256m/z	597.9256466	3.84605	neg
3.85_605.9580m/z	605.9580106	3.84605	neg
3.85_607.9542m/z	607.9542174	3.84605	neg
3.85_614.9857m/z	614.9856544	3.84605	neg
3.85_615.9132m/z	615.9132379	3.84605	neg
3.85_623.0175m/z	623.0174675	3.84605	neg
3.85_625.0145m/z	625.0144742	3.84605	neg
3.85_632.9735m/z	632.9735002	3.84605	neg
3.85_635.9780n	680.9762596	3.84605	neg
3.85_663.9169m/z	663.9169239	3.84605	neg
3.85_673.9454m/z	673.9453511	3.84605	neg
3.85_675.9418m/z	675.9417808	3.84605	neg
3.85_682.9732m/z	682.9732387	3.84605	neg
3.85_683.9010m/z	683.9009519	3.84605	neg
3.85_691.0053m/z	691.0053017	3.84605	neg
3.85_693.0022m/z	693.0021542	3.84605	neg
3.85_697.0275m/z	697.0274894	3.84605	neg
3.85_703.9651n	702.9578121	3.84605	neg
3.85_731.9036m/z	731.9036037	3.84605	neg
3.85_741.9331n/z	741.9331416	3.84605	neg
3.85_750.9607m/z	750.9606817	3.84605	neg
3.85_751.8881m/z	751.8880731	3.84605	neg
3.85_758.9927m/z	758.9926668	3.84605	neg
3.85_760.9894m/z	760.9893672	3.84605	neg
3.85_768.9483m/z	768.9483227	3.84605	neg
3.85_776.0521m/z	776.0520898	3.84605	neg
3.85_809.9205m/z	809.9204688	3.84605	neg
3.85_826.9799m/z	826.9798552	3.84605	neg
3.85_828.9771m/z	828.9771071	3.84605	neg
3.85_844.0403m/z	844.0403115	3.84605	neg
3.85_846.0370m/z	846.0370125	3.84605	neg
3.85_877.9082m/z	877.9082167	3.84605	neg
3.85_894.9667m/z	894.9667184	3.84605	neg
3.85_962.9531m/z	962.95312	3.84605	neg
3.87_204.0400n	249.0381325	3.868533333	neg
3.87_227.1403m/z	227.1402545	3.868533333	neg
3.87_228.0338m/z	228.0338189	3.868533333	neg
3.87_239.0094m/z	239.0093994	3.868533333	neg
3.87_242.0768n	241.0695338	3.868533333	neg
3.87_245.0127m/z	245.012688	3.868533333	neg
3.87_306.1075m/z	306.1074731	3.868533333	neg
3.87_315.0725m/z	315.0725328	3.868533333	neg
3.87_317.9821m/z	317.982103	3.868533333	neg
3.87_339.0075m/z	339.0075266	3.868533333	neg
3.87_374.0945m/z	374.094523	3.868533333	neg
3.87_385.0131m/z	385.0131329	3.868533333	neg
3.87_394.0564m/z	394.0564169	3.868533333	neg
3.87_397.0244m/z	397.0243894	3.868533333	neg
3.87_453.0007m/z	453.0006914	3.868533333	neg
3.87_475.9898n	520.9880651	3.868533333	neg
3.87_538.0477m/z	538.0476767	3.868533333	neg
3.89_166.0241n	211.0225396	3.8906	neg
3.89_167.0325m/z	167.0325145	3.8906	neg
3.89_233.0045m/z	233.0045012	3.8906	neg
3.89_242.0285m/z	242.0285197	3.8906	neg
3.89_247.0201m/z	247.0201442	3.8906	neg
3.89_247.0281m/z	247.0281349	3.8906	neg
3.89_256.9756m/z	256.9756165	3.8906	neg
3.89_266.0282m/z	266.0281911	3.8906	neg
3.89_300.0526m/z	300.052604	3.8906	neg
3.89_300.9921m/z	300.9920735	3.8906	neg
3.89_310.0371m/z	310.0370695	3.8906	neg
3.89_315.0078m/z	315.0077913	3.8906	neg
3.89_320.9654m/z	320.9654475	3.8906	neg
3.89_323.0747m/z	323.0747465	3.8906	neg
3.89_324.9629m/z	324.9629211	3.8906	neg
3.89_328.0751n	309.0572279	3.8906	neg
3.89_345.0572m/z	345.0571956	3.8906	neg
3.89_350.9770m/z	350.9769578	3.8906	neg
3.89_358.9503m/z	358.9503051	3.8906	neg
3.89_367.0379m/z	367.0379327	3.8906	neg
3.89_368.9793m/z	368.9793426	3.8906	neg
3.89_372.9663m/z	372.9663455	3.8906	neg
3.89_374.9842m/z	374.9842212	3.8906	neg
3.89_399.9849m/z	399.9849486	3.8906	neg
3.89_408.0597m/z	408.0597262	3.8906	neg
3.89_426.9374m/z	426.9374243	3.8906	neg
3.89_435.0267m/z	435.0266772	3.8906	neg
3.89_437.9819n	436.9667057	3.8906	neg
3.89_504.9545m/z	504.9544576	3.8906	neg
3.89_508.9412m/z	508.9412235	3.8906	neg
3.89_519.0734m/z	519.0734253	3.8906	neg
3.89_572.9422m/z	572.9421594	3.8906	neg
3.89_640.9304m/z	640.9304083	3.8906	neg
3.89_722.9331m/z	722.9330882	3.8906	neg
3.91_180.0400n	179.0326825	3.912566667	neg
3.91_217.0066m/z	217.0065996	3.912566667	neg
3.91_236.9914m/z	236.9913873	3.912566667	neg
3.91_248.0662n	293.0645138	3.912566667	neg
3.91_283.0801m/z	283.0801234	3.912566667	neg
3.91_316.0538n	361.0519767	3.912566667	neg
3.91_316.1518m/z	316.1517884	3.912566667	neg
3.91_331.9981m/z	331.9980797	3.912566667	neg
3.91_340.0724m/z	340.0724148	3.912566667	neg
3.91_350.0836m/z	350.0836232	3.912566667	neg
3.91_382.9952m/z	382.9951512	3.912566667	neg
3.91_392.0108m/z	392.0107955	3.912566667	neg
3.91_392.9505m/z	392.9504722	3.912566667	neg
3.91_399.0392m/z	399.0392453	3.912566667	neg
3.91_440.9540m/z	440.9539647	3.912566667	neg
3.91_443.9633m/z	443.9632826	3.912566667	neg
3.91_459.9984m/z	459.9983792	3.912566667	neg
3.91_518.9701m/z	518.9700571	3.912566667	neg
3.91_543.9917m/z	543.9917126	3.912566667	neg
3.91_586.9577m/z	586.9577135	3.912566667	neg
3.91_604.9443m/z	604.9442979	3.912566667	neg
3.91_654.9454m/z	654.9453727	3.912566667	neg
3.94_199.0588m/z	199.0587641	3.9351	neg
3.94_205.0409n	409.0731609	3.9351	neg

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15389.63787	14759.56606	15517.56748	14853.03622	16790.69603	17140.44653	18239.7065	15857.17198	17314.62782
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3947.123974	4189.048099	3807.151117	4342.993804	5742.660232	5474.024495	5430.20114	4899.711139	5225.924108
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402.3075864	420.2946245	501.6137306	238.9553274	318.5162764	441.6642827	588.2342251	649.6024857	570.8280136
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2447.973827	2571.344738	2644.57075	2780.381255	2993.412789	3142.556353	2365.320744	2370.708792	2658.678751
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1918.677506	1747.988035	1964.112444	2235.827172	2074.181963	2194.908583	1843.152609	1915.298772	2106.924609
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3125.224979	3780.300313	3544.055619	4238.126397	3889.51118	4073.780166	4399.241	3698.478166	4341.590083
1963.181371	1520.627357	1586.870731	0.001403199	0.001403199	0.001403199	1365.875795	1160.123611	1131.31553
3314.863468	2739.519926	2695.714932	4047.647693	3516.33631	3235.587557	3170.424488	3036.244104	3430.293288
423.3058761	404.2133468	406.8705802	518.6743567	495.8175205	485.8056946	462.9744943	401.5024938	366.7905829
1276.546897	1412.376144	1191.405982	2073.545475	2384.909573	2388.974936	1670.385283	1550.813545	1590.026411

3.94_215.9972m/z	215.9972469	3.9351	neg
3.94_234.0807m/z	234.0807063	3.9351	neg
3.94_241.0444m/z	241.0444052	3.9351	neg
3.94_251.0176m/z	251.0175749	3.9351	neg
3.94_324.0233m/z	324.0232867	3.9351	neg
3.94_359.0154m/z	359.0154319	3.9351	neg
3.94_361.0129m/z	361.0129137	3.9351	neg
3.94_371.0442m/z	371.0442496	3.9351	neg
3.94_386.0342m/z	386.0341716	3.9351	neg
3.94_386.9926m/z	386.9925861	3.9351	neg
3.94_408.0164m/z	408.0163557	3.9351	neg
3.94_438.0435m/z	438.0434868	3.9351	neg
3.94_448.9848m/z	448.9847635	3.9351	neg
3.94_454.9801m/z	454.9801183	3.9351	neg
3.94_460.0210n	459.0137156	3.9351	neg
3.94_476.0033m/z	476.0032798	3.9351	neg
3.94_477.0607m/z	477.0606791	3.9351	neg
3.94_516.9721m/z	516.9721279	3.9351	neg
3.94_527.0010m/z	527.0009907	3.9351	neg
3.94_594.9889m/z	594.9888686	3.9351	neg
3.94_662.9765m/z	662.9764885	3.9351	neg
3.94_730.9642m/z	730.9641674	3.9351	neg
3.96_141.0558m/z	141.0558228	3.957583333	neg
3.96_209.0433m/z	209.0433237	3.957583333	neg
3.96_216.0224m/z	216.0223733	3.957583333	neg
3.96_267.0019m/z	267.0019124	3.957583333	neg
3.96_267.0851m/z	267.0850967	3.957583333	neg
3.96_292.0432m/z	292.0432392	3.957583333	neg
3.96_294.0211m/z	294.0211248	3.957583333	neg
3.96_301.0807m/z	301.0807296	3.957583333	neg
3.96_334.9897m/z	334.9896666	3.957583333	neg
3.96_341.0857m/z	341.08567	3.957583333	neg
3.96_345.0184m/z	345.0183606	3.957583333	neg
3.96_360.0298m/z	360.0298379	3.957583333	neg
3.96_392.8758m/z	392.8757921	3.957583333	neg
3.96_411.1273m/z	411.1273417	3.957583333	neg
3.96_413.0059m/z	413.0059226	3.957583333	neg
3.96_428.0170m/z	428.0169549	3.957583333	neg
3.96_459.9857m/z	459.9857231	3.957583333	neg
3.96_470.9644m/z	470.9644279	3.957583333	neg
3.96_479.8686m/z	479.868596	3.957583333	neg
3.96_496.0047m/z	496.0047267	3.957583333	neg
3.96_502.1041n	547.1024316	3.957583333	neg
3.96_548.9810m/z	548.9809993	3.957583333	neg
3.96_557.2608m/z	557.2608223	3.957583333	neg
3.96_570.0917n	615.0897969	3.957583333	neg
3.96_588.9755m/z	588.9754905	3.957583333	neg
3.96_615.8435m/z	615.8435231	3.957583333	neg
3.96_616.9685m/z	616.9684859	3.957583333	neg
3.96_631.9796m/z	631.9795772	3.957583333	neg
3.96_638.0792n	683.0773019	3.957583333	neg
3.96_684.9565m/z	684.9564588	3.957583333	neg
3.96_705.0595m/z	705.0595235	3.957583333	neg
3.98_127.0401m/z	127.0401174	3.97985	neg
3.98_178.0544m/z	178.0544491	3.97985	neg
3.98_245.9941m/z	245.9940731	3.97985	neg
3.98_246.0807m/z	246.0807172	3.97985	neg
3.98_273.0132m/z	273.0131568	3.97985	neg
3.98_294.0459m/z	294.0458892	3.97985	neg
3.98_306.9667m/z	306.9666871	3.97985	neg
3.98_314.0684m/z	314.068365	3.97985	neg
3.98_324.0104m/z	324.0103849	3.97985	neg
3.98_345.0429m/z	345.0429439	3.97985	neg
3.98_371.0881m/z	371.0881031	3.97985	neg
3.98_386.9091m/z	386.9091188	3.97985	neg
3.98_391.9981m/z	391.9980711	3.97985	neg
3.98_393.9439m/z	393.94387	3.97985	neg
3.98_399.0794m/z	399.0793514	3.97985	neg
3.98_413.0307m/z	413.0307233	3.97985	neg
3.98_437.0702m/z	437.0701757	3.97985	neg
3.98_437.1067m/z	437.1067245	3.97985	neg
3.98_441.1255m/z	441.125534	3.97985	neg
3.98_454.8966m/z	454.8965849	3.97985	neg
3.98_459.0523m/z	459.0523357	3.97985	neg
3.98_481.0654m/z	481.0653657	3.97985	neg
3.98_527.0398m/z	527.0397612	3.97985	neg
3.98_595.0273m/z	595.0273452	3.97985	neg
3.98_631.0897m/z	631.0896727	3.97985	neg
4.00_166.0592m/z	166.0591705	4.002233333	neg
4.00_173.9947m/z	173.9947294	4.002233333	neg
4.00_174.9872m/z	174.987241	4.002233333	neg
4.00_188.1011m/z	188.1010754	4.002233333	neg
4.00_226.0698m/z	226.0698291	4.002233333	neg
4.00_230.9501m/z	230.9501108	4.002233333	neg
4.00_241.9863n	240.9790054	4.002233333	neg
4.00_253.0696m/z	253.0695959	4.002233333	neg
4.00_257.9692m/z	257.9691705	4.002233333	neg
4.00_270.0419m/z	270.0419294	4.002233333	neg
4.00_284.9689m/z	284.9689252	4.002233333	neg
4.00_298.9374m/z	298.9373998	4.002233333	neg
4.00_308.9661m/z	308.9660782	4.002233333	neg
4.00_311.0721m/z	311.0720622	4.002233333	neg
4.00_338.0296m/z	338.0295836	4.002233333	neg
4.00_362.0449m/z	362.04486	4.002233333	neg
4.00_366.9250m/z	366.9250153	4.002233333	neg
4.00_368.9721m/z	368.9720701	4.002233333	neg
4.00_376.9539m/z	376.9539181	4.002233333	neg
4.00_380.0671n	379.059789	4.002233333	neg
4.00_406.0169m/z	406.0168876	4.002233333	neg
4.00_434.9124m/z	434.912361	4.002233333	neg
4.00_444.9414m/z	444.9414352	4.002233333	neg
4.00_474.0044m/z	474.004421	4.002233333	neg
4.00_481.0175m/z	481.017549	4.002233333	neg
4.00_498.0203m/z	498.0202864	4.002233333	neg
4.00_502.8999m/z	502.8999474	4.002233333	neg
4.00_512.9287m/z	512.9286502	4.002233333	neg
4.00_522.8842m/z	522.8841692	4.002233333	neg
4.00_580.9162m/z	580.9162162	4.002233333	neg
4.00_609.9793m/z	609.9792852	4.002233333	neg
4.00_648.9037m/z	648.9037492	4.002233333	neg

442.4600389	389.4006387	434.489219	59.83556354	221.5721594	190.4037633	321.4792068	473.4185785	345.1968673
5575.666371	5999.157259	6318.207976	17610.76194	16447.09777	16175.24273	18797.02737	21358.97055	20555.1282
368.0100043	408.9066521	455.0136277	698.7685305	545.056209	509.2007753	517.6814871	583.1019432	551.030437
4282.772547	4616.926164	4972.828074	4571.523473	4134.598817	4470.60397	3482.014491	4034.256567	3741.81226
3059.224837	3078.298779	3255.911408	4553.901844	3836.884664	4400.358139	3931.583564	3617.61028	3901.630837
1967.255199	2147.941666	2205.407416	64.56610428	14.42361793	0.06883534	1729.468203	1750.482724	1897.585461
530.1026003	409.0553267	866.4511946	0.001403199	0.001403199	130.7824304	435.9534067	636.4734154	623.7886956
260.5257059	598.3534804	521.9938438	1.455932161	0.001403199	0.001403199	519.8901595	767.9151846	821.967606
2198.999356	2471.519592	2259.99597	12.30437356	0.001403199	0.001403199	1816.040627	1715.929993	1627.637325
942.4774407	880.9380906	955.6020297	838.410386	901.0427251	918.5597731	764.9959184	712.2437638	789.7728493
1068.059641	1316.063428	1087.51874	0.001403199	0.001403199	0.001403199	1298.981388	1081.437826	945.6919485
282.0984599	574.5962457	500.381419	2615.451493	2046.494781	2486.424333	2438.086407	2630.235686	2532.299637
2332.610273	2200.16675	2535.968451	0.001403199	0.001403199	0.695978205	1931.071062	2226.935189	1691.953925
854.0657519	1076.25662	1114.808057	1206.075704	1201.602561	881.5341186	850.9345808	670.8354263	622.7331641
20295.06616	20494.63438	21173.02476	1075.374309	1541.845324	1611.08275	18170.0327	19178.66918	17609.45788
1385.484433	1351.227023	1647.009981	0.001403199	0.001403199	0.001403199	824.3648612	922.637609	1151.668299
504.1742316	604.3778827	553.8975817	1539.513452	1311.830317	1353.256475	665.4359067	552.8251114	693.8312698
2149.388154	2123.266104	2647.305022	18.72496109	0.001403199	66.19817807	1972.364668	1901.209068	1624.95005
11530.62883	12360.94713	12814.95489	337.155637	297.7352563	394.7562345	10922.21706	11444.08214	10324.55087
7357.195451	7831.368281	8334.75015	192.9004939	237.8990845	79.05936029	6638.528775	6715.487797	6954.332458
4359.65958	5028.914217	4887.98382	0.001403199	41.32194045	34.31718675	3833.862633	4012.015656	3902.573423
2079.667795	2532.749412	2472.911961	0.001403199	0.001403199	0.001403199	2190.71968	2036.650964	2010.016217
1527.988305	1529.52813	1659.383622	1502.017018	1444.533023	1510.207176	1387.575536	1359.628058	1402.522837
6797.737877	7369.524247	7716.45507	13088.33868	13500.26977	14004.44257	7941.930913	8712.103746	8309.84932
407.4959278	432.5262806	553.1104841	276.7680931	348.6019423	502.5991305	506.0265507	559.8546498	448.6095159
543.5569564	598.277978	603.2915738	1092.501174	1100.805051	1210.574619	620.6333734	808.946064	764.8256045
462.1739616	580.5819498	555.5991407	361.9950421	550.9224023	666.1923377	639.7949882	625.4482193	723.0593635
5419.485149	5627.494127	5893.354165	3554.806251	3581.47531	3582.319394	5060.42538	5521.819384	4665.751235
326.9919855	342.4310717	287.9640957	906.2791867	837.744689	840.0605086	274.8540664	544.7593269	535.7253472
2158.724087	2740.171835	2544.064617	3302.187526	3244.017379	3380.098015	2084.260795	2589.066544	2099.563275
487.1062396	468.2704494	475.3022215	401.6653374	1148.771121	918.49929	445.1785514	684.2419701	670.9958094
4183.9395	4740.23258	5028.113039	6610.485344	6244.200645	7724.313861	4714.768918	5093.70828	5012.045537
3437.363135	4053.597432	3582.580109	6269.610372	6413.117097	7253.052708	4046.101493	4534.601849	4119.374946
3284.732255	3558.866277	3779.540209	3476.522222	3362.646304	3473.505146	3800.22458	4161.20409	3854.550698
3992.226603	3947.346569	3216.666941	3113.491811	3539.238112	3416.928709	4694.411468	2802.679551	3229.343095
28396.06913	28120.99229	29493.57193	31183.98026	28587.06753	29033.55496	27499.73732	29941.81476	29131.30936
2280.924375	2537.935366	2757.623091	4822.280045	4980.91548	5182.362669	2759.645788	2781.409429	3138.415398
2722.636328	2933.007309	3442.260046	2721.309247	3043.430545	3106.376469	3755.097395	3665.341168	3327.060399
1248.346891	1342.325089	1456.874278	2055.012819	1723.511859	1968.217426	1322.99831	1430.046181	1584.049626
320.1443148	165.0145467	388.1798435	867.3400082	960.5296334	838.1531145	334.0819342	263.3831482	257.9356541
4505.509353	4073.374868	3983.642047	3887.324202	3639.587885	3291.255903	4323.708591	3337.088068	3524.354749
2005.144341	1991.927061	1773.45873	1836.664674	2083.236917	2372.558287	2593.441222	2399.14642	2568.423683
5968.60272	5804.855269	6076.826718	6116.833876	6019.123225	6336.433931	6226.299173	6033.099131	5582.572276
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860.4992171	994.7959194	1344.550977	1993.708644	1695.355107	1258.583689	567.6252714	908.6656952	905.2019575
3534.173861	3281.056382	3721.017601	3587.206316	3432.296227	3472.663612	3262.352072	3357.145729	2915.346871
3564.783655	3202.268951	3688.246753	0.001403199	130.0247072	908.6858003	3131.614063	3055.112157	3429.258234
4231.287353	3553.564825	3604.243891	3389.541328	3892.803979	3669.633679	4392.915844	3624.480448	3412.796219
792.8992557	951.7056565	1088.858849	934.6074802	2464.417964	2061.419012	779.5722609	1132.467116	687.0720842
900.8391467	1045.620979	1027.299305	907.1196056	1115.445598	1483.87081	1061.996913	1209.968349	1400.361594
1607.829495	1908.606965	1706.925681	1976.786989	2161.315963	2008.218592	1542.35512	2085.2108	1934.216622
545.9838182	1014.411898	618.4239803	2308.125929	1723.302802	1809.788975	883.9161811	876.4493207	747.3406617
470.0036919	537.9811796	428.4761452	395.7142536	521.1635257	679.2506198	434.3868733	686.9574526	583.8875416
2305.895052	2275.988484	2436.525174	2292.59367	2269.063023	2202.732325	2436.208716	2195.812792	2355.033807
527.791934	530.2746942	581.1833859	81.89312541	0.001403199	38.53148408	25.47019788	42.22540546	18.69829097
436.2661086	542.7717836	553.9961591	758.046636	687.1132466	860.1015827	617.0840686	604.8819809	750.7617785
376.859612	400.5873483	422.5921586	4003.801917	3705.765863	3762.522746	5317.984733	6051.758609	5737.669583
789.9442553	854.8889823	950.9157265	1440.567905	1509.441165	1541.381991	1043.526768	1190.12782	1235.402441
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243.0260072	101.6140728	165.6932232	2072.700752	1741.413942	1331.883382	1583.452059	1926.855133	2093.541334
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3789.258479	4300.459224	4612.924302	3959.950266	4005.906271	4215.343836	3642.494393	4675.02778	4220.637441
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1982.887781	1723.47857	1870.379892	165.9749922	246.074155	273.6796166	1436.272603	1330.530279	1465.527837
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246.7791324	726.3346502	658.1559504	213.8081205	340.418529	331.380018	1267.778087	1271.131508	1390.234673
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1568.273127	1908.642526	1765.702612	260.9266977	249.2119198	202.2722138	1283.601386	1489.292649	1316.970146
1870.62262	2302.613975	2534.570576	1352.063878	1341.743216	967.909926	1892.629141	1693.206949	1733.712107
2435.317285	3366.305324	3297.479447	1536.311175	1795.075334	2078.213747	2078.188318	2407.709571	2381.824465
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15810.06769	17134.95969	17133.05606	4845.114737	4467.74662	4709.020063	14018.06986	15728.20997	15290.06851
9937.91814	11000.74954	11792.00964	2796.863757	2937.915791	2814.868646	9170.921854	10244.19175	9754.646771
85.97574053	68.35191537	28.21584472	46.31612594	56.14157782	69.88801387	32.4470609	69.14967835	0.001403199
6839.876688	7160.830583	7318.104545	9056.621876	8917.399972	8787.623377	8948.91109	10258.48889	9666.941591
4622.391916	4556.376823	5041.453465	1348.602772	1214.724245	1276.944895	3929.645911	4276.191485	4039.778795
26942.03039	28777.35887	30271.71712	7336.221909	7555.298156	8061.204828	25265.60162	26752.23243	26127.97975
1202.813676	1358.868015	1547.086898	1478.123514	1574.359348	1520.116776	1011.269692	1369.65553	1148.09867
11166.90783	11992.2408	12241.62945	3324.48467	3057.585064	3336.985493	10061.23475	11624.71844	10603.4038
13716.44519	14674.86339	15884.84744	9359.833763	9091.532543	9513.574593	9477.045825	10515.92688	11045.27096
911.2299868	912.9887424	1053.65736	175.0199269	198.1554007	256.2154029	895.6656178	1065.377911	867.2734072
863.1042043	723.8157297	1056.792364	0.001403199	154.9072224	131.7186582	905.3658647	864.3644943	862.7749856
17605.13668	19423.21473	19332.82743	6979.920681	7577.909451	7701.039149	16119.59129	17983.99736	17391.56404
1342.57202	1353.452835	1512.612022	3270.911037	2722.692796	2842.882952	1143.598075	1084.218391	1123.651596
8180.673511	8371.655573	9112.622881	5951.909516	5181.259393	5329.891073	5549.35117	5831.120765	5517.900135
2603.270347	2758.448681	2919.789252	3836.187615	3567.251842	3498.800547	3615.544392	3826.94294	4067.229813
2451.901798	2561.70973	2381.485814	404.7378124	573.3371259	495.8915649	2542.818451	2688.613819	2377.787353
3808.985037	4965.202383	5228.808065	464.5730408	519.5730135	305.8264633	3053.773523	4190.081171	3371.177915
15294.83543	16102.38677	16964.6033	4055.06483	4146.720992	4129.400605	13094.32378	15174.82061	14731.65163
1854.296954	2185.69082	1958.61602	2117.375794	2220.138861	2039.517338	1627.5264	2131.75557	1495.670826
4483.87641	5100.913713	5344.597596	3634.735784	2883.76773	3169.144045	3575.620591	3678.776814	3422.453357
2466.556686	2129.111365	2922.254128	254.9766604	280.6919369	600.3698075	2742.829209	2386.155768	2447.757702
13762.30341	14284.23133	14052.60394	3420.23198	3526.313438	3651.670271	12493.98491	12724.23366	12554.75358
3009.586498	3188.355277	3578.958576	2194.682109	2070.882046	2362.618128	1983.784524	2450.35326	2447.325652
1054.048762	1112.815469	1378.710669	244.6200884	1085.953187	1072.890472	1090.878975	1532.553868	1274.371818
722.3644815	986.8257641	896.8406226	1781.123547	1072.252541	1272.777233	961.5420795	983.9136937	866.7235104
1413.956447	1660.325338	1916.35676	0.001403199	501.8906058	490.5760105	1368.631674	1633.952433	1355.464224
9490.549459	9888.819663	10094.82024	2313.68601	2641.976112	2249.995311	9071.122091	9182.572425	9400.144796
1800.210292	1412.298411	1757.00535	0.001403199	262.5777492	0.001403199	1753.916416	1525.553047	1117.793764
6690.449328	7268.481968	7195.303948	1481.72449	1304.902053	1238.559001	6291.542307	5888.090469	6342.272238
1367.480873	1884.84092	1869.815327	509.4182591	1187.867467	1230.507028	1008.54783	1077.34787	979.1471943
5018.689309	5193.95819	4882.150524	932.4743948	656.4715016	874.1725916	3815.864561	3928.146587	3660.556742

4.00_653.0714m/z	653.0713608	4.002233333	neg
4.00_716.8911m/z	716.8911001	4.002233333	neg
4.02_172.9853m/z	172.985333	4.024283333	neg
4.02_262.0334m/z	262.0333928	4.024283333	neg
4.02_281.1244m/z	281.1243627	4.024283333	neg
4.02_296.0633m/z	296.0633091	4.024283333	neg
4.02_300.1284m/z	300.128374	4.024283333	neg
4.02_328.0006m/z	328.0006445	4.024283333	neg
4.02_361.0777n	406.0758275	4.024283333	neg
4.02_395.1562m/z	395.1562286	4.024283333	neg
4.02_396.0471m/z	396.0470889	4.024283333	neg
4.02_430.0322m/z	430.0322463	4.024283333	neg
4.02_541.9920m/z	541.9919971	4.024283333	neg
4.05_160.8420m/z	160.8420127	4.046666667	neg
4.05_180.0497m/z	180.0497126	4.046666667	neg
4.05_184.0616m/z	184.0615788	4.046666667	neg
4.05_192.0068n	383.0087828	4.046666667	neg
4.05_203.0021m/z	203.0020781	4.046666667	neg
4.05_278.9711m/z	278.9711068	4.046666667	neg
4.05_292.1228m/z	292.1227537	4.046666667	neg
4.05_330.0291m/z	330.0290662	4.046666667	neg
4.05_341.1469m/z	341.146889	4.046666667	neg
4.05_346.9587m/z	346.958656	4.046666667	neg
4.05_395.0032m/z	395.0031778	4.046666667	neg
4.05_414.9463m/z	414.9462512	4.046666667	neg
4.05_445.1350m/z	445.1349808	4.046666667	neg
4.05_448.0481m/z	448.0480877	4.046666667	neg
4.05_474.0633m/z	474.0632784	4.046666667	neg
4.05_482.9336m/z	482.9336417	4.046666667	neg
4.05_513.1220m/z	513.1220467	4.046666667	neg
4.05_518.9839m/z	518.9838687	4.046666667	neg
4.05_542.0509m/z	542.0508884	4.046666667	neg
4.05_654.9592m/z	654.9591604	4.046666667	neg
4.07_171.0202m/z	171.0201597	4.069216667	neg
4.07_243.1238m/z	243.1237964	4.069216667	neg
4.07_263.9351m/z	263.9351133	4.069216667	neg
4.07_269.1008m/z	269.1008473	4.069216667	neg
4.07_275.9062m/z	275.9061968	4.069216667	neg
4.07_281.1009m/z	281.1009222	4.069216667	neg
4.07_316.1881m/z	316.188091	4.069216667	neg
4.07_351.1413n	350.1340484	4.069216667	neg
4.07_374.8335m/z	374.8335018	4.069216667	neg
4.07_419.9994m/z	419.999356	4.069216667	neg
4.07_429.1385m/z	429.1385412	4.069216667	neg
4.07_663.8471m/z	663.8471076	4.069216667	neg
4.07_734.8286m/z	734.8286178	4.069216667	neg
4.09_174.0853m/z	174.0853399	4.097183333	neg
4.09_221.0126m/z	221.0126115	4.097183333	neg
4.09_227.9974m/z	227.9974334	4.097183333	neg
4.09_229.9931m/z	229.993123	4.097183333	neg
4.09_260.9878m/z	260.9878066	4.097183333	neg
4.09_294.9533m/z	294.9533499	4.097183333	neg
4.09_313.8808m/z	313.8807662	4.097183333	neg
4.09_315.0725m/z	315.0724969	4.097183333	neg
4.09_333.0527m/z	333.0526966	4.097183333	neg
4.09_395.0598m/z	395.059835	4.097183333	neg
4.09_425.2186m/z	425.2186085	4.097183333	neg
4.09_443.8312m/z	443.8311748	4.097183333	neg
4.09_454.8485m/z	454.8484726	4.097183333	neg
4.09_463.0476m/z	463.0476134	4.097183333	neg
4.09_547.8562m/z	547.856232	4.097183333	neg
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4.09_588.8250m/z	588.8249517	4.097183333	neg
4.09_656.8125m/z	656.8124558	4.097183333	neg
4.09_802.8161m/z	802.8160595	4.097183333	neg
4.11_183.0048m/z	183.0047985	4.113883333	neg
4.11_184.0075m/z	184.0075441	4.113883333	neg
4.11_197.0820m/z	197.0820379	4.113883333	neg
4.11_241.0696m/z	241.0695805	4.113883333	neg
4.11_276.0007m/z	276.0006731	4.113883333	neg
4.11_293.0622m/z	293.0621795	4.113883333	neg
4.11_306.1018m/z	306.1018433	4.113883333	neg
4.11_334.1331m/z	334.1330856	4.113883333	neg
4.11_345.1557m/z	345.1557267	4.113883333	neg
4.11_355.0108m/z	355.0107867	4.113883333	neg
4.11_360.9745m/z	360.9745028	4.113883333	neg
4.11_372.0008m/z	372.0007745	4.113883333	neg
4.11_377.9999n	422.998325	4.113883333	neg
4.11_383.0840m/z	383.0839924	4.113883333	neg
4.11_409.8776m/z	409.8775995	4.113883333	neg
4.11_428.9619m/z	428.9618565	4.113883333	neg
4.11_459.0868m/z	459.0868052	4.113883333	neg
4.11_501.8636m/z	501.8636206	4.113883333	neg
4.11_511.1048m/z	511.1048128	4.113883333	neg
4.11_558.9732m/z	558.9731926	4.113883333	neg
4.11_654.8697m/z	654.8696769	4.113883333	neg
4.14_207.0662m/z	207.0662383	4.136366667	neg
4.14_225.0746m/z	225.0746147	4.136366667	neg
4.14_226.9664m/z	226.9663719	4.136366667	neg
4.14_265.9800m/z	265.9799562	4.136366667	neg
4.14_282.9895m/z	282.9895115	4.136366667	neg
4.14_289.9369m/z	289.9369476	4.136366667	neg
4.14_300.0185m/z	300.0184558	4.136366667	neg
4.14_300.0726m/z	300.0725611	4.136366667	neg
4.14_310.5533m/z	310.5532655	4.136366667	neg
4.14_311.0589n	310.051659	4.136366667	neg
4.14_319.0562n	637.1052332	4.136366667	neg
4.14_344.0452m/z	344.045247	4.136366667	neg
4.14_344.5469m/z	344.5469086	4.136366667	neg
4.14_344.9818m/z	344.9817819	4.136366667	neg
4.14_350.9770m/z	350.9770203	4.136366667	neg
4.14_355.0362m/z	355.0362038	4.136366667	neg
4.14_355.5382m/z	355.5382301	4.136366667	neg
4.14_378.0389m/z	378.038876	4.136366667	neg
4.14_378.5406m/z	378.5405762	4.136366667	neg
4.14_380.8632m/z	380.8632294	4.136366667	neg
4.14_381.8682m/z	381.8681567	4.136366667	neg
4.14_383.8653m/z	383.8653397	4.136366667	neg
4.14_389.0300m/z	389.0300357	4.136366667	neg
4.14_389.5318m/z	389.5318222	4.136366667	neg

952.5347839	1201.824831	1126.813284	662.95923	926.56506	1004.834219	997.348104	1398.442968	1205.60867	
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158.8485572	0.001403199	162.0629074	16.94208108	11.69927894	56.95870464	109.9243987	172.5529757	157.9261145	
762.7625686	658.9129311	736.1515419	679.2038775	695.2723863	784.0424534	901.8362051	822.7930304	789.2685833	
1412.13529	1551.041693	1633.006209	213.2408113	509.5493105	457.005935	1200.267618	1493.383714	1479.449825	
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64.5167439	106.9682225	258.4257702	571.6604773	409.9525153	443.8613397	202.034437	128.5165501	70.93484213	
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4201.388049	4562.861085	4817.79911	5201.250785	4993.982133	5192.327323	4658.770045	5327.314634	4845.392579	
484.1879224	527.4565657	752.3794697	488.9327235	666.9125663	740.4284165	542.4022689	716.9540148	554.3684074	
327.2478577	440.2210121	450.2183013	665.8012383	391.776993	657.1330584	572.3272649	450.1501266	413.6075358	
2035.268907	2383.937358	2173.657166	2859.387798	2763.998408	2942.54507	2920.431635	3274.350466	2828.118891	
1744.340609	2517.615831	2769.136031	819.4921456	1380.598652	1459.269696	1359.383737	1572.817588	1534.495882	
685.8197952	569.3751297	606.6585361	493.7487411	540.7001068	501.8381742	655.0131891	544.02861	530.3513169	
549.201008	516.8221295	543.3275172	923.7522801	837.8372804	864.3918582	661.2227972	650.9759742	726.1662112	
158.6495782	107.8621387	217.0743704	154.3270939	182.0976377	164.6332149	134.7804035	193.2733145	183.972976	
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218.5396009	336.1614649	288.3744455	471.2140468	487.9219654	552.1849752	205.4341274	381.7090302	441.8817913	
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1078.209601	922.5261237	842.90873	781.0353523	865.3696155	638.2770901	990.314814	871.7562313	908.2612394	
135.8483661	238.7912734	57.24057102	400.548342	289.4387393	219.0189439	199.5774772	366.9256937	256.8878562	
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68.18629429	38.85221848	31.19132463	110.7142506	65.43041338	62.92586154	61.89235576	41.90490961	70.19610761	
991.9397213	1003.019522	1031.13067	343.4976409	445.5560285	401.2944382	514.9238819	648.3082915	596.8499676	
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628.616659	627.3595142	694.9280745	756.6019084	997.7655262	936.9113011	1165.280125	949.5335083	788.3347755	
3805.563687	3517.811631	3717.267893	841.6864957	572.0491951	663.3364646	3250.846003	3322.421919	3458.51693	
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350.2496317	278.2501207	404.3156762	606.8563256	482.4359672	448.3763866	140.5055556	344.8951766	238.3586127	
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1122.112425	1365.347788	1148.896782	834.6648815	970.2857534	815.5147225	662.6533997	753.8545914	731.7221131	
5766.744261	4114.063177	4641.070415	4043.110835	3579.447649	4131.094617	6177.44584	3425.508726	4504.282116	
596.6537138	552.7498257	347.5693132	613.8309544	904.6711524	739.2268926	432.3417206	464.7446442	672.1413423	
10715.72269	9403.38786	8405.071938	8484.091109	8005.578856	7123.143184	10477.40798	7861.526701	7892.66683	
5504.477931	4489.764869	4093.682418	3166.801112	3997.472963	4260.367873	6245.772001	3691.081323	4271.545553	
7995.584886	6219.782533	5687.337945	5001.018319	5589.30459	6300.576455	7422.340647	5421.989418	5436.924749	
497.1580318	446.0062774	496.9652016	482.624553	481.9704647	420.252934	656.9257903	531.6640711	627.7628517	
373.3694726	321.4668191	469.2575077	358.9484921	295.9356627	340.9417951	398.8587632	404.761753	317.4914721	
504.1267075	502.3067521	541.1491638	498.203621	476.0219384	441.8006414	412.5971873	485.8191738		
451.4043303	438.9121676	500.4980139	434.5817771	546.7426394	428.9181363	448.751635	390.7168217	398.5672805	
0.001403199	0.001403199	0.001403199	7370.854097	6160.47104	6479.795094	0.001403199	0.001403199	0.001403199	
334.0718136	199.3008415	355.6543143	299.5102738	326.4328465	422.1679878	345.5143188	360.9319148	304.2335645	
306.605839	389.2303874	424.0816138	1389.222091	1158.244323	1361.612394	671.9333181	543.5843964	460.4845765	
130.3239403	138.0956932	155.8934428	651.2442037	535.5488137	668.6498066	179.1780632	213.07993	410.7930223	
445.6997937	463.99062	459.5648074	280.3146585	183.6465009	244.8385427	606.1209364	514.6370201	485.4514728	
4641.547862	4858.791116	4442.589743	5872.891546	5123.977577	5584.203416	22008.14426	20645.70922	20951.65453	
2067.823384	1777.819319	1893.342124	2320.99628	2495.425517	2269.436515	2727.197842	2358.122947	2357.514854	
339.085886	224.5631557	175.1528466	115.1972151	232.0969957	398.9929169	1272.372691	1202.221245	1062.733904	
1922.209924	2039.364767	1848.777636	2314.80418	2272.537647	2249.596967	9491.007707	9215.417862	8706.001441	
2037.319994	2039.940824	2029.461768	2806.631994	2444.325085	2421.878458	3013.683465	3019.878812	2792.822442	
3616.018557	3291.371592	3684.074721	3361.603582	3617.321713	3883.056687	4321.377533	3509.966283	4093.484205	
1534.43265	1191.427624	1332.41455	1434.057024	1571.020401	1528.297458	1736.061374	1508.626747	1715.197448	
548.2952404	705.0442583	565.6342741	684.9311503	615.2015454	496.3481236	617.8976749	690.1475205	440.9632632	
6917.191931	5761.179274	5527.505156	5830.21555	6700.843392	5956.664809	7140.170619	5367.774859	5997.113192	
568.1390824	748.0516057	1025.636328	873.8829922	1166.86441	1010.117321	683.1807259	957.5928081	837.1003788	
363.5965924	489.8776348	575.5212722	93.51597279	474.9188962	449.3495508	3096.566301	2814.161061	2654.817644	
4106.571054	3886.461982	4021.325647	4637.27506	4514.216289	4066.088436	5660.667087	4224.672624	4939.779772	
480.3228238	529.8085304	523.9430286	148.7227814	200.1637264	192.6851672	706.6629014	659.560489	644.3514269	
645.9261634	739.283223	690.0450236	978.4738787	987.7304719	1018.239522	1043.412112	808.1645804	889.7269219	
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1137.435891	1190.470731	1213.92956	1097.197818	1006.800558	1018.903212	915.1047429	884.6389023	892.6151223	
3584.158657	3561.328148	3623.578439	8777.318473	7279.046225	7892.380837	3846.865962	3364.694774	3238.507404	
671.8717367	616.8608704	702.2881224	841.3657198	748.1554671	922.3411996	894.3270885	958.7710907	1033.541828	
903.759504	622.6363153	703.3996728	162.2493161	127.8702602	102.0030615	526.6028342	380.9096241	499.6899395	
960.3582488	807.1081207	1112.35466	655.8334858	411.2604774	402.2075132	722.6206929	638.6133003	632.7634937	
384.7178543	420.400753	507.1783822	3408.456532	2467.398964	2751.179494	54.30450147	0.001403199	0.001403199	
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273.6063149	127.2581817	294.0593133	3034.971099	2499.396729	2210.140471	570.7512699	479.6597394	313.2030357	
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127.7691631	157.7852481	314.2421389	1418.812287	1137.295636	1030.51706	0.001403199	0.001403199	0.001403199	
316.4349664	250.1279517	204.5937941	186.6344467	402.0884329	389.1064008	1593.489269	1647.816334	1442.481752	
1862.989057	1581.413267	1606.541312	3988.125966	3772.969708	3716.670409	2135.465414	1637.515916	1499.394271	
196.4639057	218.4046776	206.2834179	1227.558701	939.8663916	1127.242052	0.001403199	0.001403199	0.001403199	
0.001403199	0.001403199	38.75633241	391.2897816	275.4024675	343.0691903	0.001403199	0.001403199	0.001403199	
121.973707	277.7432685	0.277303882	1448.96517	1384.206566	1244.425942	1.834181854	58.53141874	64.94723856	
0.001403199	0.001403199	47.91610239	458.9469746	258.154012	201.2761508	0.001403199	0.001403199	0.001403199	
280.9984082	239.6090098	469.8293459	502.4568191	569.7474736	669.6096309	653.4952609	458.0604544	579.5639176	
628.0742408	711.5835076	565.2696505	667.4814123	654.9146786	734.6127986	1172.601719	743.7591629	429.2645902	
414.9840623	312.8780279	344.3044984	450.6233306	589.7793495	439.2760612	551.0567276	438.0956917	329.2229663	
124.6312439	211.5795558	203.1905076	1578.439397	1318.864286	1327.344922	0.001403199	9.983573562	0.001403199	
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4.14_401.0055m/z	401.005476	4.136366667	neg
4.14_418.9646m/z	418.9645942	4.136366667	neg
4.14_428.1199m/z	428.1199241	4.136366667	neg
4.14_434.1306m/z	434.1306117	4.136366667	neg
4.14_446.9062m/z	446.9062439	4.136366667	neg
4.14_451.1249m/z	451.1248682	4.136366667	neg
4.14_468.9931m/z	468.993055	4.136366667	neg
4.14_502.1183m/z	502.1182598	4.136366667	neg
4.14_514.8936m/z	514.8936395	4.136366667	neg
4.16_123.0327m/z	123.0326587	4.15895	neg
4.16_197.8899m/z	197.889864	4.15895	neg
4.16_233.0126m/z	233.0126374	4.15895	neg
4.16_250.0334m/z	250.0334326	4.15895	neg
4.16_254.5181m/z	254.5180529	4.15895	neg
4.16_255.0236n	254.0162937	4.15895	neg
4.16_261.9864m/z	261.9864309	4.15895	neg
4.16_267.0236m/z	267.0236194	4.15895	neg
4.16_288.5118m/z	288.5117657	4.15895	neg
4.16_301.0002m/z	301.0001609	4.15895	neg
4.16_320.0753m/z	320.0753402	4.15895	neg
4.16_322.0037m/z	322.0036905	4.15895	neg
4.16_322.5054m/z	322.5054102	4.15895	neg
4.16_333.0183m/z	333.0182999	4.15895	neg
4.16_340.0028m/z	340.0028061	4.15895	neg
4.16_354.0910n	353.0876164	4.15895	neg
4.16_371.0056m/z	371.0055717	4.15895	neg
4.16_407.9904m/z	407.9903722	4.15895	neg
4.16_409.0753m/z	409.0752985	4.15895	neg
4.16_471.1850m/z	471.1850091	4.15895	neg
4.16_473.0290m/z	473.029047	4.15895	neg
4.16_531.0217m/z	531.0217297	4.15895	neg
4.16_541.0164m/z	541.0164265	4.15895	neg
4.16_543.9652m/z	543.9651903	4.15895	neg
4.16_597.0430m/z	597.0429945	4.15895	neg
4.16_611.9526m/z	611.9525976	4.15895	neg
4.18_153.0534m/z	153.0533909	4.181333333	neg
4.18_204.0277m/z	204.0276691	4.181333333	neg
4.18_235.0189m/z	235.0189477	4.181333333	neg
4.18_347.0361m/z	347.0361304	4.181333333	neg
4.18_392.0183n	391.0110073	4.181333333	neg
4.18_415.0236m/z	415.023624	4.181333333	neg
4.18_415.1913m/z	415.191307	4.181333333	neg
4.18_462.0836n	461.0680052	4.181333333	neg
4.18_529.0551m/z	529.0551356	4.181333333	neg
4.19_112.9824m/z	112.9824294	4.18978333	neg
4.19_124.0165m/z	124.0165259	4.18978333	neg
4.19_158.0540m/z	158.0540296	4.18978333	neg
4.19_179.0329m/z	179.0328916	4.18978333	neg
4.19_218.9881m/z	218.9881056	4.18978333	neg
4.19_220.0647m/z	220.0647386	4.18978333	neg
4.19_234.1065m/z	234.1064987	4.18978333	neg
4.19_236.9911m/z	236.9910941	4.18978333	neg
4.19_247.0201m/z	247.0201165	4.18978333	neg
4.19_276.0913m/z	276.0912702	4.18978333	neg
4.19_276.9555m/z	276.95551	4.18978333	neg
4.19_278.9524m/z	278.9524375	4.18978333	neg
4.19_286.9845m/z	286.9844927	4.18978333	neg
4.19_298.9375m/z	298.9374733	4.18978333	neg
4.19_300.1453m/z	300.1453407	4.18978333	neg
4.19_303.9747m/z	303.9746563	4.18978333	neg
4.19_309.9738n	308.9665055	4.18978333	neg
4.19_310.9844m/z	310.9844228	4.18978333	neg
4.19_315.0078m/z	315.0078108	4.18978333	neg
4.19_318.9217m/z	318.9216812	4.18978333	neg
4.19_344.9430m/z	344.943035	4.18978333	neg
4.19_347.1351m/z	347.1351027	4.18978333	neg
4.19_360.9285m/z	360.9285373	4.18978333	neg
4.19_366.9250m/z	366.9249598	4.18978333	neg
4.19_368.9217m/z	368.9216783	4.18978333	neg
4.19_371.9621m/z	371.9620684	4.18978333	neg
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4.19_376.9539m/z	376.9539112	4.18978333	neg
4.19_382.9951m/z	382.9951416	4.18978333	neg
4.19_393.9438m/z	393.9437679	4.18978333	neg
4.19_423.0371m/z	423.0371177	4.18978333	neg
4.19_426.0421m/z	426.0420561	4.18978333	neg
4.19_426.1502n	425.1428769	4.18978333	neg
4.19_434.9123m/z	434.9123199	4.18978333	neg
4.19_444.9414m/z	444.9413969	4.18978333	neg
4.19_450.9825m/z	450.9824882	4.18978333	neg
4.19_454.8964m/z	454.8964308	4.18978333	neg
4.19_460.9834m/z	460.9833546	4.18978333	neg
4.19_461.9313m/z	461.9313041	4.18978333	neg
4.19_488.0934n	533.0915847	4.18978333	neg
4.19_494.0296m/z	494.0296171	4.18978333	neg
4.19_502.8999m/z	502.8999267	4.18978333	neg
4.19_512.9286m/z	512.9286349	4.18978333	neg
4.19_518.9700m/z	518.9700439	4.18978333	neg
4.19_562.0170m/z	562.0169702	4.18978333	neg
4.19_580.9161m/z	580.9160863	4.18978333	neg
4.19_648.9036m/z	648.9035548	4.18978333	neg
4.19_654.9454m/z	654.9454243	4.18978333	neg
4.21_206.9970m/z	206.9970288	4.212116667	neg
4.21_248.0963m/z	248.0963118	4.212116667	neg
4.21_256.9761m/z	256.9761409	4.212116667	neg
4.21_270.9895m/z	270.9895051	4.212116667	neg
4.21_325.9566m/z	325.956607	4.212116667	neg
4.21_329.0256m/z	329.0255895	4.212116667	neg
4.21_342.1671m/z	342.1671406	4.212116667	neg
4.21_380.9791m/z	380.9791365	4.212116667	neg
4.21_385.0213m/z	385.0213229	4.212116667	neg
4.21_386.9092m/z	386.9092405	4.212116667	neg
4.21_570.8374m/z	570.8373811	4.212116667	neg
4.23_203.0794n	202.072302	4.234483333	neg
4.23_216.1363n	261.1342895	4.234483333	neg
4.23_264.9345m/z	264.9344759	4.234483333	neg
4.23_272.0964m/z	272.0963712	4.234483333	neg
4.23_277.0281m/z	277.0280756	4.234483333	neg
4.23_283.0799m/z	283.079939	4.234483333	neg
4.23_297.0051m/z	297.005126	4.234483333	neg

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787.8350245	581.458644	622.3928775	2007.026659	1563.746626	1629.193944	728.744614	689.4116279	421.9965221	
1241.720222	1304.183797	1474.240104	299.6548962	407.1277335	398.696478	439.4824659	263.292224	367.2732322	
1753.972154	1550.425713	1644.499309	1984.265472	1721.307395	2007.64311	1795.600872	2158.956956	1880.882238	
5238.466638	5142.91549	4455.95383	4655.602744	5571.93842	4888.312933	6433.33012	5309.927624	5460.663813	
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4312.205427	4151.225058	3992.311892	2008.894376	1689.236842	1657.778737	5888.358036	5318.89318	5021.05118	
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464.7868487	476.8425433	534.0336039	2222.729246	1497.541331	1704.869255	0.001403199	0.001403199	0.001403199	
6213.752466	5583.433825	5854.687915	17015.86964	12994.50611	14885.69315	224.7245169	159.097906	220.2466009	
777.0928213	841.0050732	865.6892089	725.4935875	532.9922862	816.4255357	874.5399362	911.0721349	771.2857096	
177.8384905	191.8938188	196.1953105	307.6652583	220.720365	140.9235813	162.7262944	165.0396337	186.2968953	
167.9121717	125.503264	142.0511253	647.4939961	515.0603321	593.5960803	0.001403199	0.001403199	29.5308917	
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556.9926598	725.3919727	613.5130785	1649.237076	1669.73576	1671.041052	68.41780106	165.0509024	78.89636757	
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2059.633	1833.930263	1778.53226	2826.992278	1995.954583	2242.977778	2579.351879	1960.764249	1975.254062	
2615.59246	3306.678955	3522.130354	3550.199407	2012.9436	2681.013199	4915.454227	2009.36632	2486.630917	
1364.283262	1143.118775	1330.679723	1309.650056	1207.581307	1207.619514	1797.791232	1255.144254	1461.531936	
1395.328571	1732.41769	1702.004413	2531.518629	1744.786963	1790.281337	2082.707529	2119.249401	1699.782252	
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713.0441378	612.5236159	656.3354713	810.0057029	636.8809714	666.3920095	775.4748917	529.7760101	643.4473722	
177.0489325	161.211622	263.5681129	236.6637123	271.6131686	201.6422891	292.8751096	162.6479521	239.9999608	
2328.034056	1846.805789	2043.746175	927.2130903	880.0995668	903.0140224	1451.031747	1260.425237	1431.97747	
3066.704517	2804.081639	2991.513741	1027.734314	815.4533552	978.8714007	1137.3236	1157.476902	1110.047546	
1559.346229	1290.064789	1349.011976	236.9859759	512.8200599	458.9840253	1078.776802	882.0808716	1147.854468	
1365.243882	1247.02485	1187.109475	1158.474747	995.7301054	1020.361999	1780.883128	1190.827372	1246.726673	
5321.18212	4682.338611	4961.810229	3983.751395	3286.507857	3811.364252	5030.658849	3173.11683	3584.63266	
2636.878055	2664.938599	2407.135594	2806.69804	1840.081789	2431.911786	2041.220496	1434.469912	1878.223508	
51.53575436	118.7337946	54.3059153	50.67622226	68.52468142	44.72348415	145.0475703	58.12737889	58.64074366	
4210.93299	4106.027924	4031.692274	739.2874124	708.2073055	942.8355903	3927.262221	3640.039064	3709.585396	
232.823328	183.1043797	182.8742525	264.9965462	255.4083529	250.6336463	219.0189611	177.6466917	206.9553382	
6687.819686	6723.608846	6772.88195	7089.669416	6482.519751	8480.982376	6727.751437	6006.57861	5752.504996	
369.4384883	499.7919292	479.4633359	64.13716868	0.001403199	0.001403199	426.0798023	476.2531531	310.6345407	
507.6123588	423.182904	445.0344927	305.0983131	355.8373682	451.9652952	900.2775146	473.79877	665.364521	
130.6450521	103.1373337	119.5676037	25.37122032	95.94951558	112.4653485	0.001403199	61.52230453	52.20681748	
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5637.792011	4852.251504	4814.010679	6306.053469	6146.203227	7441.495958	5906.121215	4459.695677	4905.106411	
1627.00994	1609.645384	1598.964073	1396.842463	1150.536442	1454.002073	1817.265505	1621.806784	1362.698974	
8521.9105	7509.499511	7571.804149	3814.788827	3963.894038	4634.170161	9114.721943	7920.357089	7798.386803	
1879.46531	1392.973992	1449.054418	239.5696345	324.5198101	322.3271908	1729.711252	1523.080936	1392.795669	
36680.15943	32139.45596	34451.87914	5856.05277	5446.929006	6983.118638	35026.22683	31069.79779	30644.80941	
2314.475807	1804.089561	1833.074588	250.4336333	250.1412301	268.6808894	2413.671827	2198.722697	1901.36	
627.3996328	440.5227295	540.7466831	320.5501518	257.2187724	370.4858323	684.0831326	870.4117413	674.5801869	
9533.113308	8868.614412	9445.387452	2314.147172	2159.367324	2880.707368	9354.816488	9117.080246	8408.921733	
40991.07542	35764.56486	37381.61169	6592.214653	6354.686507	7874.855959	38425.24773	35388.16363	34221.4428	
1318.965198	1210.223683	1085.96734	362.227795	304.6855924	397.084662	1031.756347	900.5222167	730.6379217	
4449.828975	3508.352284	3716.294783	4865.142287	4722.211735	6090.127748	4082.852072	3397.564438	3804.864977	
2376.313114	2428.047183	1972.540137	263.9739436	204.3604135	284.6116582	2118.467606	1831.830098	1631.561745	
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1746.84472	1564.571125	1483.014476	202.3809739	112.7963007	137.7267824	1767.827506	1444.029461	1302.306568	
439.5287074	469.9109642	513.0025686	74.80626209	148.8850201	53.17824319	572.1138112	567.1626652	440.4797229	
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35292.91232	30883.93285	32534.87742	5458.684173	5264.553745	7505.114676	34462.78321	30734.98664	29781.76421	
3279.163081	3218.112556	2876.16126	4146.058072	3391.345347	4765.632658	3520.099007	2617.263138	2702.246407	
2979.383266	2879.528948	2342.008	485.5402851	421.7202381	617.517892	2781.362269	2617.909153	2505.041595	
2036.340004	1579.676861	1808.438827	398.2550693	381.6811859	400.140599	2222.03851	1419.586451	1275.633805	
3738.090634	3126.182567	3405.899314	2449.724228	2160.88741	3310.531381	4844.921453	3625.449313	3477.717385	
3378.827891	3141.494154	2622.87184	3896.059537	3785.225721	4833.62528	3797.004307	2687.32032	2699.707108	
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20354.95645	17043.94155	17097.90156	2927.29444	2969.86949	3759.846731	19083.36592	15808.03038	15575.55243	
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3168.700733	2680.136475	2844.848567	102.5621632	423.7173274	258.1282192	2413.027049	2187.812544	1945.460234	
8078.218585	8831.77029	9516.999952	1526.583979	1331.813044	474.5645436	6050.756511	6714.431936	6533.480337	
1851.724838	1561.290803	1461.120581	295.5143603	200.6184101	225.6841956	1603.837374	1476.584061	1544.346609	
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12637.73885	11884.73092	11459.19198	1631.451361	2107.96986	2471.757586	12997.09828	11387.28222	10896.42728	
2251.944975	1689.257852	1500.483343	2124.190883	2218.284247	2674.597729	2162.589221	1181.427166	2003.364775	
1873.035737	1336.584351	1706.669668	1427.802259	1095.506333	1689.844984	2521.128096	1276.794169	1835.105961	
8530.830941	8562.571969	7905.436571	1371.548289	1355.766812	1444.513759	9273.445085	7779.33704	7759.804804	
5682.895174	5498.414325	5428.145079	478.3023705	784.5741627	1143.478447	6123.917388	4707.721518	5013.523702	
1184.822373	1223.346638	1277.086698	2202.136743	1949.142757	2242.979405	1174.643634	1400.484126	1287.788287	
368.0383194	111.1726054	168.4592952	28.85891912	0.001403199	72.76147461	329.3585194	137.2624061	184.2487166	
4822.335898	5140.808532	5447.76025	5441.444616	5218.463391	6373.394766	5397.699915	5860.755205	5693.604117	
733.8519274	588.5841674	546.6406805	69.98531614	107.1762338	323.9570026	460.2116722	451.2175854	532.2195954	
1684.481402	1546.841421	2019.360156	1311.66867	1108.347754	1085.671781	1751.264295	1862.554817	1915.33302	
1135.122852	535.8552544	621.8261696	58.15442848	103.4598851	100.8033231	893.4687658	896.2113254	1067.145446	
642.2108523	613.6965643	800.8107014	851.8301786	771.1559025	869.1927086	391.0955549	384.7015514	224.9195856	
711.8065265	1100.851516	818.5994094	1259.994494	1044.86932	1196.35294	242.2282989	485.2897125	419.6765147	
604.218553	1000.753124	783.8527405	744.406156	662.1940754	522.0031869	334.7544168	399.9432316	405.5841331	
1685.694823	1953.011635	2370.335981	462.5676133	587.3923827	801.0648221	2215.924188	2444.563427	2000.9982	
2180.565854	1281.182552	1484.240881	63.01773076	96.08569065	295.6568104	1586.214898	1230.719477	1498.212096	
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124.9302351	32.55378176	237.7797295	230.3081111	99.62566642	246.969985	86.43589478	0.001403199	172.8489064	
1111.742652	1155.460318	1156.478882	1413.580315	1417.236971	1353.952796	1438.403899	883.2460469	1224.631752	
7026.75253	7472.951643	7554.563083	6935.514993	6388.511165	6523.044344	4586.185516	5351.289979	4974.300604	

4.23_303.1200m/z	303.1199951	4.234483333	neg
4.23_317.9942m/z	317.9941672	4.234483333	neg
4.23_322.0971m/z	322.0970841	4.234483333	neg
4.23_332.0814m/z	332.0813669	4.234483333	neg
4.23_348.9616m/z	348.9616478	4.234483333	neg
4.23_378.0950m/z	378.0950213	4.234483333	neg
4.23_394.0134m/z	394.0134018	4.234483333	neg
4.23_416.9490m/z	416.948962	4.234483333	neg
4.23_421.0208m/z	421.0207684	4.234483333	neg
4.23_425.1069m/z	425.1069461	4.234483333	neg
4.23_432.9803m/z	432.9802676	4.234483333	neg
4.23_439.8893m/z	439.8893004	4.234483333	neg
4.23_462.0012m/z	462.0011539	4.234483333	neg
4.23_529.9883m/z	529.9882821	4.234483333	neg
4.23_597.9748m/z	597.9747971	4.234483333	neg
4.23_665.9631m/z	665.96307	4.234483333	neg
4.26_259.0281m/z	259.0280815	4.2568	neg
4.26_281.9811n	326.9793945	4.2568	neg
4.26_316.1768m/z	316.1767703	4.2568	neg
4.26_350.9285m/z	350.9284667	4.2568	neg
4.26_363.9844n	362.9771371	4.2568	neg
4.26_445.1336m/z	445.133577	4.2568	neg
4.26_473.1302m/z	473.1301929	4.2568	neg
4.26_487.1098m/z	487.1098163	4.2568	neg
4.26_498.9520m/z	498.9519701	4.2568	neg
4.26_214.0067m/z	214.0066942	4.278183333	neg
4.28_269.9610m/z	269.9610373	4.278183333	neg
4.28_271.9580m/z	271.95805	4.278183333	neg
4.28_275.0123m/z	275.0123004	4.278183333	neg
4.28_296.9799m/z	296.9798923	4.278183333	neg
4.28_337.9486m/z	337.9486245	4.278183333	neg
4.28_347.9773m/z	347.9773384	4.278183333	neg
4.28_357.9329m/z	357.9329203	4.278183333	neg
4.28_357.9854m/z	357.9854161	4.278183333	neg
4.28_364.9673m/z	364.9672529	4.278183333	neg
4.28_379.9146m/z	379.9145801	4.278183333	neg
4.28_405.9359m/z	405.9359022	4.278183333	neg
4.28_415.9649m/z	415.9648542	4.278183333	neg
4.28_432.9551m/z	432.9550908	4.278183333	neg
4.28_446.9940m/z	446.9939924	4.278183333	neg
4.28_448.9096n	493.9078469	4.278183333	neg
4.28_453.9883m/z	453.988267	4.278183333	neg
4.28_470.0697m/z	470.0697018	4.278183333	neg
4.28_473.9234m/z	473.9233596	4.278183333	neg
4.28_481.9366m/z	481.9366262	4.278183333	neg
4.28_488.1129m/z	488.1129328	4.278183333	neg
4.28_497.1607m/z	497.1607472	4.278183333	neg
4.28_507.9993m/z	507.9992872	4.278183333	neg
4.28_514.9811m/z	514.9811355	4.278183333	neg
4.28_551.9399m/z	551.9399021	4.278183333	neg
4.28_556.1003m/z	556.100295	4.278183333	neg
4.28_566.9391m/z	566.9390987	4.278183333	neg
4.28_582.9690m/z	582.9690303	4.278183333	neg
4.28_587.1298m/z	587.1298123	4.278183333	neg
4.28_619.9273m/z	619.9273139	4.278183333	neg
4.28_650.9565m/z	650.9564979	4.278183333	neg
4.28_655.1170m/z	655.1169981	4.278183333	neg
4.28_681.9860m/z	681.9860153	4.278183333	neg
4.28_687.9147m/z	687.9147158	4.278183333	neg
4.28_718.9439m/z	718.9438967	4.278183333	neg
4.28_755.9021m/z	755.9021302	4.278183333	neg
4.28_786.9308m/z	786.9307553	4.278183333	neg
4.30_201.0770m/z	201.0770193	4.300033333	neg
4.30_203.0327m/z	203.0327048	4.300033333	neg
4.30_211.9156m/z	211.9156034	4.300033333	neg
4.30_256.0804m/z	256.0804186	4.300033333	neg
4.30_260.0962m/z	260.0962487	4.300033333	neg
4.30_271.0204m/z	271.0203969	4.300033333	neg
4.30_301.9719m/z	301.9719101	4.300033333	neg
4.30_312.1432m/z	312.1432136	4.300033333	neg
4.30_324.0160m/z	324.0160138	4.300033333	neg
4.30_324.0679m/z	324.0679108	4.300033333	neg
4.30_331.9523m/z	331.9522595	4.300033333	neg
4.30_339.9453m/z	339.9452592	4.300033333	neg
4.30_369.9591m/z	369.9590509	4.300033333	neg
4.30_407.9325m/z	407.9325133	4.300033333	neg
4.30_422.9259m/z	422.9259181	4.300033333	neg
4.30_425.9203m/z	425.9203497	4.300033333	neg
4.30_500.9426m/z	500.942612	4.300033333	neg
4.30_516.8965n	561.894833	4.300033333	neg
4.30_536.8848m/z	536.8848003	4.300033333	neg
4.30_541.9108m/z	541.9108239	4.300033333	neg
4.30_568.9298m/z	568.9297922	4.300033333	neg
4.30_609.8983m/z	609.8983291	4.300033333	neg
4.30_636.9178m/z	636.9177644	4.300033333	neg
4.30_677.8856m/z	677.8856281	4.300033333	neg
4.30_823.8894m/z	823.8893931	4.300033333	neg
4.32_212.0644m/z	212.0643546	4.3224	neg
4.32_266.9946m/z	266.99463	4.3224	neg
4.32_315.0724m/z	315.0724243	4.3224	neg
4.32_324.0779n	369.0828448	4.3224	neg
4.32_334.9820m/z	334.9819809	4.3224	neg
4.32_337.0543m/z	337.054328	4.3224	neg
4.32_415.0604m/z	415.0604137	4.3224	neg
4.32_511.1348m/z	511.1348191	4.3224	neg
4.34_208.9989m/z	208.9989262	4.344733333	neg
4.34_218.1035m/z	218.1035015	4.344733333	neg
4.34_219.0275m/z	219.0275365	4.344733333	neg
4.34_233.0070m/z	233.0069889	4.344733333	neg
4.34_240.0104m/z	240.0103526	4.344733333	neg
4.34_242.0169n	287.0151486	4.344733333	neg
4.34_274.1120m/z	274.1120347	4.344733333	neg
4.34_276.9862m/z	276.9861803	4.344733333	neg
4.34_281.1007m/z	281.1006599	4.344733333	neg
4.34_293.0626m/z	293.0625587	4.344733333	neg
4.34_301.1295m/z	301.1294593	4.344733333	neg
4.34_310.0048n	355.002615	4.344733333	neg
4.34_318.1383m/z	318.1382512	4.344733333	neg
4.34_342.1292n	323.1113554	4.344733333	neg
4.34_348.0589n	347.0515812	4.344733333	neg

345.5910267	193.6936294	226.055609	289.2991023	404.6532924	208.8525574	236.6448086	360.7104121	175.3728599	
206.6805701	165.7609679	263.9299321	217.1657324	335.5434488	318.5963058	303.1240709	253.7284012	183.8607876	
356.3971208	401.8251421	470.1616705	1353.636174	1213.558238	1390.228981	541.2091102	524.5577936	636.4623051	
394.4704326	504.2206422	490.4625526	627.9931279	430.4659876	530.7406807	439.1800981	494.192961	619.7072121	
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115.1597076	348.1976729	253.0111743	65.02064721	0.001403199	60.20774322	158.5894699	153.0275726	243.2616112	
4739.480872	4598.125932	4906.932978	5293.45016	5307.14319	4511.870357	5387.905247	5955.484797	5117.243497	
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1648.649429	1562.900273	1582.024428	1363.209959	1760.120618	1455.014798	1062.081452	1172.917818	1149.535374	
1041.661907	1145.460938	962.606956	875.1144499	1090.917527	943.2010754	1092.631042	750.2344131	862.9582465	
4348.175325	3709.489959	4732.165659	4196.361355	4379.051578	4235.949088	4620.121685	4428.659661	4388.938584	
3296.157941	3246.685985	3740.511422	3172.777396	3360.228656	3064.090295	3374.016019	3854.554373	3074.455173	
4202.899134	4374.953179	4415.403197	3148.5545	3505.172858	2941.423459	4065.013741	4372.168137	3531.911609	
2290.735175	2913.260332	3357.99931	2622.018205	2353.480051	2671.875487	2562.87376	3346.748241	2623.528641	
3189.92658	3098.446213	3131.080681	1895.356217	1780.551859	1939.029994	2318.064322	2862.832353	2513.065969	
8078.688853	8795.202764	9296.143597	3043.991326	2585.783436	2325.525431	6831.466811	7335.418442	6961.472377	
1130.048403	1144.660803	1082.014914	1743.804614	1878.056421	1511.908792	909.8280503	1088.523067	770.6836058	
1996.722094	2055.600734	1968.904159	2795.51317	3059.376072	2851.84995	3357.869939	2559.848434	2656.277947	
11541.10359	11980.57891	11813.0258	6412.8548	5942.698033	5991.691859	9441.799854	10619.30802	8972.967515	
1297.362692	1350.825259	1646.598074	1425.114842	1637.955407	1555.482442	1149.146691	1635.135072	1920.868647	
1503.273702	2039.850447	1633.992082	1049.473369	1209.726105	1012.943636	1379.73748	1370.353134	1107.156213	
398.952146	442.3691078	450.2561206	180.3829317	189.9376542	188.7621075	943.9397103	1053.897023	785.3729523	
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4025.437688	4562.740043	4158.749401	347.5870724	215.7476172	304.9744873	3666.608907	4168.214198	4234.508429	
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4665.098684	4594.159488	5324.126342	263.8079489	157.6907536	153.0920769	3633.789354	4219.816635	4187.451521	
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4310.27234	3710.897507	2728.171665	120.5376931	221.8385321	81.61936778	3396.378946	2964.096959	2781.213736	
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1221.044736	1401.819238	1204.894478	0.001403199	0.001403199	0.001403199	819.3544965	1313.756682	1144.333315	
6255.253706	7270.415639	8106.505654	86.74543126	165.4002185	0.001403199	4880.863886	6008.112814	5671.16585	
13973.03573	16128.78934	14416.77497	179.9143982	211.2618529	41.61627003	9826.149622	13191.19317	10452.63949	
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6795.704879	6414.70926	8163.044126	47.65800416	85.28190544	0.001403199	5011.074016	4814.735785	4572.740366	
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17222.40303	19097.62689	17088.44652	1501.021765	882.6846971	878.116108	17409.22716	16904.67677	15355.86177	
4464.481772	4142.736096	5543.979189	0.001403199	0.001403199	0.001403199	2615.579255	3710.287115	2177.416818	
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2328.883676	2163.187232	2277.222769	2913.324004	2711.879422	2849.125625	2386.730405	2492.778198	2178.355934	
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306.8146171	193.7073838	109.087989	595.9654467	571.8540637	616.0596756	49.89596127	0.001403199	134.3029884	
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2371.789981	2337.312421	2803.6277	5202.821978	4353.35278	4048.770693	2734.787577	3080.565973	3292.045002	
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1230.980183	1412.482496	1377.972254	2108.29936	1519.138469	1889.151798	1357.450265	1476.173864	1443.844432	
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4.34_361.9346m/z	361.9346338	4.344733333	neg
4.34_367.0656m/z	367.0656009	4.344733333	neg
4.34_377.9920n	422.9901884	4.344733333	neg
4.34_381.9580n	762.927638	4.344733333	neg
4.34_410.0892m/z	410.0892028	4.344733333	neg
4.34_412.9612m/z	412.9612238	4.344733333	neg
4.34_416.0403m/z	416.040282	4.344733333	neg
4.34_416.0464n	461.0445413	4.344733333	neg
4.34_429.9218m/z	429.9217961	4.344733333	neg
4.34_445.9788n	490.9775791	4.344733333	neg
4.34_454.0189m/z	454.0189188	4.344733333	neg
4.34_480.9488m/z	480.948835	4.344733333	neg
4.34_484.0277m/z	484.0276677	4.344733333	neg
4.34_497.9097m/z	497.909692	4.344733333	neg
4.34_513.9653n	558.9650113	4.344733333	neg
4.34_522.0064m/z	522.006371	4.344733333	neg
4.34_527.0398m/z	527.0397762	4.344733333	neg
4.34_548.9364m/z	548.9363718	4.344733333	neg
4.34_565.8970m/z	565.8969926	4.344733333	neg
4.34_581.0573m/z	581.0573253	4.344733333	neg
4.34_589.9940m/z	589.9940187	4.344733333	neg
4.34_595.0272m/z	595.0271569	4.344733333	neg
4.34_604.0745m/z	604.0745459	4.344733333	neg
4.34_616.9237m/z	616.9237246	4.344733333	neg
4.34_626.9527m/z	626.952731	4.344733333	neg
4.34_665.0070m/z	665.0070013	4.344733333	neg
4.34_684.9113m/z	684.9113315	4.344733333	neg
4.34_694.9401m/z	694.9401323	4.344733333	neg
4.34_732.9946m/z	732.9946493	4.344733333	neg
4.37_121.9440m/z	121.9440344	4.367166667	neg
4.37_182.0558n	181.0485124	4.367166667	neg
4.37_197.9868m/z	197.9868431	4.367166667	neg
4.37_232.9869m/z	232.9869104	4.367166667	neg
4.37_241.9849m/z	241.9848754	4.367166667	neg
4.37_250.0390m/z	250.0389771	4.367166667	neg
4.37_266.0260m/z	266.0259621	4.367166667	neg
4.37_306.9946m/z	306.9946222	4.367166667	neg
4.37_317.0232m/z	317.0232438	4.367166667	neg
4.37_349.1143m/z	349.1142636	4.367166667	neg
4.37_358.1874m/z	358.187442	4.367166667	neg
4.37_363.1665m/z	363.166488	4.367166667	neg
4.37_392.0184n	437.0162417	4.367166667	neg
4.37_413.1432m/z	413.1432333	4.367166667	neg
4.37_419.0449m/z	419.0449109	4.367166667	neg
4.37_428.9618m/z	428.9618251	4.367166667	neg
4.37_458.9985m/z	458.9985493	4.367166667	neg
4.37_462.9540m/z	462.9539522	4.367166667	neg
4.37_473.0678m/z	473.0678447	4.367166667	neg
4.37_520.9858m/z	520.9857623	4.367166667	neg
4.37_588.9732m/z	588.9731737	4.367166667	neg
4.37_656.9604m/z	656.9603939	4.367166667	neg
4.39_1025.1072m/z	1025.107178	4.3893	neg
4.39_1121.3814m/z	1121.381357	4.3893	neg
4.39_146.0652m/z	146.0652226	4.3893	neg
4.39_318.0309m/z	318.0308679	4.3893	neg
4.39_355.1377m/z	355.137717	4.3893	neg
4.39_364.0363n	409.0340099	4.3893	neg
4.39_391.0347m/z	391.0347049	4.3893	neg
4.39_399.0787m/z	399.0786658	4.3893	neg
4.39_413.0161m/z	413.0161388	4.3893	neg
4.39_416.0690m/z	416.0689676	4.3893	neg
4.39_427.1226m/z	427.1225582	4.3893	neg
4.39_457.0375m/z	457.0374809	4.3893	neg
4.39_461.0675m/z	461.06751	4.3893	neg
4.39_465.0502m/z	465.0502259	4.3893	neg
4.39_473.0227m/z	473.022705	4.3893	neg
4.39_474.0271m/z	474.0271418	4.3893	neg
4.39_476.1133m/z	476.1132832	4.3893	neg
4.39_477.0215m/z	477.0214606	4.3893	neg
4.39_484.0565m/z	484.0565432	4.3893	neg
4.39_498.0954m/z	498.0954461	4.3893	neg
4.39_500.0213n	545.0089714	4.3893	neg
4.39_525.0283m/z	525.0282686	4.3893	neg
4.39_535.0537m/z	535.0536596	4.3893	neg
4.39_566.0831m/z	566.0831432	4.3893	neg
4.39_593.0124m/z	593.0124404	4.3893	neg
4.39_603.0412m/z	603.0412472	4.3893	neg
4.39_620.0313m/z	620.0312901	4.3893	neg
4.39_634.1747m/z	634.1747729	4.3893	neg
4.39_671.0290m/z	671.0289935	4.3893	neg
4.39_702.1619m/z	702.1618696	4.3893	neg
4.39_728.9875m/z	728.987457	4.3893	neg
4.39_739.0164m/z	739.0163986	4.3893	neg
4.39_743.1305m/z	743.1305071	4.3893	neg
4.39_753.1591m/z	753.1591136	4.3893	neg
4.39_770.1472m/z	770.1472212	4.3893	neg
4.39_807.0035m/z	807.0035211	4.3893	neg
4.39_821.1469m/z	821.1469015	4.3893	neg
4.39_835.2901m/z	835.2900624	4.3893	neg
4.39_874.9907m/z	874.990692	4.3893	neg
4.39_889.1334m/z	889.133441	4.3893	neg
4.39_903.2772m/z	903.2772262	4.3893	neg
4.39_942.9790m/z	942.978998	4.3893	neg
4.39_957.1207m/z	957.1206905	4.3893	neg
4.39_971.2645m/z	971.2645072	4.3893	neg
4.41_262.9846m/z	262.9846225	4.411115	neg
4.41_290.1071m/z	290.1071032	4.411115	neg
4.41_306.1383m/z	306.1382792	4.411115	neg
4.41_357.0829m/z	357.0829559	4.411115	neg
4.41_358.0158m/z	358.0157798	4.411115	neg
4.41_360.0703m/z	360.0702761	4.411115	neg
4.41_383.0529m/z	383.0529336	4.411115	neg
4.41_401.0839m/z	401.0839113	4.411115	neg
4.41_406.0401m/z	406.0400665	4.411115	neg
4.41_413.0423m/z	413.0423327	4.411115	neg
4.41_437.0500m/z	437.0500222	4.411115	neg
4.41_442.1617m/z	442.1617241	4.411115	neg
4.41_443.0688m/z	443.068805	4.411115	neg
4.41_456.9331m/z	456.9330955	4.411115	neg
4.41_464.1440m/z	464.143995	4.411115	neg

384.3800625	458.8417474	578.7835293	782.2928103	751.576429	557.5204842	441.0189697	543.8153674	588.3897144	
468.8743112	263.5465335	416.6608501	789.3367513	695.3385087	378.7312587	271.7689343	520.343483	668.4284519	
9426.968003	9251.743917	8811.620091	13721.91117	10633.3828	10316.23872	9908.283909	10848.82821	10972.2003	
4659.939843	3785.099875	4156.088818	5606.036436	4741.697903	4786.933494	4083.741209	4310.976478	4529.574342	
639.1758747	740.5561734	728.3209787	476.8694229	459.6115946	323.5461516	358.3212001	486.7820053	585.1553018	
811.4283427	1083.82571	978.5732928	1733.941175	1438.180764	1226.667116	1374.470536	1091.890317	1155.48168	
1606.150072	1754.097048	2002.275726	262.0133639	175.247132	184.6522966	945.9204881	1633.068553	1116.429827	
875.2746998	1356.286014	1645.977091	2387.84291	1759.755998	1459.368683	1083.762107	2464.962603	2000.053933	
747.3234678	1044.930623	920.5365606	1377.558938	1044.797661	1234.747233	1462.681384	1498.422184	1146.102133	
9955.203387	11049.42559	10943.45571	15955.08606	11821.60313	12736.51341	12131.34652	12623.17965	12218.00574	
1991.205502	2712.18857	2462.451857	128.7830357	124.5285478	125.7414812	1595.98732	2530.480579	2305.650527	
1833.317523	1381.52944	1533.70304	2948.346211	2274.415554	1959.256053	2039.745154	2176.779434	1996.657174	
885.9278583	766.2429133	772.8833641	0.001403199	0.001403199	2.354704023	510.654621	568.2901917	380.5313169	
817.016491	546.5410123	1025.460112	1356.821613	686.7599985	778.8573195	920.6520631	872.6670074	940.5219624	
8231.91781	8654.760659	7525.429171	11699.28418	8923.593334	9102.696409	9954.567454	9700.029864	9480.769515	
1275.217337	1453.291232	1090.848605	55.1734934	111.5492872	114.7094434	984.290938	1565.456552	1228.719091	
3989.930771	4184.523757	3736.018672	1180.927433	1131.273375	1422.425889	3439.270661	4213.547768	3297.362851	
1624.841642	1502.898346	1420.237903	2273.41962	2375.700245	1771.76938	1190.75048	2058.854178	1735.955018	
589.217773	961.9801192	570.170441	1099.011967	1039.54021	950.7164415	708.65627	1059.412816	565.6223679	
662.9696937	641.3683894	813.1485058	1788.435506	1125.414105	829.2506922	850.4166732	686.7906219	725.3493113	
1362.887219	1949.907607	1516.373211	98.36974483	64.60735327	127.3583116	1294.867623	1878.858566	1642.733434	
3329.439073	2710.418331	2985.660654	1308.733949	979.7518105	946.5005464	2839.60569	2422.024463	2561.806723	
1203.299733	617.1453001	1239.325416	0.001403199	0.001403199	0.001403199	271.5366918	891.0114899	834.2209157	
1809.48263	1627.340011	1297.195556	2565.981852	2261.083659	1789.145039	2069.313157	2078.469744	2117.965295	
7364.355708	7118.869352	7869.802764	10882.11276	8795.82548	8505.702485	9646.946185	8943.345216	8358.159102	
1950.606349	1599.290492	1656.819721	2634.169294	1921.153073	1519.051435	1187.922332	2240.107611	2141.326048	
1602.814318	995.7874826	1404.419587	2312.689966	2349.404074	2017.437428	1430.209356	1877.819061	1589.157485	
6467.870406	5867.132292	6016.156741	10115.98153	8147.853467	7535.101158	8584.134888	7424.706543	7279.895045	
1689.001087	1248.574429	1345.452156	2559.021074	2200.528607	1696.136284	1306.97952	2508.536392	2009.134052	
171.3119225	135.8325617	144.9830756	163.3935019	221.5904419	212.5721594	230.3540696	181.062179	168.7739052	
13986.28836	16463.16106	17832.36542	25860.14754	18738.01624	14157.68911	11627.09191	14091.69251	13224.80761	
735.4481856	1033.618687	1148.830966	2482.114731	2080.687849	2089.995368	2224.021857	2585.748265	2726.842751	
427.8102766	222.4760484	239.034691	233.0083256	123.5286134	243.3758308	351.5221216	311.731617	245.9216375	
0.001403199	48.36865389	55.94639541	135.0234935	146.8210269	41.49105355	42.622388	123.5527776	0.001403199	
705.6847194	711.0546338	816.8248121	1438.767983	991.46702	1091.041871	523.8484069	544.5674012	529.4833955	
751.9606703	980.60232	881.1513594	1643.794383	1010.486385	707.6603478	581.555503	667.8794262	695.3870733	
972.0593571	1153.296739	1201.651366	2189.677167	1215.851688	944.6682695	607.1339611	926.9425354	1003.707385	
6724.895812	8196.004983	7972.118365	12195.95903	8723.340493	8345.551732	5495.354813	6192.396261	5893.89011	
886.2034704	1004.119609	1356.953151	2741.9313	1793.080235	1742.061153	1270.962718	1789.872036	1250.590581	
8700.918956	9365.168329	9388.735775	7286.976056	6182.959547	6161.194013	7236.862998	8723.153149	8184.008795	
7541.388997	7262.293032	7534.825999	7647.666549	5876.987973	6669.418716	6319.093923	6459.113043	6545.86431	
6874.042428	6232.91997	6263.275596	5542.09222	3363.733017	4256.243857	3042.825351	5022.366202	3991.525343	
2299.522211	1823.446481	2125.299919	1593.616451	1145.038796	1586.445011	2500.158799	3315.717693	2841.244115	
1121.845143	1462.23938	1507.289441	2330.469765	1814.425643	1854.028858	1551.462277	1848.522826	1755.299595	
936.9303918	409.9869158	495.9527785	1009.19482	833.310922	1351.502673	1063.708224	914.9914389	487.119953	
928.0531143	891.7477333	677.4347812	771.0913923	659.4958022	591.715738	441.0292949	604.7014389	655.5270385	
488.4092667	663.8965288	578.3483978	778.4850997	400.6178702	380.0966186	354.2799765	182.5457001	482.7856503	
1044.356053	1409.345553	1550.988902	380.2657115	453.9055361	536.5359174	2019.077706	2275.011711	2152.232582	
2898.474325	2722.748327	2601.642912	5445.363639	2938.450893	3547.837711	3006.465351	2491.10316	2735.273547	
2028.078656	2050.469113	1869.759817	3727.054907	2441.264944	2781.807981	1595.633699	807.2622591	1718.677982	
1616.742426	1247.435872	1271.341085	2986.221739	1996.790501	2204.698165	1411.51502	1353.726715	1627.003078	
1921.975286	3394.754319	3579.058205	3139.345037	1564.40123	2609.665155	4416.233067	2494.079071	2748.624969	
0.001403199	7992.140781	7281.545621	0.001403199	0.001403199	0.001403199	0.001403199	6820.265747	6799.178039	
717.0848745	661.3543008	913.1113711	612.3608711	570.743324	434.2424888	751.6325589	1001.519639	942.0147582	
1514.152693	606.6489691	263.1779679	820.9954576	344.744355	1324.750842	1455.550123	1852.94714	1235.519104	
3339.214001	3701.140826	2752.348587	2704.166392	2760.915066	2813.755804	2063.416467	2127.638009	2995.369918	
11250.42369	9776.617861	7545.494452	5934.797519	5294.428517	5346.623624	9554.690424	8906.48972	9520.603045	
66108.07431	69941.79607	69965.72887	3498.324309	2941.346145	2938.081527	46444.24397	53845.50259	51981.47059	
142727.5658	141983.5119	134531.8931	125871.5309	116934.3583	119650.939	165437.5446	160053.8201	168458.9387	
22803.15751	24866.72903	26218.02693	35.77961034	452.9274363	339.0385647	15614.73773	16367.09299	16587.34585	
9190.492624	8244.015948	8456.887033	8247.989996	7928.451842	7765.897548	11043.26249	9903.65278	11908.20378	
2383.750039	2173.601032	2570.693794	1333.278732	1587.379832	1896.521342	2265.781994	1570.236613	2178.062411	
18787.26063	15315.94921	15888.14657	16870.97775	15095.25531	16572.98765	20282.1763	15749.4477	20853.07508	
365.2616752	1022.646235	1137.753375	2351.621991	1604.150082	1898.62515	537.63905	955.7387339	736.2015203	
795.395428	1355.403944	1530.349845	1944.695707	1171.980147	1228.399278	1730.322138	1370.072346	1087.454396	
548.1519214	584.7033098	398.2959855	634.7343605	326.3594355	132.2269497	744.8369164	290.7192041	622.0204404	
432.2977249	804.0552102	0.001403199	953.0992564	1417.15331	1066.959025	417.9817909	385.9368781	984.6020959	
7669.384	8133.459849	8830.236888	281.3220133	0.001403199	0.001403199	5852.44795	6563.978201	5273.84232	
6355.952877	5878.378587	4883.837956	4994.662771	3711.871288	3851.996	5328.052293	5365.444902	5975.064711	
7204.550677	5979.198831	5854.134373	7448.570529	5915.22566	6986.776546	8045.432896	8640.334976	6721.754361	
10911.83166	10939.47966	12166.60038	197.9581181	315.6811656	315.4231182	10399.19018	12067.17694	9581.211166	
8330.836313	7186.97388	4993.201773	2530.567975	2510.214358	2286.738716	5081.642602	6250.992805	4936.953759	
11506.94416	10175.37133	10200.7074	26125.65042	25490.13785	23413.00645	14234.52006	10801.18743	11888.16924	
48043.3864	48308.9836	42893.97791	49913.2105	46063.70049	47998.39739	61246.86083	52554.39807	58367.58178	
3022.267577	3127.870466	2974.28446	0.001403199	0.001403199	426.6261164	3287.399665	3026.533447	2849.790275	
9447.576807	7407.486261	4677.425128	8396.218263	7435.102148	8944.351583	10549.81836	7105.709423	9306.396617	
31725.88568	29048.13848	26872.371	32113.36046	32185.15058	33100.77219	40070.86865	35704.86523	40595.03847	
2561.759976	1528.272018	2836.419778	3310.205503	3210.121057	3027.474129	4125.396574	3386.1093	4220.394047	
7277.480388	10045.87528	8081.878541	3462.871922	2914.318433	4981.250271	7995.695996	9444.334509	9602.297536	
18930.99897	18424.45174	18494.55296	24290.39703	22070.14143	22776.88119	25319.99516	21396.78695	25270.78822	
2206.089426	3166.005077	2281.006298	2235.605381	2420.200444	1068.253705	2931.982085	2031.492676	4659.84761	
3561.711362	2541.451096	942.168918	2963.338899	3326.504591	3853.306816	3811.744523	1786.068512	3830.076058	
13860.25022	10375.77568	11973.05977	14693.40948	16565.97243	16520.86746	18822.15351	12938.99107	17244.07141	
4390.451781	5994.945484	6980.540998	2219.102784	4076.284837	3451.486089	5349.743664	5526.177353	5781.913151	
23850.90656	22837.78251	19980.81793	14060.64383	11705.06241	14425.77322	26577.60292	24377.84904	25088.79935	
1354.97511	904.7946051	2143.645755	581.8010977	783.5117322	1116.852302	2371.319413	1803.211475	2478.736118	
9297.104881	9024.388077	5118.463569	12829.20346	11404.24826	11663.09789	13429.52596	9098.94869	9710.18182	
12360.55831	10663.50071	12235.22355	12106.0533	10512.98329	11774.41514	17503.53031	16403.95117	16803.84318	
25501.08253	34998.11481	35560.82911	11070.8564	6074.137838	8304.903262	26114.82803	39023.55835	44451.64006	
4769.001119	3040.807288	2641.868781	7198.193342	6697.476459	6997.998418	6997.956066	4096.089773	3986.361867	
9635.864723	9077.917301	6972.430726	6732.911741	5672.340443	7863.454856	8847.508651	10230.16478	13892.29689	
8798.830781	11497.00572	10243.42745	3249.949726	3121.426358	2454.906495	7172.101733	12948.97605	10822.1535	
795.3479912	2788.333434	579.453353	3313.086597	4138.267567	2368.41892	2858.532932	949.1228943	1266.368242	
5688.036711	5349.612224	5064.943665	6242.585821	5570.330203	5345.066074	6153.73615	4446.054681	8245.531674	
4789.54518	5990.068005	6156.777342	2869.890611	2382.619288	1476.207283	7384.047782	6494.816406	9639.934139	
1346.557099	1625.364265	1578.753178	673.6826271	896.8191455	742.6309767	1112.285903	1023.777085	1663.040413	
204.3460216	77.36562671	51.11384823	1209.308108	634.3767823	656.2810224	486.2466509	400.3932018	526.4589937	
772.0226201	804.534082	847.4459745	1324.335783	1428.926757	1184.944953	312.321951	626.4905682	593.5458501	
15614.43223	17406.33691	17785.76517	5843.982026	5762.226962	5022.705106	12520.80683	14618.76646	12878.61215	
1307.538642	1199.57161	1223.749528	995.1326472	686.3858692	722.2837361	1197.990454	1109.10886	1565.04527	
2704.925429	2664.859105	2656.251339	2326.716335	2820.611886	2049.499272	2470.081056	3189.624983	3400.899794	
5254.021475	4950.627267	5609.150231	3468.659484	3133.789028	3555.63501	4832.785529	4787.500876	5175.12268	
3128.469339	2463.361087	2748.981179	2464.872277	2512.992177	2062.883048	3347.718864	2906.22709	3372.291708	
1115.280533	944.457553	691.56112	1387.232832	1069.44245	847.8527177	1483.870536	1285.231583	1594.228009	
2196.767887	1593.390761	1638.605272	0.001403199	0.001403199	0.001403199	114.8824699	2003.177246	955.7789134	
4161.533754	3621.130897	3956.519304	822.8543099	580.9829704	869.5303676	2285.941088	2209.970703	3049.751563	
9143.793193	11018.30994	11707.54743	2975.176459	2547.861469	3054.76649	6576.391101	9964.512315	8823.125379	
2972.897738	2428.296718	2323.559737	3009.577279	2614.711339	2841.308277	3352.574681	2816.537819	3210.821288	
1325.885888	1412.748048	1015.656824	819.4303656	724.6230564	608.7805062	892.6055419	1200.448154	974.143218	
106933.7228	130101.2254	125679.877	41358.89583	34232.13336	34825.58559	93751.4078	110311.9943	107588.0467	

4.41_515.0661m/z	515.0660808	4.41115	neg
4.41_522.1025m/z	522.1024722	4.41115	neg
4.41_534.9790m/z	534.9790398	4.41115	neg
4.41_552.0443m/z	552.0443071	4.41115	neg
4.41_580.1315m/z	580.1314726	4.41115	neg
4.41_590.0901m/z	590.0900983	4.41115	neg
4.41_600.1193m/z	600.119341	4.41115	neg
4.41_612.9964m/z	612.9963951	4.41115	neg
4.41_648.1193m/z	648.1192871	4.41115	neg
4.41_658.0774m/z	658.0773828	4.41115	neg
4.41_660.9996m/z	660.9996408	4.41115	neg
4.41_668.1066m/z	668.1066493	4.41115	neg
4.41_736.0939m/z	736.0939028	4.41115	neg
4.41_750.2373m/z	750.2373168	4.41115	neg
4.41_787.0161m/z	787.016097	4.41115	neg
4.41_801.1595m/z	801.1594974	4.41115	neg
4.41_804.0809m/z	804.0808677	4.41115	neg
4.41_818.2252m/z	818.2251857	4.41115	neg
4.41_872.0689m/z	872.0688635	4.41115	neg
4.41_886.2114m/z	886.2113773	4.41115	neg
4.43_186.0294n	371.0444	4.432683333	neg
4.43_200.0661n	399.1275502	4.432683333	neg
4.43_208.0617m/z	208.0617311	4.432683333	neg
4.43_236.0097m/z	236.0096603	4.432683333	neg
4.43_238.0068m/z	238.0068128	4.432683333	neg
4.43_247.0646m/z	247.0646303	4.432683333	neg
4.43_262.0137m/z	262.0136955	4.432683333	neg
4.43_276.0492m/z	276.049179	4.432683333	neg
4.43_278.9829n	323.9810009	4.432683333	neg
4.43_290.0283m/z	290.0283163	4.432683333	neg
4.43_290.0648m/z	290.064774	4.432683333	neg
4.43_296.5092m/z	296.5092476	4.432683333	neg
4.43_298.0008m/z	298.0007956	4.432683333	neg
4.43_299.0151m/z	299.0150545	4.432683333	neg
4.43_301.0004m/z	301.0004149	4.432683333	neg
4.43_303.9972m/z	303.9971883	4.432683333	neg
4.43_305.9943m/z	305.9943036	4.432683333	neg
4.43_314.0260m/z	314.0260154	4.432683333	neg
4.43_317.9902m/z	317.9902196	4.432683333	neg
4.43_318.0654m/z	318.0654134	4.432683333	neg
4.43_320.1176m/z	320.1175709	4.432683333	neg
4.43_331.0163m/z	331.0162918	4.432683333	neg
4.43_371.9846m/z	371.9846234	4.432683333	neg
4.43_373.9816m/z	373.9816377	4.432683333	neg
4.43_379.1508m/z	379.150802	4.432683333	neg
4.43_382.0135m/z	382.0134668	4.432683333	neg
4.43_391.9689m/z	391.9689048	4.432683333	neg
4.43_394.0299m/z	394.0298734	4.432683333	neg
4.43_403.0215m/z	403.0215083	4.432683333	neg
4.43_407.0418m/z	407.0418539	4.432683333	neg
4.43_413.9508m/z	413.9507668	4.432683333	neg
4.43_434.0531m/z	434.0530565	4.432683333	neg
4.43_439.9721m/z	439.972054	4.432683333	neg
4.43_450.0010m/z	450.0009606	4.432683333	neg
4.43_466.9913m/z	466.9913176	4.432683333	neg
4.43_467.1149m/z	467.1148577	4.432683333	neg
4.43_505.0375m/z	505.0375094	4.432683333	neg
4.43_507.9595m/z	507.9595423	4.432683333	neg
4.43_517.9884m/z	517.9884442	4.432683333	neg
4.43_527.9433m/z	527.9433369	4.432683333	neg
4.43_573.0248m/z	573.0247664	4.432683333	neg
4.43_575.9473m/z	575.9472843	4.432683333	neg
4.43_583.0535m/z	583.0534773	4.432683333	neg
4.43_585.9759m/z	585.9758983	4.432683333	neg
4.43_600.1681m/z	600.1681032	4.432683333	neg
4.43_602.9663m/z	602.966279	4.432683333	neg
4.43_603.0899m/z	603.0898907	4.432683333	neg
4.43_651.0414m/z	651.0414433	4.432683333	neg
4.43_653.9637m/z	653.9636809	4.432683333	neg
4.43_711.9219m/z	711.9218571	4.432683333	neg
4.43_719.0289m/z	719.028903	4.432683333	neg
4.43_721.9507m/z	721.9507136	4.432683333	neg
4.43_789.9381m/z	789.9381189	4.432683333	neg
4.43_857.9240m/z	857.923959	4.432683333	neg
4.45_173.0933m/z	173.0932825	4.454616667	neg
4.45_235.0168m/z	235.0167992	4.454616667	neg
4.45_246.0807m/z	246.0806606	4.454616667	neg
4.45_262.5154m/z	262.5153566	4.454616667	neg
4.45_275.0036m/z	275.0035506	4.454616667	neg
4.45_290.9714m/z	290.9714334	4.454616667	neg
4.45_296.0075m/z	296.00752	4.454616667	neg
4.45_307.5002m/z	307.500214	4.454616667	neg
4.45_314.0682m/z	314.0681793	4.454616667	neg
4.45_401.0550m/z	401.0550449	4.454616667	neg
4.45_417.1405m/z	417.1404841	4.454616667	neg
4.45_436.9750m/z	436.9750149	4.454616667	neg
4.45_444.2069m/z	444.2068725	4.454616667	neg
4.45_445.2086m/z	445.208637	4.454616667	neg
4.45_455.1564m/z	455.1563851	4.454616667	neg
4.48_167.0350m/z	167.0350264	4.477166667	neg
4.48_242.0131m/z	242.0131046	4.477166667	neg
4.48_243.0813m/z	243.0812943	4.477166667	neg
4.48_306.1020m/z	306.1019886	4.477166667	neg
4.48_376.1336m/z	376.1335882	4.477166667	neg
4.48_460.8834m/z	460.8833685	4.477166667	neg
4.48_649.0452m/z	649.0451964	4.477166667	neg
4.50_248.0963m/z	248.0963499	4.49925	neg
4.50_260.0963m/z	260.0963114	4.49925	neg
4.50_277.0695m/z	277.0695085	4.49925	neg
4.50_283.0880n	328.0840399	4.49925	neg
4.50_379.0996m/z	379.0995712	4.49925	neg
4.50_393.1418m/z	393.1417966	4.49925	neg
4.50_415.9648m/z	415.9647676	4.49925	neg
4.50_445.1717m/z	445.1716762	4.49925	neg
4.50_452.0588m/z	452.0588348	4.49925	neg
4.50_482.9338m/z	482.9337865	4.49925	neg
4.50_483.9524m/z	483.9523663	4.49925	neg
4.50_520.0466m/z	520.0465939	4.49925	neg
4.50_603.0043m/z	603.0043066	4.49925	neg
4.50_704.8157m/z	704.8157163	4.49925	neg

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8598.392463	8491.006188	10290.83549	3003.757078	3572.186571	3030.301638	8007.722532	7579.095935	6881.247228
3263.031964	3099.182827	2627.472531	2910.784711	2448.343444	2821.576662	3113.127313	1813.534152	3407.875163
4285.111323	3672.059561	3610.725065	5417.060517	3962.592197	4592.222822	6476.480464	3585.893263	6003.50593
7065.735982	7240.315514	8909.831833	812.1299322	0.001403199	340.6292197	2357.374543	4348.253403	3564.100652
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27853.06381	31539.97658	31823.96715	14836.41117	11220.91006	12139.57297	27369.86675	25850.84363	30897.07315
3430.584817	3153.383225	1828.162595	2107.251431	2215.570458	2606.585846	3055.995412	2578.411974	3392.923761
5116.184977	5125.955123	5737.553349	322.8488472	537.6141588	0.001403199	1340.240716	1997.338501	2272.876717
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3903.641639	2127.964489	3058.253232	6392.157452	4196.532623	6747.490786	7347.173782	4296.242162	4190.721978
16723.61459	15577.88656	19877.20386	9728.997122	7946.980314	9240.08036	15405.25948	17208.34311	17058.77362
10572.0055	9665.681616	12886.77063	7022.112321	5743.482919	5917.506402	9446.839705	9288.268461	11920.88308
18730.10006	19791.99516	22143.06855	4280.186133	2449.60895	3997.728262	17429.32396	17482.39374	19364.87827
3673.753709	5319.943717	4732.588577	1111.614798	1069.151843	855.4310751	2647.141395	3044.398071	2611.165994
6174.935252	6033.929469	5767.958752	1157.132646	732.0479273	1188.564413	4187.093165	1750.705688	3419.307626
7187.456709	5485.333162	10001.61273	3509.426318	4534.048067	3917.910238	8050.384761	5562.963165	6434.077842
8150.00925	9341.056739	10052.64234	3101.830549	1991.164407	1576.996415	9876.002717	9978.622484	9240.170992
5813.651486	2475.908204	5034.394516	2346.396965	1749.954542	2515.547015	5924.245776	4070.906124	4356.108079
9431.218057	4692.596243	7827.763205	1956.630007	1050.499771	0.001403199	6676.063752	5773.190674	7225.398991
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4127.550251	3528.452248	3462.952415	1917.458512	1582.113827	1666.813944	2985.570845	3154.366328	3199.340927
1917.067088	1600.757977	1394.334535	793.3848824	803.376656	825.9174518	1249.449165	1583.130109	1609.737945
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275.1470053	542.7391736	603.3915355	0.001403199	0.001403199	0.001403199	390.103191	154.5754414	349.0029987
4690.130155	5870.398685	5895.808201	1056.875033	834.1613751	902.1255624	4863.052988	6015.098217	5036.938391
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2389.216521	1877.820975	1713.703827	2029.86722	1365.709282	1981.642359	2497.373341	1573.329243	1749.878586
1432.190724	2175.363461	1481.2021	2106.092299	2058.505687	1693.85322	1285.219655	2001.154354	2020.180603
53618.43462	51166.13687	49405.11396	31288.63838	29625.15045	30846.91213	47359.84398	42178.99853	43667.94545
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385.2788053	430.8529718	398.7876281	175.297529	131.2799979	172.5062113	354.2132484	407.4939333	390.9585985
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85.47554317	56.03616538	59.46255014	649.9155505	701.7207209	569.1458104	1273.749119	1160.650673	1200.098232
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266.8777569	258.8697748	283.5442296	47.14563956	0.001403199	76.66206072	25.63718287	294.1724439	269.9387063
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263.980372	413.2498897	305.8579679	391.0968858	452.9557251	693.2463969	274.0765531	304.3977687	455.2410624
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601.6948159	826.3307227	832.3973767	1008.926996	693.9362509	811.3972705	468.2053194	800.1852423	893.2922264
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3162.96041	3524.455254	2829.822536	4274.146997	4117.967909	4619.922521	4158.466327	3720.888511	4247.863527
1748.213822	1977.439608	1684.285787	0.001403199	0.001403199	0.001403199	1610.589054	1639.899794	1621.086461
482.3989557	438.5409971	516.0442084	1319.611095	1113.297866	1284.171314	1366.837878	1452.344116	1089.469537
1026.171436	144.7698857	4027.432987	339.1938781	129.254194	244.1893044	300.4557936	0.001403199	472.3410224
1293.035476	1681.777758	925.2298756	1341.129149	1498.847267	1212.794605	2044.169264	1728.571204	2038.223337

4.50_717.0323m/z	717.0322945	4.49925	neg
4.52_138.0278m/z	138.0278106	4.521733333	neg
4.52_163.0765m/z	163.0765383	4.521733333	neg
4.52_194.0515m/z	194.0515435	4.521733333	neg
4.52_213.9640m/z	213.9640324	4.521733333	neg
4.52_239.0540m/z	239.0540358	4.521733333	neg
4.52_247.0201m/z	247.0201449	4.521733333	neg
4.52_259.5300m/z	259.5300285	4.521733333	neg
4.52_271.1554m/z	271.1553874	4.521733333	neg
4.52_276.1277m/z	276.1276678	4.521733333	neg
4.52_278.1070m/z	278.1070002	4.521733333	neg
4.52_281.9858m/z	281.9858035	4.521733333	neg
4.52_285.1710m/z	285.1709754	4.521733333	neg
4.52_298.1097m/z	298.1096651	4.521733333	neg
4.52_300.1452m/z	300.1452135	4.521733333	neg
4.52_307.5678m/z	307.5677975	4.521733333	neg
4.52_308.0730m/z	308.0730229	4.521733333	neg
4.52_309.0725m/z	309.0724554	4.521733333	neg
4.52_329.0234m/z	329.0234302	4.521733333	neg
4.52_348.9774m/z	348.9773675	4.521733333	neg
4.52_355.0108m/z	355.0108448	4.521733333	neg
4.52_376.9930m/z	376.9930012	4.521733333	neg
4.52_377.0599m/z	377.059889	4.521733333	neg
4.52_397.0108m/z	397.010828	4.521733333	neg
4.52_400.0487n	399.0414102	4.521733333	neg
4.52_411.8814m/z	411.8814368	4.521733333	neg
4.52_444.9807m/z	444.9806942	4.521733333	neg
4.52_464.9982m/z	464.9981781	4.521733333	neg
4.52_477.0541m/z	477.0541487	4.521733333	neg
4.52_501.1982m/z	501.1982275	4.521733333	neg
4.52_512.9678m/z	512.9678395	4.521733333	neg
4.52_535.0167m/z	535.0167183	4.521733333	neg
4.52_670.9922m/z	670.9921964	4.521733333	neg
4.54_257.0492m/z	257.0492479	4.54425	neg
4.54_275.0599m/z	275.0598724	4.54425	neg
4.54_308.0742n	615.1397549	4.54425	neg
4.54_318.1383m/z	318.1382895	4.54425	neg
4.54_344.9821m/z	344.9820828	4.54425	neg
4.54_375.0655m/z	375.0655445	4.54425	neg
4.54_386.0471m/z	386.0471	4.54425	neg
4.54_393.0500m/z	393.0499646	4.54425	neg
4.54_428.0958m/z	428.0958207	4.54425	neg
4.54_451.0322m/z	451.0321784	4.54425	neg
4.54_454.0347m/z	454.0346695	4.54425	neg
4.54_565.0580m/z	565.0580238	4.54425	neg
4.54_587.0076m/z	587.0075769	4.54425	neg
4.57_122.0374m/z	122.0373941	4.5668	neg
4.57_248.8872m/z	248.8871797	4.5668	neg
4.57_285.0960m/z	285.0959582	4.5668	neg
4.57_304.1225m/z	304.1225664	4.5668	neg
4.57_355.0031m/z	355.0031361	4.5668	neg
4.57_360.0735m/z	360.0734874	4.5668	neg
4.57_370.1024m/z	370.10244	4.5668	neg
4.57_372.8914m/z	372.8913691	4.5668	neg
4.57_385.0130m/z	385.013018	4.5668	neg
4.57_393.0916n	438.0898519	4.5668	neg
4.57_453.0009m/z	453.0009047	4.5668	neg
4.57_459.2111n	458.2027463	4.5668	neg
4.57_506.0772m/z	506.0771905	4.5668	neg
4.57_520.9878m/z	520.9878078	4.5668	neg
4.57_526.1898m/z	526.1898282	4.5668	neg
4.57_558.9652m/z	558.9652237	4.5668	neg
4.57_588.9757m/z	588.9757149	4.5668	neg
4.57_626.9527m/z	626.9527254	4.5668	neg
4.57_656.9628m/z	656.9627886	4.5668	neg
4.57_694.9409m/z	694.9409157	4.5668	neg
4.57_724.9502m/z	724.9502425	4.5668	neg
4.59_182.0944n	181.0871606	4.589283333	neg
4.59_186.0854m/z	186.08538	4.589283333	neg
4.59_226.9662m/z	226.9662391	4.589283333	neg
4.59_252.0206m/z	252.0205504	4.589283333	neg
4.59_270.1043m/z	270.1043385	4.589283333	neg
4.59_270.5129m/z	270.5128682	4.589283333	neg
4.59_271.0186n	541.0309032	4.589283333	neg
4.59_332.1168m/z	332.1167918	4.589283333	neg
4.59_343.8940m/z	343.8939906	4.589283333	neg
4.59_358.0164m/z	358.0163532	4.589283333	neg
4.59_405.0763m/z	405.0762976	4.589283333	neg
4.59_416.1390m/z	416.1390109	4.589283333	neg
4.59_473.0639m/z	473.0638776	4.589283333	neg
4.59_541.0509m/z	541.0508729	4.589283333	neg
4.59_599.1085m/z	599.1085104	4.589283333	neg
4.61_194.0389m/z	194.0388804	4.611883333	neg
4.61_248.0541m/z	248.0541412	4.611883333	neg
4.61_274.1121m/z	274.1120664	4.611883333	neg
4.61_290.0286m/z	290.0285733	4.611883333	neg
4.61_305.1070m/z	305.1069665	4.611883333	neg
4.61_359.0621n	358.0547931	4.611883333	neg
4.61_471.0970m/z	471.0970434	4.611883333	neg
4.61_494.0297m/z	494.0297462	4.611883333	neg
4.61_496.9495m/z	496.9495022	4.611883333	neg
4.61_563.0243n	562.0169898	4.611883333	neg
4.61_579.1153m/z	579.1153367	4.611883333	neg
4.61_588.8249m/z	588.8249468	4.611883333	neg
4.61_601.1242m/z	601.1241735	4.611883333	neg
4.61_603.1588m/z	603.1587592	4.611883333	neg
4.61_630.0047m/z	630.0047361	4.611883333	neg
4.61_647.1036m/z	647.1035838	4.611883333	neg
4.63_174.0853m/z	174.085349	4.632666667	neg
4.63_179.9364m/z	179.9364179	4.632666667	neg
4.63_216.1243m/z	216.1242839	4.632666667	neg
4.63_303.0465m/z	303.0465365	4.632666667	neg
4.63_354.0188m/z	354.0187672	4.632666667	neg
4.63_362.9413m/z	362.9413017	4.632666667	neg
4.63_403.0677m/z	403.0676787	4.632666667	neg
4.63_451.0833m/z	451.0833151	4.632666667	neg
4.63_564.9369m/z	564.9368853	4.632666667	neg
4.63_656.8129m/z	656.8129059	4.632666667	neg
4.63_722.8578m/z	722.8578349	4.632666667	neg
4.64_182.8967m/z	182.89674	4.641416667	neg

518.5968646	880.2910765	724.6955737	2209.619548	2277.176087	2588.07751	1192.723833	891.2654686	917.7128744
67.34341631	53.84373022	80.46870131	36.22483889	0.001403199	13.50638371	11.41001813	38.27100515	20.76087943
102.0605776	174.6599679	175.8727712	86.61845175	169.1871888	140.3844146	221.6502084	235.457478	237.1656323
84.09146539	109.9189505	107.7404621	258.2083271	221.2321651	260.1803816	168.661116	202.5747804	151.1254574
737.0424502	671.6271866	574.0532981	795.6801793	759.4544609	792.7413833	886.2418546	867.9812514	656.2563005
485.6755095	718.858255	535.8515476	795.3425631	824.1173566	793.008917	650.0872933	665.2597508	749.6182642
468.6352322	422.9242423	382.0434089	546.0090769	557.1459374	526.1653365	805.7950787	894.2814865	843.932432
0.001403199	36.08324803	30.72266061	263.6552487	359.4367816	160.8705147	0.001403199	0.001403199	0.001403199
1378.975348	1625.91894	1611.832586	1387.124217	1247.563714	1258.3111	1228.401251	1274.875748	1435.819142
637.4689396	665.7595044	672.5170141	1028.400622	1113.817992	968.1481153	689.1747936	878.8663561	836.4970175
2913.76764	3077.156265	3448.134895	3319.428251	3360.522892	2954.364319	2469.653957	2391.498114	2751.496386
187.7098418	207.0616407	113.4096981	0.001403199	0.001403199	0.001403199	149.0977322	231.8502312	195.623981
401.1475289	365.5176476	357.7673689	307.8465126	262.6584734	335.389554	169.1987747	104.482975	172.0700692
640.6256035	865.5362212	726.449937	1222.383827	1058.448529	966.6397056	821.9033639	836.4041324	1040.650798
974.0479372	916.3293742	1058.926635	673.3607597	740.4835624	792.3330088	1147.274793	1308.344096	1367.942457
51.24793889	199.0597469	144.1112306	0.001403199	72.93212119	0.001403199	0.001403199	63.37313652	55.11212031
316.8820176	224.9247777	225.9057521	150.5436888	221.4299162	175.9792389	194.183541	241.7068571	243.48602
22706.46006	9468.633426	63866.81405	9385.922316	8707.334504	8876.144137	12415.18257	12932.78603	17611.41796
1026.357853	1114.886735	1042.859027	2473.474088	2151.229795	2210.765192	1548.831102	1760.088713	1990.66391
679.2092846	1004.841287	864.1814916	1225.707711	981.8603705	1077.042919	926.1452006	979.8474526	1120.72075
6751.92055	7488.173479	7573.276109	4610.495134	4378.082014	4495.202945	12167.79265	13915.61394	13328.36936
3402.168641	3612.046949	3466.32167	2259.148335	2464.455713	2394.288457	7034.614905	7521.858062	7768.818528
7400.990313	1055.570447	24018.35419	1680.031828	1552.825776	1298.211221	1373.455622	1460.782231	3770.226166
742.8221263	744.2918858	388.6724677	1713.787568	1807.732609	1455.605082	872.4166036	1060.792664	1378.68023
4803.293697	820.3043239	16946.29963	1096.77467	694.0694602	786.9075302	1010.910401	1055.616651	2725.926809
6171.307802	5311.97976	3775.841807	4012.561217	3887.982365	4139.310271	5716.947784	4567.666029	5018.687493
2477.52149	2642.059575	2737.964832	1976.144809	1739.442172	1797.187639	5511.63045	5382.653168	5572.438608
352.4380835	401.6811415	319.722718	1073.230854	1144.022251	1115.910361	701.0827965	889.0939424	863.3317889
755.3878364	1184.288284	776.5165101	1002.106971	853.6690953	843.3049017	1019.772372	1158.964817	972.3220726
1584.437147	1826.279994	1909.901395	639.8875162	543.3394043	679.8249569	1252.041802	1174.822272	1312.938239
1596.324158	1548.023033	1517.682658	1066.882586	969.5375222	931.6879039	2801.275183	3011.979647	3402.343953
1596.070876	301.9905144	6437.774613	376.8559894	234.8600306	293.7974041	381.0897653	204.5172806	889.6956574
563.1020847	0.001403199	1613.347399	123.0103948	0.001403199	157.3354775	0.001403199	192.5744365	236.0093173
448.9280586	508.8553259	484.7876551	164.0732463	225.062101	184.1909335	439.513324	398.4055436	372.3015628
1368.451031	1526.214835	1462.837447	587.0723278	521.8297151	586.6371453	831.3787438	1236.169764	1062.501925
3423.333549	4406.527137	4812.99387	1870.535701	1990.989049	1854.105614	2349.107957	2759.954764	2945.736507
291.6182507	344.6999493	283.9811158	149.2135462	228.9001416	303.989987	202.2861756	261.878899	296.2402042
530.4074798	504.4171625	418.5863189	297.3528636	434.9764979	367.3071682	948.2975188	1120.120609	1108.437268
448.0776609	526.8407896	262.2688676	414.4516352	559.821111	536.255966	749.742922	582.2446872	834.7936853
2253.463357	2214.806914	2210.510747	1514.065236	1498.931616	1331.335641	1225.898726	1676.004257	1583.951056
2572.136135	3584.53237	3502.000797	325.0328245	341.765981	292.5549213	1017.118675	1003.862697	1813.779134
84.03984904	0.001403199	174.5374122	190.7899788	164.943978	158.7867573	0.001403199	112.6113319	125.2297329
9589.366146	10802.05524	10690.37388	6206.540824	5805.496521	6012.279143	7656.295182	7951.726939	8433.296047
1203.156818	1128.584265	1190.241851	937.2619161	978.3770474	1181.187345	528.3460642	830.4132156	773.5771072
76.5831903	328.8997853	269.1244573	154.0536466	1590.639526	1210.169211	89.66018444	0.001403199	0.001403199
1380.97297	1700.073828	1554.757066	740.6610114	774.8809587	700.8401537	692.1618533	1150.033475	1253.320569
83.92013393	43.41128629	58.50845263	58.68892181	44.2613539	49.46932673	12.7342046	38.17745408	34.52120848
951.2145475	772.4896875	558.7187513	578.2224299	667.2417093	686.436954	997.7202198	697.5950762	872.9942291
511.5358239	454.7860527	400.6512645	753.7850753	648.208098	587.0244232	505.8193296	552.316992	502.694659
711.7638736	983.2197949	866.9027843	806.6981098	633.5262694	687.7997088	885.1361627	949.5018026	1105.879411
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114.3156563	189.0812254	94.15170288	456.3835241	470.2621792	370.5587304	143.5554696	201.7611465	220.4822876
2139.629654	1837.490526	1531.844437	4475.93145	4265.580614	3965.825352	1840.224928	2380.298348	2291.782078
812.6529117	699.2759781	500.6121512	681.6696775	865.3369262	688.518311	975.5988772	832.6414337	1175.554547
2312.544263	2280.601265	2159.248645	1494.957251	2655.344647	2698.532702	1944.363803	2197.258863	1913.499015
1319.823144	1533.961921	1459.072921	2658.406421	2504.579244	2470.83955	1661.117324	1925.231436	1805.49153
2303.464765	2719.599827	2592.297262	2447.445274	3248.671043	2752.857155	2408.610517	2161.877129	1832.553902
2711.31476	2622.982786	2739.629901	4229.353998	4231.216618	3546.341039	3573.43438	3552.117431	3558.528852
615.3730555	894.6036131	827.3332072	1885.764554	1705.210113	1173.69991	903.838391	1311.755983	780.1605342
1907.868274	1856.393131	1920.066583	2139.176555	2226.974398	2194.270261	1860.906088	1794.130954	1815.106161
857.0444416	1057.780878	945.0538947	1410.245781	1060.644158	1282.597893	1423.3608	1375.638144	1396.647754
2814.514406	2625.930573	2277.007579	1055.887513	1044.975928	1115.816896	1943.200928	1562.674835	1674.971759
2040.289871	1711.415931	1808.778323	1929.840504	2003.144631	2186.064211	1596.44066	1656.791308	1826.75449
1719.922324	2133.962793	1609.287386	849.325279	744.6299462	776.4763109	1498.420306	1554.11541	1264.174269
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1756.449651	1782.942424	1422.892629	810.1867064	571.7658168	621.8969591	948.8814378	1038.681554	1338.826454
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137.7934304	108.8271503	78.02149091	93.70668208	159.7401042	106.1829455	91.26227863	79.99818222	64.82821135
707.8050721	795.9546687	573.3507483	792.7599857	783.5677146	768.4781672	902.2113345	815.712416	953.3234597
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1155.943603	2617.585927	2726.283884	1589.877288	1320.8.10251	12448.23068	1522.215387	950.3934512	4554.405304
2374.228731	3415.217267	3468.128414	3399.776744	3386.277258	3139.867627	2404.299715	3195.895429	3597.60083
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646.5613066	572.8585403	544.8012306	420.6095892	432.6438057	431.7609822	756.8787303	559.319232	708.9215742
5589.21548	5692.695673	5078.277231	6223.25998	6659.13884	5163.848317	5433.789261	5606.276104	6175.141636
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3732.319253	3080.62468	2728.752806	4201.464944	4548.559019	4206.502578	4146.087634	3494.811357	4390.261084
2228.644387	1980.680956	2305.619898	2720.318991	2565.330749	2124.481533	2386.176629	2541.279631	2700.434404
196.6099361	471.2469221	746.2961602	952.5424073	1269.692027	747.6731791	0.001403199	0.001403199	0.001403199
56.59236249	79.59580027	56.60728968	150.9460783	147.6985556	140.1327043	95.5735927	136.0461546	158.1099419
825.3112574	845.377069	756.9376368	987.1165134	1078.732695	1255.141522	165.0402946	799.0732958	918.4820002
102.7711008	77.35478179	168.8387753	651.8354983	457.685432	259.7398326	523.7722226	391.1033914	565.6629248
1447.979936	1432.096904	1516.222043	1324.501292	1356.316028	1055.172258	1923.729243	1464.539045	1977.586011
576.922204	597.4672633	550.6067353	348.1148546	225.4362697	215.9383092	322.7512625	429.3795252	444.6201654
13220.26605	13009.03446	12624.97825	20353.54666	20827.48814	18231.61886	16090.60612	13130.17644	19232.22064
2053.248272	2181.487595	2177.214939	1587.402227	1407.265594	851.0936052	2134.861803	1867.943999	2677.041142
3701.312996	3415.55315	3046.754131	6019.911239	5972.590286	4851.949881	4600.076135	3625.793271	4937.350894
2593.811523	2132.843628	1989.912031	2859.161983	2686.792849	2959.773643	3498.590041	2541.68934	2691.600471
2362.448038	2435.040833	2260.384422	6688.735348	6626.968881	6145.605746	2972.915458	2851.01526	3287.111872
2241.16652	2443.120627	2624.223284	0.001403199	0.001403199	0.001403199	1554.302307	1430.6965	1620.04576
3559.892048	2386.638952	2507.533942	2872.665227	2613.082816	3554.041017	4238.309962	2924.58709	2296.64141
1646.999543	1840.32602	1792.457466	1717.427971	1562.212161	1332.336531	1288.235032	1212.172853	1045.579521
5812.160324	5517.102247	5699.634014	4083.054155	3824.462612	3562.949642	5616.294539	4903.816814	6439.878501
636.6384443	701.3307478	786.3088146	1654.147866	1963.974399	1719.754989	966.0121501	858.3241425	1355.671775
308.7154861	436.9887622	542.2080607	0.001403199	0.001403199	0.001403199	381.0239312	161.3834763	0.001403199
43.98355949	69.61425659	33.99975163	52.99207147	88.49044946	64.12464302	110.3420119	57.98405853	89.13605415
972.9126921	923.092096	728.5222008	935.8433593	866.3035431	1052.5291	1141.993488	873.1791251	1058.919749
214.294598	314.272155	278.044148	553.3402196	525.2216673	496.2854318	338.9279144	234.5170403	202.8501933
1008.480912	878.9835314	815.6099479	1024.72152	817.7566492	850.2209337	1217.531979	1088.528977	1171.11519
592.9258868	587.1079425	445.4084005	0.001403199	0.001403199	0.001403199	47.6822219	0.001403199	81.41297366
2791.942973	2149.136684	2068.215279	2430.042204	2846.674385	2716.237671	3439.857561	2638.491102	2998.528385
2311.215869	1602.917365	1999.586991	2171.271869	2413.927062	2947.652171	8887.165463	8481.124946	4646.620658
836.6666078	813.2177359	596.2274054	1462.032107	1475.143976	1257.01653	1343.549412	1187.469039	1106.652056
1903.969137	1252.198585	995.1695427	2034.212494	1681.848595	1671.317801	2307.534875	1907.415298	2193.596825
1741.452881	1685.489319	1514.027261	1619.722781	1333.160375	1838.502454	1872.639268	1103.781384	1207.345625
2079.124933	1591.168495	2238.847981	2803.933704	2670.688256	3153.451429	3335.011392	2379.46986	2860.283522
1938.353234	1431.186499	1270.82025	1292.455633	1240.577491	1230.21904	1641.622683	1150.700248	1554.950842

4.64_259.0282m/z	259.028164	4.641416667	neg											
4.64_299.9718m/z	299.9717757	4.641416667	neg											
4.64_300.9745m/z	300.9744593	4.641416667	neg											
4.64_310.0006m/z	310.0006119	4.641416667	neg											
4.64_330.0209m/z	330.0209142	4.641416667	neg											
4.64_331.9228m/z	331.9228132	4.641416667	neg											
4.64_339.0158m/z	339.0158008	4.641416667	neg											
4.64_342.0832m/z	342.0832018	4.641416667	neg											
4.64_391.2241m/z	391.2241073	4.641416667	neg											
4.64_545.8538m/z	545.8537617	4.641416667	neg											
4.64_560.1873n	559.1800708	4.641416667	neg											
4.64_570.8375m/z	570.8374811	4.641416667	neg											
4.64_589.1534m/z	589.153381	4.641416667	neg											
4.64_654.8700m/z	654.8699642	4.641416667	neg											
4.66_113.0196m/z	113.0196356	4.660483333	neg											
4.66_238.0702m/z	238.0702298	4.660483333	neg											
4.66_244.1272m/z	244.1272473	4.660483333	neg											
4.66_263.9352m/z	263.9351635	4.660483333	neg											
4.66_271.1167m/z	271.1166949	4.660483333	neg											
4.66_318.8723m/z	318.8723224	4.660483333	neg											
4.66_339.0594m/z	339.0594479	4.660483333	neg											
4.66_366.0784m/z	366.0783528	4.660483333	neg											
4.66_370.0968m/z	370.0968055	4.660483333	neg											
4.66_377.9881m/z	377.9880996	4.660483333	neg											
4.66_406.1802m/z	406.180174	4.660483333	neg											
4.66_417.0759m/z	417.075891	4.660483333	neg											
4.66_430.1356m/z	430.1356189	4.660483333	neg											
4.66_446.9064m/z	446.9063689	4.660483333	neg											
4.66_461.0320m/z	461.0319828	4.660483333	neg											
4.66_519.1507m/z	519.1506542	4.660483333	neg											
4.66_553.0510m/z	553.0509752	4.660483333	neg											
4.66_597.0074m/z	597.0074154	4.660483333	neg											
4.66_621.0385m/z	621.0385471	4.660483333	neg											
4.66_689.0259m/z	689.0259048	4.660483333	neg											
4.68_186.1069m/z	186.106901	4.682483333	neg											
4.68_368.1069m/z	368.1069414	4.682483333	neg											
4.68_395.0597m/z	395.0597313	4.682483333	neg											
4.68_463.0478m/z	463.0478391	4.682483333	neg											
4.68_531.0350m/z	531.0349964	4.682483333	neg											
4.68_955.0216m/z	955.0216011	4.682483333	neg											
4.70_126.8811m/z	126.881056	4.703166667	neg											
4.70_155.0715m/z	155.071477	4.703166667	neg											
4.70_224.0874m/z	224.0873668	4.703166667	neg											
4.70_232.0593m/z	232.0592884	4.703166667	neg											
4.70_239.0539m/z	239.0538613	4.703166667	neg											
4.70_240.0856m/z	240.085559	4.703166667	neg											
4.70_246.1429m/z	246.1428815	4.703166667	neg											
4.70_271.0913m/z	271.0912643	4.703166667	neg											
4.70_276.1275m/z	276.1275176	4.703166667	neg											
4.70_277.0901n	322.0885813	4.703166667	neg											
4.70_278.1435m/z	278.143545	4.703166667	neg											
4.70_280.0205m/z	280.0205163	4.703166667	neg											
4.70_307.1400m/z	307.1399915	4.703166667	neg											
4.70_308.0729m/z	308.0729369	4.703166667	neg											
4.70_314.0568m/z	314.0568769	4.703166667	neg											
4.70_376.0604m/z	376.0604281	4.703166667	neg											
4.70_418.9163m/z	418.9163306	4.703166667	neg											
4.70_444.0479m/z	444.0478779	4.703166667	neg											
4.70_526.0511m/z	526.0511301	4.703166667	neg											
4.70_594.0387m/z	594.0386999	4.703166667	neg											
4.70_662.0262m/z	662.0261627	4.703166667	neg											
4.70_730.0138m/z	730.0137721	4.703166667	neg											
4.70_798.0007m/z	798.0007324	4.703166667	neg											
4.70_954.5193m/z	954.519276	4.703166667	neg											
4.73_187.1170m/z	187.1169811	4.725416667	neg											
4.73_207.9773m/z	207.9772527	4.725416667	neg											
4.73_209.1028n	254.1011233	4.725416667	neg											
4.73_211.0978m/z	211.0977644	4.725416667	neg											
4.73_222.0903m/z	222.090315	4.725416667	neg											
4.73_273.0805m/z	273.0805479	4.725416667	neg											
4.73_320.0737m/z	320.0736736	4.725416667	neg											
4.73_329.0233m/z	329.0232981	4.725416667	neg											
4.73_344.1166m/z	344.1166165	4.725416667	neg											
4.73_368.0812m/z	368.081225	4.725416667	neg											
4.73_369.0259m/z	369.0258742	4.725416667	neg											
4.73_380.0474m/z	380.0474373	4.725416667	neg											
4.73_380.1173n	379.1100618	4.725416667	neg											
4.73_396.1000m/z	396.1000009	4.725416667	neg											
4.73_401.9952m/z	401.9951771	4.725416667	neg											
4.73_444.1875m/z	444.1875444	4.725416667	neg											
4.73_447.0977m/z	447.097749	4.725416667	neg											
4.73_448.0349m/z	448.0348693	4.725416667	neg											
4.73_464.9979m/z	464.997866	4.725416667	neg											
4.73_469.9825m/z	469.982497	4.725416667	neg											
4.73_507.0995m/z	507.0995267	4.725416667	neg											
4.73_516.0224m/z	516.0223511	4.725416667	neg											
4.73_636.1267m/z	636.1267199	4.725416667	neg											
4.73_683.9737m/z	683.9737346	4.725416667	neg											
4.73_704.1138m/z	704.1137552	4.725416667	neg											
4.73_751.9611m/z	751.9610613	4.725416667	neg											
4.73_865.9878m/z	865.9878228	4.725416667	neg											
4.75_138.8602m/z	138.8601952	4.747466667	neg											
4.75_208.0536m/z	208.0535779	4.747466667	neg											
4.75_224.1024n	269.1007768	4.747466667	neg											
4.75_260.0962m/z	260.0962229	4.747466667	neg											
4.75_266.0202m/z	266.0202338	4.747466667	neg											
4.75_276.0490m/z	276.0490087	4.747466667	neg											
4.75_303.0462m/z	303.0462252	4.747466667	neg											
4.75_320.0389m/z	320.0389124	4.747466667	neg											
4.75_320.1538m/z	320.1538293	4.747466667	neg											
4.75_334.0078m/z	334.0077617	4.747466667	neg											
4.75_344.0208m/z	344.0208113	4.747466667	neg											
4.75_349.0800n	697.165786	4.747466667	neg											
4.75_349.1507m/z	349.1506701	4.747466667	neg											
4.75_354.0785m/z	354.0784895	4.747466667	neg											
4.75_366.0020m/z	366.0020429	4.747466667	neg											
4.75_376.2343m/z	376.2343369	4.747466667	neg											
4.75_412.0241m/z	412.0241143	4.747466667	neg											
4.75_414.0648n	395.0469614	4.747466667	neg											
4.75_422.0661m/z	422.0660648	4.747466667	neg											

2245.316092	2229.41648	2769.444141	1971.896188	1829.863093	2185.22157	1273.819316	1708.746975	1434.054022						
83.01760817	101.1300883	90.32744436	281.8183178	145.4402177	231.8735841	231.617976	225.7222381	53.87218239						
553.9229575	514.1455209	592.4319645	700.4526575	627.3972718	792.0651306	680.3876699	539.5596954	708.106665						
2310.082025	2134.905487	1893.495261	3783.306526	3651.812605	3775.727131	3186.556361	3197.913639	2911.234639						
291.4322854	189.1818166	189.6808281	222.8304841	179.6046739	144.9677717	54.26911512	48.38609505	61.8242992						
2721.20495	2330.589656	2443.329015	3074.768503	3160.851667	3464.978547	3833.150262	2444.494958	3231.730008						
764.4830336	720.9738149	834.8876255	0.001403199	0.001403199	0.001403199	3345.881101	3471.179176	2325.693778						
618.5698289	219.4919206	278.437147	1664.642364	1961.628748	1940.706141	833.3443217	599.5868452	264.3909709						
71.73170196	133.2876938	163.1550465	161.7148962	128.0209446	181.2164793	110.4592514	54.89167404	73.70494813						
2538.86834	1707.585441	1666.537065	2253.67062	2811.27903	3027.135781	2513.278472	1949.209568	1814.532604						
4021.455092	3107.834062	4515.976345	3685.680081	4110.811053	3951.180825	684.6416968	1212.16058	677.2914444						
4208.546013	3795.423712	3260.449044	4501.720232	5531.058828	5258.64092	5365.866696	4267.064303	5563.270666						
640.6692148	924.0541032	973.7963829	0.001403199	105.6885872	0.001403199	969.8218392	913.5246368	555.2751532						
2531.2747	2153.940417	1763.926968	2956.696487	3240.358016	3765.974231	3644.016697	3024.652802	2085.591673						
222.1127788	215.3255616	125.00749	245.9651014	259.7289554	355.2972628	362.3923894	325.3238493	266.340561						
546.6881588	443.6538915	589.4934524	697.7359089	501.2328587	548.0825901	577.0329331	712.3414153	484.049315						
199.5504361	217.0229012	187.4082116	402.9787915	538.2739633	459.3969988	176.3746631	187.9202251	328.3882822						
1256.823322	1105.541413	955.1520301	1418.706047	1380.848044	1463.454923	1536.015083	1284.993494	1492.24927						
1061.729823	823.6619549	1141.804449	993.9166479	869.5734418	1053.615677	990.223113	1143.192797	693.9056173						
1433.081288	985.4391744	975.0274508	1199.650825	1052.813503	1139.848312	1478.781445	993.0213824	1135.406388						
795.3870089	608.8662376	686.4404875	1803.887999	1792.82755	1937.040588	1049.978212	1133.653038	672.2537875						
658.1603571	363.3691978	520.1760849	953.3752447	1020.739805	1341.038318	754.9276603	792.916513	615.6452685						
2445.699185	2361.955141	2901.887899	2273.621337	1964.326483	2076.967624	4378.798691	4697.263519	3241.688285						
981.8775771	263.0860362	759.233921	1413.938538	1620.564926	1483.994649	1134.674816	953.7060662	298.5402983						
400.3189676	454.7439385	314.8579597	1308.274347	1140.740842	1472.220798	698.7802918	655.4682939	533.5568275						
4167.666137	3642.34162	4284.229717	9381.468512	10002.59403	5646.611472	5934.143097	4267.870574							
267.6626155	366.0030887	512.1045144	0.001403199	54.4751003	0.001403199	422.3801698	539.7036858	343.1672979						
3955.450811	3007.909336	3383.370647	4716.741932	4708.27917	4706.045389	5020.159529	3689.122971	3827.436545						
3192.624889	3035.984895	2863.071079	4350.887053	4605.684435	4495.797563	5541.497881	4361.257252	3597.853379						
0.001403199	109.0178175	196.8698721	123.6966995	341.2864047	90.99458066	459.9039251	496.9272957	110.2666747						
1916.328031	2151.789031	1888.458609	3041.7	3508.9549	4098.952738	2846.242142	2997.11835	1630.629311						
1233.967702	1614.146581	1126.536818	1332.928768	1491.598538	2170.427453	1531.317319	1719.249402	1602.98846						
1017.454108	1090.101927	1241.508371	2353.166822	2082.238803	2418.307551	1564.914499	1611.013931	942.7009896						
595.1799704	210.3612375	352.3932551	1531.174017	1526.076666	2008.749352	1142.126831	1246.169685	280.9219351						
96.30297141	13.04802984	55.38012222	0.001403199	56.33754606	51.53685791	0.001403199	0.001403199	75.37838539						
270.4761768	238.7339361	318.1216781	113.3359731	8.16189867	0.001403199	93.61978738	0.001403199	0.001403199						
4555.072379	4332.09017	5059.250732	3011.533262	2066.506413	2494.467641	5679.469979	5249.039583	4760.646624						
2139.888443	2350.902759	2926.437462	1750.303846	1004.33792	1329.749696	2748.593781	2314.276818	3324.573373						
1033.977394	1200.74386	1277.715754	747.4191322	130.0170411	524.5764222	1298.016686	1608.233913	1880.627569						
501.9682115	943.1750391	1863.017271	2457.03151	2162.575919	1811.741884	1096.480282	707.0909424	1522.124484						
278.7677435	181.0429184	183.7270755	215.2650254	182.2349571	144.3302223	257.3248875	207.0021171	193.4352992						
726.2787866	556.1858704	641.291762	723.3306117	772.2762017	813.9634131	853.4153054	632.1679612	787.3730463						
164.5020927	139.572828	231.4570192	208.3669719	144.1136164	210.2284753	260.5370374	146.3976269	173.681301						
559.8690403	622.379348	652.7082912	1036.669408	943.1637803	1134.982107	523.2919526	467.9875099	560.5721393						
520.7647442	525.5525154	727.5034231	989.4729047	949.3092585	1114.712268	801.8248414	666.3802602	698.6711509						
4052.113924	4068.873866	4452.952476	5754.749716	5268.517889	5256.556114	6036.207034	6510.751236	6219.305758						
496.7193769	773.1172482	731.0740444	835.6336173	707.7240633	787.0706036	417.1354988	468.5544052	627.7861772						
887.1877414	922.7355333	777.19383	717.9817129	921.2606569	996.9768968	1058.879809	956.2118412	1058.948063						
200.7325918	328.968988	316.2758536	422.7638503	337.2976632	394.8403535	392.3874648	484.133935	268.3862867						
26111.38256	23255.55155	23268.60264	25586.19408	28285.86981	27170.07228	30084.71157	24765.39955	28252.90509						
347.1687308	172.1962197	432.7392633	395.1199223	299.6366928	266.1473279	319.9636658	389.8859352	243.7876227						
728.41731	897.60834	685.3848478	51.11447156	83.68093123	49.43853381	135.5434504	152.8437195	180.5335077						
960.1671096	1100.851154	1105.183496	628.1473777	672.0660182	677.219474	850.3489514	1074.541592	983.5566218						
1236.99662	1551.293742	1308.256083	1898.020548	1599.297824	1480.707132	2038.087434	2192.644062	1910.218477						
905.9130389	644.355812	879.6340767	667.5667655	679.0243087	927.1007857	1022.486868	875.3400393	791.9098763						
1296.500074	1058.870263	1140.387546	1737.316621	1501.260733	1397.723625	1478.923614	1862.992255	1624.516644						
969.7298906	616.1932088	851.9005773	804.5305428	1317.949753	1541.884673	1656.885977	819.7725393	906.7625384						
1062.505742	815.5138816	1237.602826	1189.351097	1099.905174	1097.704452	1593.12799	1107.084396	1188.785695						
8219.10665	7920.359764	7529.034038	9767.44375	9750.928226	10290.36725	11134.12141	8167.762128	9411.008607						
6119.94943	5278.990862	5063.900355	6641.035288	7596.03565	7089.144854	7204.921322	6105.370405	6625.68836						
4221.240007	5041.909147	4430.657916	5133.783192	5433.405711	5500.160967	6153.785882	4339.214553	4988.826691						
3203.481602	3046.19498	3355.583461	4056.272922	4328.094192	3348.986129	4955.609534	3261.933487	5091.116448						
2321.391803	2233.049906	2078.377373	3224.689061	1951.258228	2632.899337	3660.156812	2126.747426	2647.099648						
829.592155	911.3413472	1151.993478	1913.888597	1798.588094	1377.364149	1314.899223	1761.830597	1436.251097						
14405.32539	13041.62249	13158.1517	14034.05	14949.91436	14863.45515	16271.41317	14177.79004	14824.09871						
90.82982286	0.001403199	165.9477315	0.001403199	78.76752431	35.71532737	80.30654329	41.57846069	32.13027109						
57733.50267	54241.81107	53339.51643	57261.35668	62443.04261	62665.39748	66088.99717	57359.87948	59865.22819						
1512.268367	1433.337068	1618.976538	1692.516646	1641.36891	1642.617822	1725.996659	1679.892913	1437.194829						
689.3049837	296.3704495	532.3187551	667.0227218	680.1231734	805.0662199	760.1412748	738.1568493	457.4404767						
388.2985786	143.9475125	327.6925416	517.2152207	715.5295434	423.3405687	389.5607752	405.8677737	98.20742099						
406.9310044	537.320758	496.3929955	554.4477757	931.2918485	649.8108285	677.1887278	541.6044773	748.3515579						
2657.858473	3002.458789	2600.937441	4262.588112	4520.744457	4257.19678	2583.403054	2583.476702	2781.870043						
619.6398995	578.3803898	510.3548015	1202.679142	1007.393851	1028.046412	806.0840298	824.0926285	624.4072677						
5839.740845	6313.860881	6051.574196	7802.930054	7470.410852	7182.73357	8243.538816	8372.57639	7875.862843						
1713.679546	1629.221555	1597.490491	889.3545319	769.1733543	538.8792165	1183.372104	1375.423734	1050.430902						
1839.659075	1098.415844	1431.790398	2001.280471	2143.478387	2011.452075	2192.511304	1616.564298	1900.772157						
8596.156378	8875.647798	8965.738338	16062.87254	15179.41005	15346.09858	9141.512186	10101.05075	9970.36431						
377.0461577	364.7956679	347.1235101	777.6171766	658.1863405	797.271832	461.7654894	469.2962952	384.2168666						
2675.204038	3619.674058	3125.056099	1232.877926	1491.083021	1220.877926	2661.444618	2713.054562	2946.067333						
4045.90253	4620.735243	5364.178308	2707.262214	2524.37173	2978.201302	2834.301858	3314.417764	2687.00043						
3507.69097	3769.019696	3661.285496	7839.524641	7631.706366	7579.685336	3657.973999	4396.790989	3766.540438						
1988.027337	1573.42058	1713.189103	1544.624415	1979.255783	1996.498026	2201.692997	1330.471863	2083.946803						
1426.802011	1240.299263	1618.024215	1849.795282	2004.049944	2038.073763	1174.252559	907.3041496	1058.281428						
2334.226005	2774.812267	2900.106759	2446.745115	645.8743383	1109.27057	2170.744488	2344.928282	2491.98438						
1288.135388	1859.04368	1408.903408	156.5384707	395.8577562	204.9787058	1347.998659	1294.788132	1103.211178						
1375.338273	1369.910338	1240.088802	1654.459398	1906.032967	1451.426193	1937.179799	1417.161922	1330.615007						
1857.947149	2704.886567	2805.400797	707.7258401	767.5875091	941.002521	1277.511051	2023.114593	2547.116423						
3851.046521	4248.736117	3976.446967	1721.9386	2592.513842	2316.436225	3895.344445	3938.703901	4144.913719						
1311.281773	2185.190134	1897.016721	432.1582193	630.0202274	311.5520407	1235.206533	1081.891275	1655.154626						
3562.924049	3641.976487	3521.544319	1801.258068	1710.825425	1512.624979	2450.284788	3076.729507	3955.156968						
1481.614496	487.5902662	1320.613815	1758.038439	2102.600481	1793.209498	1888.439954	1796.963379	1153.777017						
198.6962534	156.4956042	153.692129	262.949793	241.8463477	184.9238748	228.3809039	201.4177945	162.1267542						
118.0196488	170.9220751	98.27256959	99.01813028	123.3046284	119.6157812	137.1581274	59.16941929	90.08611914						
82408.62749	87424.9668	88605.09704	76653.98124	76509.89172	74503.09635	78452.61387	95536.99315	83222.07831						
39.68842954	0.001403199	61.98800385	855.7915555	742.0635529	671.3689455	1077.419784	1083.927622	807.9240131						
6010.642988	5849.467055	6452.039478	2664.346883	2926.147676	2532.592561	5109.00723	6040.312569	5656.014575						
53859.37273	55048.11004	55852.42712	24482.97795	26105.09457	25137.60599	46585.56908	53239.32484	48445.50986						
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879.349436	533.0443604	752.0839511	412.0524498	332.3520998	377.8643556	717.578815	832.8499008	206.820498						
654.3792445	317.2037595	788.1753297	1239.472018	1231.308098	1174.655621	588.6720748	576.913063	283.687063						
3146.274077	3328.326221	3397.557499	1313.197636	1392.095398	1209.572337	2722.48671	2717.344147	3195.757427						
1142.107571	1064.109157	1168.150798	838.9097808	870.9285938	706.2656379	748.816062	1213.183243	605.689415						
3266.711754	3061.360531	3171.212506	3911.720154	3549.738994	3085.836809	2617.304828	3835.243479	3655.518571						
3619.667249	3920.899799	3798.479432	4667.030121	4585.726356	4882.538675	4588.628773	4445.73007	4659.676541						
2037.656291	2547.779757	2226.736018	1998.6847	2023.505177	1977.734358	2351.010527	2106.859252	2307.529643						
1026.980275	841.112475	965.1859859	950.3280504	842.0467286	800.8417587	1163.197266	882.5855013	459.9822154						
1301.749468	1399.782535	1519.497751	2229.768023	1944.756146	2356.741813	1572.66069	1820.766872	1271.597272						
16842.861	15506.32462	17527.19359	7571.590588	8230.644883	7990.827746	15613.86487	15333.27461	14764.37712						
7775.574086	7366.335927	7778.853714	4851.005511	6955.41073	6312.066537	7971.274674	8176.117424	6489.58437						
2014.549568	2447.988414	2240.715289	2122.123154	2454.373107	2112.050549	2566.266057	1655.98568	2094.887198						

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4.86_280.5987m/z	280.5986676	4.858383333	neg
4.86_326.1612m/z	326.1611862	4.858383333	neg
4.86_338.0838m/z	338.0837834	4.858383333	neg
4.86_381.1664m/z	381.1663558	4.858383333	neg
4.86_441.1234m/z	441.1234342	4.858383333	neg
4.86_605.1061m/z	605.1060654	4.858383333	neg
4.86_741.0807m/z	741.0807183	4.858383333	neg
4.86_809.0682m/z	809.0682381	4.858383333	neg
4.88_196.0712n	195.0639498	4.880083333	neg
4.88_255.0198m/z	255.0197554	4.880083333	neg
4.88_313.0820m/z	313.0819885	4.880083333	neg
4.88_321.0102m/z	321.0101615	4.880083333	neg
4.88_322.1275m/z	322.1274606	4.880083333	neg
4.88_390.1149m/z	390.1149241	4.880083333	neg
4.88_401.0466m/z	401.0466371	4.880083333	neg
4.88_403.1612m/z	403.161206	4.880083333	neg
4.88_416.0167m/z	416.0166695	4.880083333	neg
4.88_425.1434m/z	425.1433514	4.880083333	neg
4.88_456.9852m/z	456.9851678	4.880083333	neg
4.88_465.0996m/z	465.0996316	4.880083333	neg
4.88_481.2447m/z	481.2447313	4.880083333	neg
4.88_533.0870m/z	533.0870226	4.880083333	neg
4.88_537.0221m/z	537.0221098	4.880083333	neg
4.88_660.9478m/z	660.9478407	4.880083333	neg
4.88_738.9640m/z	738.9639862	4.880083333	neg
4.88_806.9512m/z	806.9512314	4.880083333	neg
4.90_241.0696m/z	241.0695841	4.902316667	neg
4.90_251.0174m/z	251.0174033	4.902316667	neg
4.90_253.0227m/z	253.0226764	4.902316667	neg
4.90_260.0542m/z	260.0541786	4.902316667	neg
4.90_268.0076m/z	268.0076285	4.902316667	neg
4.90_280.0416m/z	280.04159	4.902316667	neg
4.90_307.5497m/z	307.5496761	4.902316667	neg
4.90_331.0392m/z	331.0391933	4.902316667	neg
4.90_340.9943m/z	340.9943464	4.902316667	neg
4.90_348.0291m/z	348.029106	4.902316667	neg
4.90_358.1875m/z	358.1874781	4.902316667	neg
4.90_388.9977m/z	388.9976654	4.902316667	neg
4.90_417.0901m/z	417.0901083	4.902316667	neg
4.90_445.1727m/z	445.1726946	4.902316667	neg
4.90_445.1903m/z	445.1903319	4.902316667	neg
4.90_467.0140m/z	467.0139608	4.902316667	neg
4.90_484.0042m/z	484.0042473	4.902316667	neg
4.90_485.0775m/z	485.077513	4.902316667	neg
4.90_524.9723m/z	524.9723617	4.902316667	neg
4.90_535.0016m/z	535.0016485	4.902316667	neg
4.90_592.9601m/z	592.9600947	4.902316667	neg
4.90_602.9891m/z	602.9890671	4.902316667	neg
4.90_605.0091m/z	605.0091185	4.902316667	neg
4.90_663.0621m/z	663.0620895	4.902316667	neg
4.90_670.9769m/z	670.9768759	4.902316667	neg
4.92_166.0333m/z	166.0332502	4.92485	neg
4.92_203.0022m/z	203.0021706	4.92485	neg
4.92_217.0352n	216.0279148	4.92485	neg
4.92_238.0699m/z	238.0698943	4.92485	neg
4.92_251.0903m/z	251.0902508	4.92485	neg
4.92_251.5143m/z	251.5143087	4.92485	neg
4.92_273.9867m/z	273.9867407	4.92485	neg
4.92_279.0237m/z	279.0237067	4.92485	neg
4.92_284.0156m/z	284.0154603	4.92485	neg
4.92_297.1323m/z	297.1323396	4.92485	neg
4.92_313.1278m/z	313.1277902	4.92485	neg
4.92_314.0560m/z	314.0559986	4.92485	neg
4.92_314.5576m/z	314.5575837	4.92485	neg
4.92_348.2031m/z	348.2030844	4.92485	neg
4.92_352.0029m/z	352.0029452	4.92485	neg
4.92_354.0575m/z	354.0574738	4.92485	neg
4.92_368.1153m/z	368.1153401	4.92485	neg
4.92_374.2187m/z	374.2187256	4.92485	neg
4.92_416.1906m/z	416.1905966	4.92485	neg
4.92_419.9906m/z	419.9905595	4.92485	neg
4.92_428.2374m/z	428.2374157	4.92485	neg
4.92_429.1382m/z	429.1382346	4.92485	neg
4.92_439.0711m/z	438.0710694	4.92485	neg
4.92_484.1784m/z	484.1783913	4.92485	neg
4.92_511.1048m/z	511.1047694	4.92485	neg
4.92_555.9653m/z	555.965258	4.92485	neg
4.92_565.1132m/z	565.1131851	4.92485	neg
4.92_595.0742m/z	595.0742442	4.92485	neg
4.92_623.9530m/z	623.9529846	4.92485	neg
4.92_625.1121m/z	625.1120736	4.92485	neg
4.92_629.1195m/z	629.1194836	4.92485	neg
4.95_224.0026m/z	224.0026253	4.94705	neg
4.95_232.1313n	213.1134528	4.94705	neg
4.95_270.1429m/z	270.1429382	4.94705	neg
4.95_281.9058m/z	281.9057504	4.94705	neg
4.95_302.1434m/z	302.1433844	4.94705	neg
4.95_363.1564m/z	363.1564308	4.94705	neg
4.95_364.1118n	363.1045296	4.94705	neg
4.95_392.0814m/z	392.0814304	4.94705	neg
4.95_453.0865m/z	453.0865478	4.94705	neg
4.95_506.2246m/z	506.2246121	4.94705	neg
4.95_530.1303m/z	530.1302503	4.94705	neg
4.95_535.0474m/z	535.0473754	4.94705	neg
4.95_540.2536m/z	540.2535706	4.94705	neg
4.95_562.1549m/z	562.154924	4.94705	neg
4.95_589.1538m/z	589.1537644	4.94705	neg
4.95_603.0348m/z	603.0348285	4.94705	neg
4.95_636.1410n	635.1337166	4.94705	neg
4.95_817.1146m/z	817.114595	4.94705	neg
4.97_263.9352m/z	263.9352007	4.969683333	neg
4.97_272.1870m/z	272.1869943	4.969683333	neg
4.97_290.1072m/z	290.1071984	4.969683333	neg
4.97_297.1942n	342.1924537	4.969683333	neg
4.97_355.0402m/z	355.0402451	4.969683333	neg
4.97_355.5421m/z	355.5421224	4.969683333	neg
4.97_397.1517m/z	397.1516841	4.969683333	neg
4.97_637.0855m/z	637.0854853	4.969683333	neg
4.99_235.1421n	234.1348674	4.99225	neg
4.99_246.0967m/z	246.0966905	4.99225	neg
132.6232259	92.32528925	168.8332928	141.0305452	214.6476623	176.6099227	337.1753713	188.38097	141.5743369
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737.0502797	818.1547686	906.0959237	862.4825553	988.458011	980.6554209	643.9995624	671.3753052	733.5507104
1969.313337	1910.833527	2155.040318	1822.770733	1700.329609	1421.761913	1883.938732	2325.381204	1933.975839
3412.991885	3638.346302	3936.440228	4036.45112	4329.149461	4074.830778	4404.487448	4713.998134	4935.97645
2453.396943	2525.582128	2420.41956	3065.387802	2928.785965	2989.401839	296.5770606	124.76309	245.0346591
6071.225625	6725.368604	6344.246069	8211.280227	7651.243068	8620.036857	9460.340653	8445.876302	8308.309973
2532.243837	2422.218668	2741.644309	3803.925207	3575.783705	4577.209509	3605.440632	3845.36616	3948.469703
2267.804396	2077.804936	2286.343866	2798.756247	2737.864347	3327.925686	3445.956932	3305.658691	2583.123974
33825.47874	35720.84862	36971.55167	35350.77002	36433.503	36493.95147	26242.67205	27462.38103	26141.90972
826.8838378	755.9270031	865.744239	542.4835177	899.835309	940.7848269	570.5220709	686.3754425	594.3866113
342.367829	344.9640668	447.4073311	0.001403199	0.001403199	0.001403199	521.1518901	737.1341787	572.1269604
3452.890362	3612.254419	3259.90819	3088.141174	3777.492502	3385.01164	2439.916595	2639.823372	2740.816296
3339.437296	3604.186189	3930.204651	2134.334961	2199.373706	2308.139799	3255.373368	3634.977913	3948.968703
1599.833587	1496.409762	1859.785487	906.6899715	1009.69702	912.0400911	1615.874361	1331.518031	1354.769588
3042.361263	3509.617701	3538.922279	83.83563076	170.2035124	54.6176619	5741.792885	5525.338428	6023.801051
33944.73881	36176.63013	35970.51976	38026.59817	39089.52617	38062.62153	38206.91445	37747.99077	35286.66729
1194.79063	1097.285358	1649.30211	1605.329168	1399.553796	1288.653202	1230.421997	1140.316419	1229.28893
5388.254418	6307.353515	6307.928673	5616.650143	5646.005143	5909.707662	6042.160649	6332.726504	7089.4471
2105.285047	1833.805406	2100.684457	2074.810174	2222.068503	1851.02316	1749.633279	1533.47905	1469.18291
2535.116853	2320.086365	2310.523417	4521.527603	5103.023488	4225.133443	3066.574796	3500.693139	3452.300882
516.3299312	679.8825791	834.4629527	920.1764889	1489.685525	1197.301142	867.2175301	689.0069396	1031.85306
684.4423275	1100.562237	977.1223689	2140.740158	2024.475325	1540.390518	1380.462518	950.0151075	1204.278673
1518.033369	1584.49202	1599.383024	24.19269378	7.474354841	0.001403199	3138.260137	2915.961572	2718.188984
1028.8082	1295.89443	1257.640856	1301.869374	1444.995455	1581.935312	838.5185726	1287.685819	817.5802694
3483.108059	4019.886324	2905.862741	3099.381699	3027.946372	3508.85186	2559.758034	2547.077408	3185.221117
1536.044889	1376.444994	1094.934976	2342.010009	1004.298233	1744.973755	1077.220078	1335.544983	2035.019525
1349.370397	1214.49721	1247.252899	1411.809788	1213.085959	1389.441118	1095.464563	1023.870357	1126.744771
1007.893115	1246.36209	1199.04688	1215.276959	1230.006847	1327.42651	1453.358582	1543.812205	786.8947534
3033.495823	3162.339743	3342.517541	3014.873881	3477.507384	3012.640181	2291.283615	2612.59968	2308.301262
880.3402712	943.1998257	969.1268818	336.0985285	286.1913095	233.2691124	551.2036855	607.3914261	363.1422288
1832.739268	2184.928583	2247.125941	2350.845817	2117.308066	2520.963068	1996.198568	2069.945568	2155.280451
2019.093225	2323.083828	2484.280679	2257.096805	2438.442398	2419.916844	1746.658205	1929.566718	1746.874909
181.0556645	410.9100807	703.01707	630.7041652	328.3916253	588.1545495	582.0900661	481.8355687	403.1379163
16123.4529	16634.36327	16793.10793	17485.47296	17262.63531	17406.14713	13547.98294	13798.8425	13196.98878
816.6607169	684.0910423	701.9409674	267.7333132	582.6756239	437.5539034	381.0961106	439.7464695	375.9338739
1516.903159	1697.265565	1452.649141	1691.970941	1803.635065	1820.800249	1450.38604	1186.407476	1515.979692
336.3032145	438.6387084	433.4279981	252.0877188	283.3441698	217.7385352	291.1719999	300.7042387	409.8647745
2991.30314	3173.098143	2711.130807	2824.178626	3436.194988	2807.723591	2208.253984	2963.165022	2087.522312
2912.112583	2767.805427	3315.089631	3379.676581	4174.489911	4050.168126	3464.47446	3982.873388	3070.818206
8685.256485	8516.40383	9741.034833	14504.04271	16437.07874	14819.46374	11348.78794	11603.0204	11231.10258
1727.583941	1966.795442	2333.612715	3416.010265	2604.965021	2461.071851	1934.123332	1928.454285	2082.246105
9672.535185	9086.907891	10178.42116	9819.583308	11319.74527	10336.95145	7453.293138	7988.878032	7675.335556
1122.467483	1334.725226	1424.326916	738.0205351	1268.923866	1254.162327	1076.681726	1239.82328	609.2749265
1370.229906	1163.408543	1534.441045	2093.034547	2315.828746	2026.460515	1515.82001	1704.857936	1670.157808
1668.219982	1465.212769	1815.536314	1347.010403	1699.228015	1660.283384	1487.145413	1485.556336	919.7004886
7539.256287	8379.667813	8027.014754	8629.6278	9174.011682	8303.686987	6233.608113	6393.22958	6417.93724
1332.614792	1382.604202	875.0583666	893.6776316	970.7900163	1767.336771	1406.815808	1484.656601	178.058959
6120.20187	6650.823273	7173.044856	6452.163443	6749.229965	6927.883986	5789.557613	4703.060871	4929.297822
906.8076942	753.3035495	585.5861301	0.001403199	0.001403199	97.70266777	1942.284828	1725.787636	818.938118
1352.390299	1119.255671	894.0174818	1583.180623	2103.422876	2293.246236	1997.901718	2044.179344	730.6744666
5220.917095	6064.726126	5164.088129	5318.794135	5784.325008	6344.836545	5087.729143	4149.266495	4599.022055
512.0598174	488.3049654	607.4378121	636.9368412	519.292229	620.6648979	738.7316929	612.1682483	729.8185433
2712.479857	3232.16896	3242.184075	1808.48671	1764.248754	1761.607988	2620.793947	2714.614489	2769.720258
12152.90894	12710.69547	13464.18578	1492.725934	1613.527484	1416.213502	2584.076843	2957.454228	2881.484067
778.0922406	938.2010136	1034.448646	2124.667704	2024.433434	1964.716561	877.1828042	909.8306117	1000.875355
698.0873948	860.4406635	733.9875229	808.1010244	889.430783	759.6598382	536.9695639	524.9232483	620.5585665
2951.505453	3006.883954	2915.605283	3378.013373	3704.879685	3594.365698	546.7935144	570.6083083	377.6328653
973.1836176	962.3822834	1063.00052	130.3223689	91.98853517	114.5046779	168.0775423	244.4182396	99.7117737
1182.743421	1416.89754	1430.602519	152.4324497	267.5011021	321.2806699	280.4860969	391.6386871	276.2033016
8232.262261	8937.994696	8940.124847	1211.542829	1112.704241	1184.233453	1964.420069	1982.13916	1896.265412
1282.432126	1220.400202	1566.469526	1264.48301	1911.413183	1578.688714	1381.293271	1576.351215	1088.139774
607.4994523	440.4298706	699.0386946	626.6312607	619.4177334	544.4233838	459.6951038	397.5120458	414.3677947
1366.417336	1210.37625	1347.979793	1975.365247	1551.583665	1739.648268	1368.398938	1754.951994	1650.610562
75.30984164	58.95046188	268.2181401	495.8017816	318.1589282	318.4458613	162.7703101	180.6371004	180.8466695
399.660839	463.2772202	551.8794313	2389.882024	2178.116815	1951.485861	648.7343405	792.8005892	751.2350622
4484.794924	4789.906915	5182.319851	585.3877997	532.9829222	519.6666851	1002.450511	903.5789642	1178.761945
263.7008679	513.6915168	555.5067479	1174.873168	1035.81268	943.3177549	590.3126516	655.1063411	478.8470709
614.033535	714.9040853	875.3973387	636.8338971	436.4044024	469.3348659	1004.44863	700.2237356	950.5838491
663.0860366	929.0942281	915.7825329	1100.493074	1240.251524	1136.714695	975.4483498	999.2508941	695.5618589
482.7416513	579.6117503	507.9781127	1963.864182	1931.636532	2046.566392	641.0381711	959.7090854	773.8931507
3731.508139	4444.476875	4280.461277	395.446688	373.3377906	542.6774643	813.1271047	888.1109831	991.8827547
322.4231674	330.0959362	135.016001	425.258748	353.308933	522.856086	315.2436574	342.3768413	305.8972905
15907.04788	17867.06089	17994.22386	16585.6826	16619.86846	17604.90365	17328.50726	17702.40028	16600.41803
673.2138732	795.2459149	823.2717875	577.6343083	565.3069818	712.2017716	368.9947317	316.8887634	358.6918299
139.2910058	448.6414244	234.6229255	1277.3622	1228.053309	1224.54544	282.5222858	358.1855582	313.6670304
942.6632361	1337.501717	971.9791497	946.794367	924.4589521	1106.50789	654.8529168	902.0380478	575.9332097
1836.016005	2575.314053	2438.626066	152.6015064	172.7618727	0.001403199	488.7631672	201.5767593	178.1195352
3724.326025	3644.622187	3819.176935	3306.787613	4388.290453	3323.193382	4358.528402	3895.748291	3014.111712
1390.822147	1485.934199	1584.36211	2026.606034	3467.722319	3342.672473	2414.378535	2536.785431	1333.540634
1737.231811	1785.44359	1469.753367	0.001403199	234.4545324	273.546632	410.6694451	134.6846848	159.2839585
1658.041563	2447.487778	2206.494972	0.001403199	0.001403199	0.001403199	262.6097849	188.4522171	237.3220558
3476.660344	3264.33039	3770.195959	5279.259687	4897.497887	5749.624054	3979.099285	4447.193004	3736.331428
115.5169655	31.49430012	26.80174856	144.301739	59.07841085	141.7114242	253.9983881	286.0926529	232.3689324
1969.064994	2137.78514	2338.396002	2127.714393	2328.234946	2533.14431	2142.511098	2002.135734	1635.123184
0.001403199	227.6546503	128.0576133	145.7989661	128.0747729	207.21731	48.61716282	38.61326218	142.935926
1681.533392	1572.175735	1538.122355	1504.716748	1955.807062	1554.095262	2087.151436	1559.494342	1655.805989
501.805654	509.0277424	689.0964766	1155.001297	1205.200388	910.3390097	553.7271147	445.8775864	594.8382158
2026.272573	1587.772998	2883.645488	2432.310884	2785.108192	1776.846177	3399.953174	2006.470181	3433.566347
3333.602737	3464.259913	3520.229084	4055.817455	3252.014587	3272.366403	92.33119727	0.001403199	111.9956607
670.8828141	721.919762	1012.605413	427.1945827	112.7159138	111.0102323	474.0471455	587.8820317	371.2712663
3071.635696	3025.781492	3270.175849	3575.638646	3136.217626	3550.886083	306.5235109	489.025528	257.464014
1073.970532	705.4106023	1134.97002	3066.101061	2800.299308	2929.692249	1526.64258	1827.590615	1665.905779
392.7889942	138.5235166	163.2064473	473.8924777	623.1296331	473.9086398	428.7244809	250.5970383	127.7857164
0.001403199	0.001403199	0.001403199	3321.377455	3252.014587	3272.366403	92.33119727	0.001403199	111.9956607
165.4350112	208.2584407	156.1311566	237.1881434	239.6907926	0.001403199	316.1525519	107.200119	0.001403199
1405.14483	1853.575211	1438.348134	0.001403199	19.12633394	0.001403199	835.7824734	902.5113747	840.3253336
501.6547686	514.095796	286.3399197	0.001403199	0.001403199	0.001403199	195.1451529	204.7868729	0.001403199
0.001403199	0.001403199	0.001403199	1249.729847	1442.488312	1355.153796	0.001403199	0.001403199	0.001403199
11435.1311	11753.02127	11950.8823	132.6942808	44.42256751	0.001403199	7253.665204	8776.557511	7275.586386
1631.74087	1623.878636	2046.134804	0.001403199	0.001403199	1060.378857	699.3853912	893.7923344	
375.3965696	203.8582721	374.5660012	358.5725547	502.1654676	342.1614358	422.7423456	372.6869752	400.075298
959.0146646	873.2716589	1069.931182	846.3482223	760.1573783	984.726694	861.1453029	815.6086212	678.6057761
191.9287828	123.0741598	156.8010093	281.0443998	171.1706917	207.9462322	297.0956931	189.5621972	57.38215906
72396.19208	76585.16466	78451.8284	50808.5717	48544.62046	50895.43238	72334.69687	69746.42116	68222.69775
1081.940199	1260.674433	1363.47741	1603.296715	1825.870697	1797.923799	1801.885511	1710.806679	1940.144641
225.8124473	510.0129614	410.6800062	633.0943914	629.0268821	611.3533489	574.5829901	510.9876221	458.1452995
3092.74529	3169.222173	3477.534082	3989.793691	3875.786542	4568.836611	4270.133713	3709.504072	3512.212535
4639.481499	4415.507909	4901.022765	3641.809143	4063.58946	4364.843401	4037.571391	3918.466728	4077.905951
6828.968608	6712.178207	6439.599796	6773.95931	7649.107249	7329.28199	9626.179423	8706.189796	7700.633852
142.0741911	133.5839439	186.3239723	72.83050633	0.001403199	60.6757959	119.1237305	143.3385264	93.66639912

4.99_260.0640n	519.1092537	4.99225	neg
4.99_272.1509m/z	272.1509191	4.99225	neg
4.99_284.0942m/z	284.0942201	4.99225	neg
4.99_287.1115m/z	287.1114838	4.99225	neg
4.99_361.1508m/z	361.1508025	4.99225	neg
4.99_365.1714m/z	365.171414	4.99225	neg
4.99_409.0108m/z	409.0107972	4.99225	neg
4.99_445.2075m/z	445.2074578	4.99225	neg
4.99_491.0742m/z	491.0741544	4.99225	neg
4.99_520.1077m/z	520.1076651	4.99225	neg
4.99_522.1034m/z	522.1033782	4.99225	neg
4.99_542.0889m/z	542.088911	4.99225	neg
4.99_544.0860m/z	544.085958	4.99225	neg
4.99_547.0015m/z	547.0014667	4.99225	neg
4.99_572.2540m/z	572.2540185	4.99225	neg
5.01_205.0656n	205.0482973	5.014716667	neg
5.01_250.0334m/z	250.0334298	5.014716667	neg
5.01_254.0170n	299.0151837	5.014716667	neg
5.01_262.1120m/z	262.111994	5.014716667	neg
5.01_301.0308m/z	301.0308443	5.014716667	neg
5.01_343.0390m/z	343.0390433	5.014716667	neg
5.01_361.2235m/z	361.2235194	5.014716667	neg
5.01_368.2278m/z	368.2277585	5.014716667	neg
5.01_369.0182m/z	369.0181625	5.014716667	neg
5.01_375.0653m/z	375.0653383	5.014716667	neg
5.01_391.2243m/z	391.2242939	5.014716667	neg
5.01_411.0266m/z	411.026565	5.014716667	neg
5.01_437.0058m/z	437.0057521	5.014716667	neg
5.01_443.0526m/z	443.0526014	5.014716667	neg
5.01_479.0141m/z	479.0141006	5.014716667	neg
5.01_504.9935m/z	504.9935341	5.014716667	neg
5.01_539.0857m/z	539.0856903	5.014716667	neg
5.01_572.9807m/z	572.9807468	5.014716667	neg
5.01_614.9888m/z	614.9888031	5.014716667	neg
5.01_619.0302m/z	619.0301892	5.014716667	neg
5.01_640.9678m/z	640.9678159	5.014716667	neg
5.01_682.9771m/z	682.9770893	5.014716667	neg
5.04_266.1094m/z	266.109373	5.037216667	neg
5.04_300.0856m/z	300.0856219	5.037216667	neg
5.04_310.0740m/z	310.0740616	5.037216667	neg
5.04_329.1244m/z	329.1244051	5.037216667	neg
5.04_378.0611m/z	378.0610658	5.037216667	neg
5.04_526.1167m/z	526.1167488	5.037216667	neg
5.04_540.2108m/z	540.2107972	5.037216667	neg
5.04_607.0740m/z	607.0740045	5.037216667	neg
5.06_232.0229m/z	232.0228992	5.05975	neg
5.06_232.5610m/z	232.5610377	5.05975	neg
5.06_248.0964m/z	248.0964485	5.05975	neg
5.06_258.5221m/z	258.5220963	5.05975	neg
5.06_276.0913m/z	276.0912613	5.05975	neg
5.06_303.0991m/z	303.0991066	5.05975	neg
5.06_334.1272m/z	334.1271676	5.05975	neg
5.06_344.2080m/z	344.2080104	5.05975	neg
5.06_358.1874m/z	358.1874459	5.05975	neg
5.06_366.0605m/z	366.060461	5.05975	neg
5.06_370.1314m/z	370.131441	5.05975	neg
5.06_375.1040m/z	375.104014	5.05975	neg
5.06_402.1141m/z	402.1140783	5.05975	neg
5.06_402.1890n	447.1880638	5.05975	neg
5.06_409.1720m/z	409.1719801	5.05975	neg
5.06_427.2341m/z	427.2341177	5.05975	neg
5.06_455.1022m/z	455.1021578	5.05975	neg
5.06_499.0454m/z	499.0454207	5.05975	neg
5.06_526.6185m/z	526.618493	5.05975	neg
5.06_542.2692m/z	542.2692646	5.05975	neg
5.06_567.0325m/z	567.0325251	5.05975	neg
5.06_589.1504m/z	589.1503833	5.05975	neg
5.08_179.9364m/z	179.9363958	5.080566667	neg
5.08_203.1176m/z	203.1176467	5.080566667	neg
5.08_243.0850m/z	243.0850189	5.080566667	neg
5.08_244.8882m/z	244.8882065	5.080566667	neg
5.08_259.0719m/z	259.0718834	5.080566667	neg
5.08_267.0851m/z	267.0851269	5.080566667	neg
5.08_304.0806m/z	304.0805904	5.080566667	neg
5.08_329.0235m/z	329.0234618	5.080566667	neg
5.08_385.1694m/z	385.1693535	5.080566667	neg
5.08_440.0557m/z	440.0556639	5.080566667	neg
5.08_473.0633m/z	473.0632849	5.080566667	neg
5.08_513.1711m/z	513.1710569	5.080566667	neg
5.08_540.2537m/z	540.2537141	5.080566667	neg
5.08_651.1012m/z	651.1011918	5.080566667	neg
5.10_239.0540m/z	239.0539769	5.1031	neg
5.10_326.1070m/z	326.10702	5.1031	neg
5.10_332.1543m/z	332.1542926	5.1031	neg
5.10_335.0732m/z	335.073205	5.1031	neg
5.10_347.1352m/z	347.1351875	5.1031	neg
5.10_401.0468m/z	401.046841	5.1031	neg
5.10_453.1040m/z	453.1040215	5.1031	neg
5.10_453.1569m/z	453.1568937	5.1031	neg
5.10_525.2708m/z	525.2707505	5.1031	neg
5.10_655.1217m/z	655.1217401	5.1031	neg
5.13_164.9274m/z	164.9273614	5.132616667	neg
5.13_196.0698m/z	196.0697695	5.125666667	neg
5.13_262.0254m/z	262.0253974	5.132616667	neg
5.13_264.0224m/z	264.0224456	5.132616667	neg
5.13_265.0187m/z	265.0186863	5.125666667	neg
5.13_286.1301m/z	286.1301158	5.132616667	neg
5.13_289.0445m/z	289.0445131	5.132616667	neg
5.13_313.1274m/z	313.1273667	5.132616667	neg
5.13_330.0130m/z	330.0130391	5.132616667	neg
5.13_340.0416m/z	340.0416458	5.132616667	neg
5.13_350.9286m/z	350.9285744	5.132616667	neg
5.13_357.0319m/z	357.0319374	5.125666667	neg
5.13_360.1853m/z	360.1853384	5.125666667	neg
5.13_389.1823m/z	389.1823481	5.125666667	neg
5.13_393.0933m/z	393.0933295	5.132616667	neg
5.13_398.0003m/z	398.0003381	5.132616667	neg
5.13_400.1333n	399.1296665	5.132616667	neg
5.13_408.0292m/z	408.0291905	5.132616667	neg
5.13_450.2105n	449.2032908	5.132616667	neg

3926.366689	3406.136649	3934.189699	6307.304785	5840.711949	6430.708633	5101.925184	4530.168228	5394.888702
722.267149	726.44814	773.4826988	780.5406557	1000.697967	946.4058848	1238.910315	782.5539733	893.4501562
146.4706612	72.34750667	182.181735	276.5085558	332.1818925	304.48671	236.6289508	165.7877844	133.9722321
9091.408806	9746.788817	10075.44547	8758.935513	8425.8874	9345.921642	10473.75067	8303.245841	8714.172437
98451.5618	103724.288	106611.9644	97009.36261	95370.46843	99544.53254	108468.5875	108642.5416	105977.5857
181.941165	218.7639686	209.5781362	89.2733415	117.660367	130.7530181	310.1941055	132.0856628	209.3289848
799.4576969	762.1791183	1092.421359	971.0276366	974.158141	1164.329138	713.8813454	436.8379593	345.3342559
3071.664568	3269.819508	3530.798198	470.9368718	180.0872916	101.9120768	2101.515854	2075.905061	1190.856235
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4981.589617	6414.697717	5846.083176	516.5706663	138.7888873	227.9418653	1034.176336	738.0960809	710.953452
1797.02612	1893.36125	1770.647862	0.001403199	0.001403199	0.001403199	239.1440992	134.6888733	120.7984064
1706.615613	2130.397068	1613.621533	31.09809388	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199
500.7588374	592.6306885	769.646958	0.001403199	0.001403199	0.001403199	0.001403199	290.0203438	0.001403199
1352.418165	1355.449013	1184.020567	2468.771569	2043.000261	2479.42833	2146.97678	1472.550113	1848.984564
4929.577282	5249.38536	5864.96347	6951.581929	7157.909181	7132.824559	8437.496846	6353.559573	5862.179272
2684.443346	2844.805661	2990.054427	2267.719092	2208.04141	2280.514823	2092.789277	1590.17554	1510.211324
420.464451	531.6756565	392.0090131	971.0295381	900.0112949	1205.07886	639.4389491	533.0844759	464.4149969
2254.29844	2113.943253	2002.323253	1528.099559	1528.326223	1382.117709	1547.581395	1562.836114	1282.90772
2595.284005	2499.802625	2922.58674	3107.392557	3167.42525	3469.483553	4579.746938	4442.819344	4301.939899
4812.818871	5155.729117	5437.643385	4398.915084	4465.041491	5161.865785	5423.697898	4248.717876	4686.066258
3314.575703	3107.939334	3529.37578	5197.252384	5581.840718	5656.339065	5576.7747	4098.861409	4433.320036
1044.787065	1631.82171	1210.349218	935.2929785	882.5871826	917.4954994	615.1755715	761.8519421	590.2721006
143.241179	125.4301775	208.2401593	84.65661512	150.7711722	111.5257985	164.3245551	248.8723049	114.999038
3488.353136	3517.911594	4027.012719	4000.839356	4865.845394	4779.436515	4542.586754	3848.802217	3984.293419
1317.754541	1176.694334	1189.054408	1768.197395	1838.642676	1957.046099	1518.874246	1398.400917	1329.043818
225.4916249	200.4474082	198.5812465	219.8855225	0.001403199	131.8706681	234.8441661	127.4158535	0.001403199
2174.999438	2525.535674	2425.286369	3566.859704	4004.956287	4050.306937	4284.957758	2875.863907	3001.965398
2965.031097	3270.031615	3100.023364	3198.102237	3355.431695	3728.144861	2973.932374	2830.526812	2828.175208
554.856112	636.3396298	642.9132943	998.867598	1477.344094	964.1120708	972.2948315	875.240917	737.8647823
1843.164956	1540.101959	1717.230081	3093.394593	3240.108279	2634.776929	2831.668859	2045.937515	2231.711857
1874.338588	2925.556955	2018.484206	1937.842009	2615.087615	1983.165684	1997.890426	1667.902016	1845.609091
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1686.833253	1489.818478	1775.069803	1156.621059	1575.821155	1221.632932	1607.587247	1350.541952	1208.512154
1012.645276	1077.802445	807.9519421	1596.643171	1715.485082	1724.825568	1769.630555	1338.992225	1159.368646
190.4665518	277.3433976	180.9056942	2097.879434	2186.045909	1927.595135	490.6475222	389.6068537	302.9247976
1458.742005	1304.108006	1087.625549	765.8653056	761.096015	1058.707136	1253.543652	855.547764	700.7255751
620.7454284	1050.979641	841.5049087	1867.775676	1602.502287	1790.387693	1406.511243	1044.165959	994.5808765
68.68992832	133.621561	123.6085368	208.0991566	250.9627932	204.9609425	158.9695484	162.0851881	148.3082502
303.6810045	299.1577627	392.4070463	609.0958684	627.3756285	711.3876331	482.8350173	578.0042675	447.7714211
949.2380385	1009.976408	955.5336701	1206.565721	1561.639688	1583.862681	1191.444555	961.1456458	1252.277518
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815.9044165	810.600512	640.4175555	897.2313567	702.5080576	823.9265522	953.2771454	797.6818733	712.7717614
624.6106283	678.3623189	799.1092474	1081.829124	804.6060511	737.1767911	279.5702345	177.7720718	365.9005655
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145.3748223	318.0292701	291.3222841	1428.689672	635.7349031	1091.410113	309.7595275	140.7033691	262.8647606
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97.14093253	151.0420728	210.3423715	160.1224779	260.1901049	269.3109543	25.83060014	219.4078627	202.0207025
2868.332165	2958.366931	2714.030258	17762.99734	16348.20095	18699.22513	6675.843963	5941.23996	7110.509439
449.1699413	930.7666296	398.0955043	1173.081917	1318.517339	1621.556733	30.76105047	0.001403199	0.001403199
4432.419833	4759.81685	4923.409243	5693.982988	7399.092417	8267.296704	5115.259925	4615.858778	5529.885387
2489.727839	2792.751043	2717.428325	3257.390555	3285.33285	3491.64638	2723.390429	2740.602718	3209.369474
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856.3717797	544.999198	590.8833399	1291.868531	574.0841565	1264.585006	758.4337214	656.2266174	789.3015499
177.215972	132.8542076	142.3866743	608.5036974	486.7341599	411.0939715	236.5159367	265.773243	301.3837344
1417.5671	1297.679733	1275.494923	1743.785589	1688.71528	1872.332733	1314.874859	1386.712504	1439.892539
497.9190434	312.5420124	397.9323058	217.1852544	223.9786269	51.08545798	363.821639	299.7093801	387.3058399
17939.10501	18605.44736	19608.04772	15740.41071	14980.01539	16072.59888	20031.09203	19678.96885	18106.9725
4964.371659	4629.513136	5009.718541	5663.027307	5304.708233	6070.33225	7022.701716	5977.367977	7284.235828
3036.363376	3087.507959	3230.249006	3814.680805	3907.491618	3698.537302	3148.586821	3277.31156	4012.593454
441.9614604	823.8761321	761.2904652	0.001403199	0.001403199	168.531919	337.0519134	354.501241	309.0131367
2755.923453	2394.863335	2697.673061	603.77513	341.9181051	474.2088487	3572.45973	3196.719437	3856.31816
309.3795796	0.001403199	420.9897729	90.32084262	250.6030135	307.4111924	0.001403199	0.001403199	0.001403199
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1399.398629	1480.913593	1830.293281	132.1690876	133.0408589	438.0683515	2593.262029	2516.236401	3184.086236
188.3030288	72.87621974	178.0881568	2023.669061	727.7197104	1317.822672	310.2697657	380.0302628	86.06847611
395.3823651	426.1045038	318.3034062	409.7397965	380.0615557	461.7728611	463.1957394	427.8465252	408.2442005
32.09653151	22.59500492	31.24910982	20.46488808	48.56470599	0.001403199	25.08444329	23.83372021	32.03845911
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331.734504	424.0788461	338.9346269	385.2321275	350.1332003	495.4278115	447.3667084	384.6300541	262.4332995
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1816.059202	2094.141907	1964.961213	1862.166409	1835.883601	2018.770611	2179.702276	2013.756654	2006.783579
3347.238604	3534.984077	3136.349747	3417.324165	2636.127925	3705.097746	4470.225639	3830.640621	3784.560304
839.5728154	542.1221965	468.9928218	685.9161833	580.9096298	746.1570661	829.6653589	665.8473222	523.0725314
48978.92439	52008.37443	48265.25292	79846.12487	80501.07352	84917.20152	61807.6044	54268.48619	60885.00627
671.5328144	848.7879208	910.1723452	849.4724917	275.2019162	962.9405925	1349.560925	833.4837341	1025.100968
1490.235343	1375.358665	1603.885942	1147.90842	673.3137378	1359.513309	1640.987967	1010.534683	964.88073
667.5181519	841.6752155	741.8888109	2581.814002	2062.701934	3469.901901	1340.674507	866.4199864	1067.59275
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2282.005906	2529.452411	2050.256502	2698.572484	2581.840718	3160.803361	2579.882207	2136.757308	2056.880883
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215.9853103	398.1944015	264.8211654	0.001403199	0.001403199	0.001403199	102.4120465	117.033907	104.730454
6722.816138	7622.460584	6649.11633	11400.43306	10778.23371	12994.80895	8253.679571	7533.686115	8537.460933
1600.324993	1677.16531	1852.057436	1955.598102	2489.616564	2347.891529	1937.109831	1587.785085	1611.963083
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1358.766788	1347.386165	1023.125313	2326.258853	2057.476248	2007.065997	1976.738667	2097.119717	2488.788157
312.1581781	440.5551299	258.9871738	547.2004719	590.1024943	541.3297913	580.6376008	446.2043773	766.3237737
3127.857424	3071.593589	3008.658178	762.5276056	677.7435382	700.2744908	518.97873	437.5767975	542.0348929
2461.863216	2579.094033	2072.782152	1296.626525	906.3988895	851.9472418	1366.597416	1420.157082	1973.279824
774.9261179	1141.891419	742.1357224	1721.747087	1397.000088	1527.079771	1397.75851	1640.797479	2155.130223
2440.442186	3033.047823	2181.258094	1927.401312	1959.830707	1585.251842	1788.670677	1865.017439	2214.032522
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1574.260096	1253.945362	1090.819839	1330.865052	1210.305345	1481.663278	1763.318787	1248.088114	1215.56457
397.9246134	433.0658616	206.2319413	642.0064505	537.2007935	514.2086606	598.9551289	711.1086617	669.1792595
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15163.16895	15931.19049	15410.09062	22601.60809	22710.80866	22982.95475	18664.64506	17378.11228	17693.43556
4757.796874	5845.789912	4336.3769	8342.405121	7170.124605	7950.434669	7003.127641	7669.653194	9923.269629
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5.13_465.9876m/z	465.9876038	5.132616667	neg
5.13_467.0600m/z	467.0599577	5.125666667	neg
5.13_476.0166m/z	476.0166349	5.132616667	neg
5.13_499.1803m/z	499.1803431	5.132616667	neg
5.13_535.0476m/z	535.0475995	5.125666667	neg
5.13_544.0042m/z	544.0042071	5.132616667	neg
5.13_570.8376m/z	570.837599	5.132616667	neg
5.13_603.0352m/z	603.035206	5.125666667	neg
5.13_611.9916m/z	611.9916444	5.132616667	neg
5.13_671.0228m/z	671.0227584	5.125666667	neg
5.13_679.9791m/z	679.9790906	5.132616667	neg
5.13_747.9664m/z	747.9663768	5.132616667	neg
5.16_218.9793m/z	218.9792549	5.155116667	neg
5.16_243.1239m/z	243.1238737	5.155116667	neg
5.16_282.9896m/z	282.9895821	5.155116667	neg
5.16_296.0963m/z	296.096341	5.155116667	neg
5.16_304.9716m/z	304.9715958	5.155116667	neg
5.16_333.0936m/z	333.0936052	5.155116667	neg
5.16_364.0841m/z	364.0841441	5.155116667	neg
5.16_372.9591m/z	372.9590621	5.155116667	neg
5.16_401.0813m/z	401.0813204	5.155116667	neg
5.16_461.1137m/z	461.1137268	5.155116667	neg
5.16_711.1117m/z	711.111666	5.155116667	neg
5.18_281.9059m/z	281.9058707	5.1777	neg
5.18_287.0515m/z	287.0515164	5.1777	neg
5.18_354.0976m/z	354.0975538	5.1777	neg
5.18_355.0392m/z	355.0391533	5.1777	neg
5.18_382.1219n	427.1229054	5.1777	neg
5.18_387.1851m/z	387.1851193	5.1777	neg
5.18_422.0847m/z	422.08469	5.1777	neg
5.18_423.0267m/z	423.0266903	5.1777	neg
5.18_427.1973m/z	427.1973274	5.1777	neg
5.18_431.2108m/z	431.2107605	5.1777	neg
5.18_491.0144m/z	491.0143559	5.1777	neg
5.18_497.1262m/z	497.1262192	5.1777	neg
5.18_511.1345m/z	511.1344865	5.1777	neg
5.18_519.1065m/z	519.1064834	5.1777	neg
5.18_528.1186m/z	528.1186011	5.1777	neg
5.18_565.1117m/z	565.1117025	5.1777	neg
5.18_605.0503m/z	605.0503967	5.1777	neg
5.18_633.0993m/z	633.0992792	5.1777	neg
5.20_331.1400m/z	331.1400235	5.20005	neg
5.20_430.1843n	429.1768363	5.20005	neg
5.20_481.2446m/z	481.2446166	5.20005	neg
5.20_537.0629m/z	537.0629698	5.20005	neg
5.20_541.0098m/z	541.0097727	5.20005	neg
5.22_207.0640m/z	207.0639534	5.222166667	neg
5.22_232.1313n	231.1238808	5.222166667	neg
5.22_235.0225m/z	235.0224902	5.222166667	neg
5.22_241.1446m/z	241.1446882	5.222166667	neg
5.22_252.0125m/z	252.0125251	5.222166667	neg
5.22_253.1060m/z	253.106015	5.222166667	neg
5.22_275.0516m/z	275.0515693	5.222166667	neg
5.22_321.0935m/z	321.0934616	5.222166667	neg
5.22_343.0389m/z	343.0389879	5.222166667	neg
5.22_359.1252m/z	359.1251829	5.222166667	neg
5.22_408.1849m/z	408.1849097	5.222166667	neg
5.22_411.0265m/z	411.0264809	5.222166667	neg
5.22_462.0767m/z	462.0767474	5.222166667	neg
5.22_479.0138m/z	479.0137694	5.222166667	neg
5.22_485.1178m/z	485.1178334	5.222166667	neg
5.22_553.1052m/z	553.1052357	5.222166667	neg
5.22_580.1244m/z	580.1243648	5.222166667	neg
5.22_621.0926m/z	621.0926226	5.222166667	neg
5.22_631.1213m/z	631.1213164	5.222166667	neg
5.22_689.0802m/z	689.080169	5.222166667	neg
5.22_757.0675m/z	757.0675013	5.222166667	neg
5.22_811.3608m/z	811.360801	5.222166667	neg
5.22_835.0836m/z	835.0836143	5.222166667	neg
5.22_877.3062m/z	877.3061932	5.222166667	neg
5.22_903.0715m/z	903.0715455	5.222166667	neg
5.24_266.9946m/z	266.994604	5.244033333	neg
5.24_283.9848m/z	283.9847745	5.244033333	neg
5.24_306.1383m/z	306.1383234	5.244033333	neg
5.24_334.1327m/z	334.1326932	5.244033333	neg
5.24_334.9822m/z	334.9822457	5.244033333	neg
5.24_396.1123m/z	396.1123444	5.244033333	neg
5.24_402.9695m/z	402.9694535	5.244033333	neg
5.24_550.9212m/z	550.9212791	5.244033333	neg
5.24_648.1122m/z	648.1121727	5.244033333	neg
5.26_321.1557m/z	321.1557095	5.263033333	neg
5.26_341.0338m/z	341.0338007	5.263033333	neg
5.26_347.1349m/z	347.1349329	5.263033333	neg
5.26_370.1330m/z	370.1330367	5.263033333	neg
5.26_385.1508m/z	385.150792	5.263033333	neg
5.26_425.2186m/z	425.2186054	5.263033333	neg
5.26_452.0756m/z	452.0756269	5.263033333	neg
5.26_470.9568m/z	470.9567766	5.263033333	neg
5.26_538.9444m/z	538.9444217	5.263033333	neg
5.27_216.1242m/z	216.124191	5.271716667	neg
5.27_229.0177m/z	229.0177144	5.271716667	neg
5.27_239.1290m/z	239.1290376	5.271716667	neg
5.27_319.1763m/z	319.1763329	5.271716667	neg
5.27_374.2187m/z	374.2186593	5.271716667	neg
5.27_443.1544m/z	443.1543847	5.271716667	neg
5.27_443.2087m/z	443.2087245	5.271716667	neg
5.27_445.1070m/z	445.1069953	5.271716667	neg
5.27_543.2816m/z	543.2815718	5.271716667	neg
5.27_578.1814m/z	578.181358	5.271716667	neg
5.27_601.2403m/z	601.2403378	5.271716667	neg
5.29_155.0715m/z	155.0714718	5.28555	neg
5.29_278.9711m/z	278.9711144	5.28555	neg
5.29_284.1117m/z	284.1117343	5.28555	neg
5.29_428.9617m/z	428.9617218	5.28555	neg
5.29_445.2073m/z	445.2073171	5.28555	neg
5.29_513.2344m/z	513.2343689	5.28555	neg
5.30_243.0850m/z	243.0849826	5.302883333	neg
5.30_259.5117m/z	259.5116571	5.302883333	neg
5.30_325.0389m/z	325.038927	5.302883333	neg
5.30_331.0777m/z	331.0777267	5.302883333	neg

727.8205938	635.5063905	447.8711257	934.836834	885.6528746	949.9858069	1137.964853	979.6828626	1340.443483
358.9098063	90.90662323	249.92932	7341.648253	7869.822085	8466.661529	0.001403199	0.001403199	36.23960685
3855.95574	4033.876849	2993.162468	6082.604832	5517.467349	5946.591297	5396.597707	5702.81805	6716.204124
2522.417317	2597.12785	3082.236171	3983.258985	3453.869862	4099.602918	2444.83395	2580.44833	2179.880717
0.001403199	109.9794426	0.001403199	3892.957729	3979.410715	3784.30806	0.001403199	0.001403199	0.001403199
2788.420605	3151.166113	2455.283165	4468.485029	3814.669868	4324.319999	4478.382613	4362.798799	4946.497928
4296.756186	3739.591475	3336.398689	3558.739345	3494.342847	4152.372874	5260.422465	3262.157544	4323.416096
0.001403199	0.001403199	0.001403199	2237.089118	1766.103413	2619.438419	0.001403199	0.001403199	0.001403199
2154.839184	2509.073762	1708.881886	3596.783295	3174.714841	3577.631794	2932.544442	3400.827362	3801.312178
0.001403199	0.001403199	0.001403199	1053.156217	393.9551785	1199.916473	0.001403199	0.001403199	0.001403199
1564.954542	2278.021573	1246.754328	3438.048096	2072.496641	2853.325167	2749.036659	2652.688177	3833.782624
1257.536241	1296.805501	1048.279224	2447.94547	2053.085654	2821.419715	2004.487981	2519.934431	2585.05022
577.3338536	551.4009396	482.1363488	616.1277488	310.2517462	359.8387573	621.8759458	579.3261436	960.7879776
15794.6841	18063.20582	16801.06004	26032.87109	26104.81452	26246.53674	19428.23654	19370.35797	19773.23232
1615.399468	1972.823854	1642.600709	0.001403199	0.001403199	0.001403199	1215.333497	1252.49461	1421.87933
1507.830895	1730.244562	1611.044048	866.3487384	792.7216924	898.759598	1474.696376	1478.007752	1728.706694
2574.018024	3587.771141	2969.924801	0.001403199	0.001403199	0.001403199	2203.115791	2283.817648	2344.155646
1342.150318	1801.282194	1532.261974	3138.198752	2760.06011	2572.698513	1808.248024	1909.474745	1739.289662
393.9907897	548.5400017	421.3410396	270.8699087	183.5376042	150.4098988	446.7390531	376.076524	606.0903055
2065.416762	2572.074832	1767.446085	0.001403199	0.001403199	0.001403199	1853.884044	1752.423885	1987.57079
1082.141934	1270.384865	787.0044281	1899.628335	1506.318863	1939.341153	1415.273303	1467.022823	1574.674761
437.3431749	697.9516556	663.4578986	1214.964893	1130.120832	1097.259787	605.166654	695.7841624	697.7409094
2599.897431	1825.518323	2190.283702	2187.38606	2490.917781	1928.482831	2398.414365	2083.897743	2145.076193
1520.629434	1291.10859	896.7821154	1136.824901	1145.15265	1336.808423	1681.616274	1367.716373	1432.691789
1305.380794	1411.339215	1404.698066	3791.531626	3930.691204	3369.976308	1780.364514	1641.001993	1450.375936
687.4845188	787.0667071	638.7077986	883.2649932	912.5663183	1010.106123	766.3078558	508.5962929	527.2890157
1430.136493	1186.352563	1492.71123	2995.770662	4099.584208	3600.685086	1716.030933	1728.794517	2030.790175
20823.24971	23222.99275	20254.12859	14933.02185	15797.50762	16585.34656	19162.22823	18250.6951	20553.28027
1820.290952	2128.240578	1888.452777	2345.036569	1971.215504	2000.707071	2052.193265	2587.469681	2277.118356
389.0043139	455.1795971	508.2493027	651.0481548	636.9288762	757.9012344	246.1558647	412.3575211	543.9471904
458.2677963	425.5786459	488.6585863	1008.899735	1432.834009	1458.305288	419.0993057	607.6113075	585.6517527
17993.19957	19344.32716	18764.32107	7961.821488	7809.407344	7888.078243	17361.52044	17681.19869	17407.60643
180.5497011	450.4865702	526.0976805	622.3166359	337.6678296	481.6051928	488.0111242	479.8830109	491.8764782
294.833958	129.1102004	125.6598503	1107.889822	1025.30265	881.4066609	374.9426287	372.7164885	341.3644162
4841.760624	4858.998086	3925.195342	4971.709701	4613.754742	4532.991896	4027.753074	4041.787369	4042.444981
209.8111679	154.2286032	0.001403199	220.1648274	360.4527172	373.1682932	0.001403199	0.001403199	0.001403199
523.0620153	984.7566569	676.0604954	688.5144759	1054.728822	911.1942785	536.7782799	435.9967346	674.5489524
0.001403199	0.001403199	0.001403199	333.362852	343.4121662	621.6315018	137.8772684	365.9786684	137.7634688
4500.78486	3905.367616	4329.957204	2887.904559	3317.030211	3601.592088	3750.56754	3221.015686	3610.170433
2794.576176	3720.094439	3323.85251	2059.590855	2102.518476	1991.157277	4121.120775	3826.444911	3110.625761
1505.891374	2384.259713	1448.304753	2186.634394	2258.892236	2619.652546	1943.959719	1985.344735	1925.554371
490.2558045	744.2050037	625.0258748	748.5778185	593.9807181	781.2377015	964.4143727	389.7151153	1017.513442
41869.76565	42348.14553	41486.14929	59662.51399	62992.57292	61640.04188	50313.94185	47091.6126	48975.69433
5103.130612	5544.398358	6249.691286	7969.208647	7466.533813	7479.285137	5107.008809	6074.497776	5800.786539
4849.733341	5287.412893	4120.059048	3042.609419	3049.055099	2740.123263	4764.229569	4141.55323	5459.153184
1185.055104	1143.703638	886.0916116	1714.411429	992.1819232	605.5132667	1039.266714	970.0527039	863.643057
8597.715321	8777.601773	8553.740474	9721.825415	9282.395708	9709.165722	6876.716661	6450.959933	7467.096484
4645.512911	4979.497751	4854.689473	4838.769002	5186.150624	4718.77373	4580.588245	4665.520869	4936.879785
1160.761581	931.3520058	1058.927499	74.70322382	0.001403199	0.001403199	869.1945137	728.3250552	970.4070151
603.767673	725.5559976	687.9772178	205.8496065	553.2976939	493.0045522	639.9172278	456.9712721	635.5873618
197.3592807	389.0956072	348.8505635	0.001403199	0.001403199	0.001403199	185.6520017	279.7240847	276.0980793
1475.418648	1670.964215	1299.369909	1442.68914	1362.290651	1335.015133	1572.90356	1379.120478	1663.751034
6294.765536	6012.745884	5438.855242	6527.95413	6380.050377	6134.704699	4383.268114	4248.231975	4547.67126
907.8756994	1067.56488	933.6120623	1006.650829	851.4163905	928.3924905	1198.792231	992.4117892	1033.586757
3871.276296	4279.839394	4052.167999	4646.510381	3950.157135	4280.825903	2922.997293	3051.425555	2973.670851
693.4239579	295.7478624	881.4672469	1006.497375	920.5726493	16.8211275	970.2006317	878.6299397	1009.256754
2027.640275	2089.285422	1875.463773	1704.732705	1661.187406	1704.855638	2342.603506	1924.365607	2452.237236
2968.069477	3014.392598	2813.450343	3107.641538	3071.10209	2504.02756	2186.724362	1913.605786	2086.231064
0.001403199	0.001403199	0.001403199	605.7721391	396.9389144	271.8217196	21.94381961	113.3388023	0.001403199
1862.270529	2280.296	2000.530731	1922.459595	1916.332676	1932.418213	1080.109494	1405.013629	1314.014511
10877.28856	9559.15467	9635.405202	9874.454342	10107.16709	9321.696437	12304.4645	11932.31219	13127.44435
8101.037229	7114.849335	6377.166138	7092.217849	6573.595613	6168.566139	8996.302463	8903.186418	9443.274882
2887.276628	2487.419288	2820.923723	2385.652066	2510.775203	2660.456424	3423.348856	3277.75606	4313.122517
5552.570435	4676.694526	5224.26483	5161.731766	4045.962119	3456.666149	6293.84286	6520.753674	6864.507082
24615.57107	22397.87626	22456.93484	25279.12	24224.08291	19756.40073	29981.28137	29760.78374	30375.94717
3654.219182	2529.229	3051.559429	3373.678259	2875.942531	2622.254135	3586.262962	3767.348571	4685.218153
2236.798419	1295.008118	1369.313597	2187.012542	2334.665435	1805.301755	2179.073818	2749.369234	3302.229103
645.4040339	969.5627887	1072.838781	1049.046329	860.0121579	570.9415335	1690.184291	2121.017853	693.6216086
9000.335359	7709.584975	7994.376722	9548.621392	8203.864454	6826.145729	10862.88621	10708.46877	11296.8329
1811.217463	1467.140936	1170.355701	634.1371815	503.4355684	773.1987248	2329.538934	2500.060196	1882.783051
6045.26058	4819.831018	3855.362803	5220.252704	4733.135784	4696.747902	7731.407002	6436.948145	7090.127556
8129.844775	6999.941554	7463.613794	415.8309086	446.4406387	469.0598103	7340.145569	6225.073187	7588.968596
3224.723172	2436.691046	2426.303539	0.001403199	50.36503296	95.77504491	2320.174903	1722.791788	2396.573894
4446.874212	4425.154617	4219.564655	5795.290076	6126.012195	5574.239792	4698.223881	4535.895921	4817.370188
886.9600342	964.4563699	704.3432398	1170.742216	1240.06659	1566.743041	505.7368392	102.4737816	648.5695885
4242.268417	3637.058113	3832.249623	146.3750257	458.3623012	427.984854	3759.107231	3163.109889	3446.700419
6551.613297	5879.431498	5714.421179	5437.242373	5005.920452	5023.601867	6902.041327	6466.785962	7602.370935
3864.751393	3334.920407	2997.954939	0.001403199	0.001403199	69.67624096	3351.023125	2690.75123	3708.909255
5649.773192	4970.010316	3793.843252	4543.217393	5071.273793	5229.657843	7005.655052	5053.542864	5620.325943
2089.89963	1912.651811	2025.026077	2332.973631	2078.967541	1619.638256	2564.647067	2653.710518	2531.235429
2650.838314	1980.948575	1881.520124	1867.372001	1435.039089	1720.963966	2465.872027	2131.930951	2356.615682
1602.890322	1705.791011	1524.839115	596.2653064	496.9083211	497.8844852	1602.27454	1135.827303	1622.315881
2118.015856	1930.986395	2356.207106	2703.754189	3184.276404	3233.470218	1878.228506	1871.025006	2341.6007
0.001403199	0.001403199	0.001403199	767.3854293	691.2029852	0.001403199	79.17301941	213.8365649	
40278.73269	40263.00254	41587.45748	64110.83337	65941.53474	65696.37937	47359.83714	43408.31469	48992.78525
4456.049032	3317.50793	3256.806432	5059.617913	4100.845353	3365.809087	3159.020531	2913.407244	3301.424961
0.001403199	0.001403199	0.001403199	1336.279915	1233.85316	1079.339709	0.001403199	0.001403199	0.001403199
3395.798268	3076.45382	2976.79421	0.001403199	0.001403199	0.001403199	2632.936749	2284.204575	2501.517832
1966.335777	1529.555711	1553.379746	0.001403199	0.001403199	0.001403199	1801.456605	1168.800827	1277.477344
1429.245146	931.5723712	1006.491083	2202.150621	2194.147569	2583.834027	1377.215794	955.12404	1240.626877
4473.99508	3426.61666	3746.776179	2333.435077	2357.382323	2241.091079	4746.106838	3739.227269	5146.602401
646.435826	498.9942763	376.2575012	609.2072416	493.2804651	642.8179168	606.2483849	450.5201555	675.664125
643.4681034	241.3804446	400.3247052	631.0610132	267.0113369	723.6577967	326.6679318	426.7500085	645.2651473
7317.797479	5923.247769	6326.027195	10433.5294	10851.28064	10430.73429	9493.440478	7256.926952	9914.742073
3028.889101	2448.697991	3208.828393	3978.428076	3526.924564	4374.162107	3418.269617	2996.121864	3835.947646
2.432349756	217.9812902	286.1641508	836.3565727	702.6416231	541.8935401	43.56582464	426.6437565	437.9926757
672.6920048	362.1308527	704.0796204	956.1158876	1102.272093	1018.440546	752.7316837	525.7389526	538.7763865
123939.0336	92309.64088	91520.6339	77389.68142	78409.34673	81003.35068	118497.114	87147.48606	112045.4543
1440.424159	951.2082591	1285.344218	1925.087169	1579.79031	2301.310784	1648.00901	1366.829804	2040.044318
2588.845015	1672.024275	1583.210391	984.2538598	1212.853882	872.1188947	2664.611701	1504.632618	2164.673663
449.4300661	428.1378094	373.2278775	405.5202922	445.7092243	372.5289419	536.2858477	324.4781137	372.2925938
2104.820301	2286.623174	1840.991804	1834.2813	2442.405332	2471.892841	3172.393894	1916.233398	2739.803788
512.4136001	164.3097599	239.9254977	1038.033578	482.8349661	794.1098094	178.6571976	241.5491066	341.0670098
2960.163299	2368.57931	1975.886704	1931.359152	2354.579487	2258.423027	3146.184808	1988.744617	2484.380998
2100.310048	1727.644755	2239.918196	765.0854616	1531.513624	1515.052346	1551.079479	1873.924927	1870.670087
7842.705752	6573.472653	6959.363211	7391.161909	9544.223906	9348.430233	7256.030217	5571.086042	7358.010652
964.5500443	988.3676623	1030.744391	606.7204604	858.605667	924.8613177	1373.190093	1047.447055	1564.58749
8024.537364	8040.745677	8390.903846	10808.09778	11841.21135	11240.41168	9180.998609	9586.680684	9938.729224
2360.784814	2233.380498	2179.070268	689.5711925	837.9435369	683.783909	2008.646049	1827.471163	2025.244647
943.1529024	892.2911059	895.2324718	1888.09969	2339.098056	2816.077292	1014.813823	1170.377621	1474.512657

5.30_360.1853m/z	360.1852879	5.302883333	neg
5.30_464.3020m/z	464.30204	5.302883333	neg
5.30_534.6158m/z	534.6157797	5.302883333	neg
5.30_640.1382n	685.1366135	5.302883333	neg
5.30_707.1192m/z	707.1192157	5.302883333	neg
5.30_775.1061m/z	775.1061378	5.302883333	neg
5.32_256.1556m/z	256.1556301	5.320233333	neg
5.32_264.0547m/z	264.0546505	5.320233333	neg
5.32_331.1307m/z	331.1306683	5.320233333	neg
5.32_419.1096m/z	419.1095832	5.320233333	neg
5.32_429.1381m/z	429.1381149	5.320233333	neg
5.32_453.1738m/z	453.1737924	5.320233333	neg
5.32_477.8657m/z	477.8657403	5.320233333	neg
5.32_490.2296m/z	490.2295887	5.320233333	neg
5.32_511.2179m/z	511.2178915	5.320233333	neg
5.32_521.1258m/z	521.1257676	5.320233333	neg
5.32_633.1006m/z	633.1006444	5.320233333	neg
5.32_668.2729m/z	668.2729486	5.320233333	neg
5.32_701.0885m/z	701.0884921	5.320233333	neg
5.34_164.9570m/z	164.9570486	5.3394	neg
5.34_179.0715m/z	179.071491	5.3394	neg
5.34_269.1015m/z	269.1015062	5.3394	neg
5.34_313.1273m/z	313.1272878	5.3394	neg
5.34_345.0935m/z	345.0935023	5.3394	neg
5.34_493.1693m/z	493.1693115	5.3394	neg
5.34_533.1308m/z	533.1307663	5.3394	neg
5.34_600.2854m/z	600.2853703	5.3394	neg
5.34_610.1271n	655.1260654	5.3394	neg
5.34_617.1058m/z	617.1057987	5.3394	neg
5.34_678.1136n	677.106364	5.3394	neg
5.36_230.1519n	275.1500967	5.361783333	neg
5.36_257.1008m/z	257.1008191	5.361783333	neg
5.36_335.1350m/z	335.135013	5.361783333	neg
5.36_344.2080m/z	344.2080278	5.361783333	neg
5.36_360.2395m/z	360.2395307	5.361783333	neg
5.36_386.1725m/z	386.1725498	5.361783333	neg
5.36_403.1138m/z	403.1137561	5.361783333	neg
5.36_461.0629m/z	461.0629107	5.361783333	neg
5.36_471.1012m/z	471.1011542	5.361783333	neg
5.36_539.0881m/z	539.0881612	5.361783333	neg
5.36_549.1184m/z	549.1183922	5.361783333	neg
5.36_605.0430m/z	605.0430365	5.361783333	neg
5.36_607.0772m/z	607.0772344	5.361783333	neg
5.36_685.0931m/z	685.0930661	5.361783333	neg
5.38_246.0755m/z	246.0750534	5.384216667	neg
5.38_254.1399m/z	254.1398802	5.384216667	neg
5.38_285.1345m/z	285.134539	5.384216667	neg
5.38_329.0702m/z	329.0702257	5.384216667	neg
5.38_411.1275m/z	411.1275463	5.384216667	neg
5.38_481.2444m/z	481.2443504	5.384216667	neg
5.38_490.1036m/z	490.1035534	5.384216667	neg
5.38_491.0637m/z	491.0636765	5.384216667	neg
5.38_523.1414m/z	523.1414107	5.384216667	neg
5.38_540.2534m/z	540.2533649	5.384216667	neg
5.38_548.1497m/z	548.1497033	5.384216667	neg
5.38_591.1284m/z	591.1284419	5.384216667	neg
5.41_145.0618m/z	145.0618171	5.406433333	neg
5.41_226.1682n	207.1503513	5.406433333	neg
5.41_269.2767m/z	269.2767375	5.406433333	neg
5.41_270.1581n	269.1507978	5.406433333	neg
5.41_282.9919m/z	282.9918861	5.406433333	neg
5.41_305.1274m/z	305.1273614	5.406433333	neg
5.41_328.1588m/z	328.1587954	5.406433333	neg
5.41_358.1612n	403.1612303	5.406433333	neg
5.41_422.1160m/z	422.1160096	5.406433333	neg
5.41_444.1779m/z	444.1778711	5.406433333	neg
5.41_463.0844m/z	463.0844346	5.406433333	neg
5.41_471.1486m/z	471.1486096	5.406433333	neg
5.41_531.0717m/z	531.0717017	5.406433333	neg
5.41_533.0688m/z	533.0688782	5.406433333	neg
5.41_541.2657m/z	541.2657287	5.406433333	neg
5.41_558.0913m/z	558.0912958	5.406433333	neg
5.41_561.2909m/z	561.2909067	5.406433333	neg
5.41_567.1675m/z	567.1675289	5.406433333	neg
5.41_569.2070m/z	569.2069676	5.406433333	neg
5.41_599.0597m/z	599.0597038	5.406433333	neg
5.41_599.2247m/z	599.2247408	5.406433333	neg
5.41_637.1947m/z	637.1947124	5.406433333	neg
5.41_677.0758m/z	677.0758416	5.406433333	neg
5.41_697.2658m/z	697.2658477	5.406433333	neg
5.41_745.0633m/z	745.0632669	5.406433333	neg
5.41_745.2284m/z	745.2283516	5.406433333	neg
5.41_773.1693m/z	773.1693334	5.406433333	neg
5.41_793.3596m/z	793.3595952	5.406433333	neg
5.41_881.0376m/z	881.0376361	5.406433333	neg
5.43_216.1241m/z	216.1241496	5.428733333	neg
5.43_246.5767m/z	246.5767007	5.428733333	neg
5.43_266.0179m/z	266.0179223	5.428733333	neg
5.43_269.0354m/z	269.0353633	5.428733333	neg
5.43_294.0574m/z	294.0573881	5.428733333	neg
5.43_321.0933m/z	321.0932938	5.428733333	neg
5.43_330.0046m/z	330.004639	5.428733333	neg
5.43_335.0258m/z	335.0258397	5.428733333	neg
5.43_345.0546m/z	345.0545602	5.428733333	neg
5.43_349.1507m/z	349.150708	5.428733333	neg
5.43_355.0098m/z	355.0098459	5.428733333	neg
5.43_358.1217n	357.1193324	5.428733333	neg
5.43_362.0448m/z	362.0448155	5.428733333	neg
5.43_392.9846m/z	392.9845853	5.428733333	neg
5.43_397.1846m/z	397.1845598	5.428733333	neg
5.43_405.0101m/z	405.0100559	5.428733333	neg
5.43_413.0420m/z	413.0420201	5.428733333	neg
5.43_418.2449m/z	418.2448605	5.428733333	neg
5.43_430.0321m/z	430.0320895	5.428733333	neg
5.43_441.1486m/z	441.1485787	5.428733333	neg
5.43_465.9793m/z	465.9793137	5.428733333	neg
5.43_481.0295m/z	481.0295038	5.428733333	neg
5.43_490.9849m/z	490.9848872	5.428733333	neg
5.43_498.0199m/z	498.0199395	5.428733333	neg
5.43_499.1071m/z	499.1071375	5.428733333	neg

2275.592462	1743.873631	1970.419359	2166.486059	2226.415532	2893.539815	1738.271302	1121.1424	1749.972922
1184.828154	1745.275408	1613.652791	337.8616758	362.4534036	483.2453128	1939.843225	1276.962213	1873.347972
793.7076997	427.5611312	733.1067193	669.8473746	733.4374201	599.846197	694.9717279	589.8587634	962.969587
7091.739019	6919.757434	7605.674455	0.001403199	0.001403199	0.001403199	0.001403199	80.72444534	125.0458109
2926.231586	2743.316848	3134.250018	0.001403199	0.001403199	0.001403199	348.3237182	0.001403199	0.001403199
2365.493552	2747.397959	2092.374403	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199
663.7879411	742.1291607	790.0157703	782.0998336	1127.165193	1177.0826	1065.881434	868.0647231	1265.268286
582.3615778	548.1350488	725.3471493	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	35.15849823
388.1531268	624.207812	715.1314941	806.9225173	1271.278093	1170.694002	690.9598938	444.6703492	700.2742696
647.1766259	755.1435313	1060.730452	704.7177963	1673.109351	1271.935397	1016.32813	773.4002075	1334.274558
10954.35282	10122.87885	13475.57198	11286.12611	17445.2481	16829.26628	13967.25451	12918.00395	18032.79688
2140.816325	1701.3913	1970.985432	847.7188316	901.5694197	919.1982843	1355.813041	1296.877849	1812.747303
3227.073142	2814.851348	2923.049716	3525.493973	3412.168309	3132.952962	4140.179961	2671.773612	3969.547374
1250.565155	1447.464959	1898.131931	2371.059408	2987.626192	2988.392433	3662.794648	3716.892	4921.209629
298.1561188	1009.741622	736.5262707	659.8943248	367.3409278	610.7465119	1064.173959	1076.430782	1259.598704
2350.38251	1620.03943	2304.622711	5506.927094	5620.768628	5091.71963	2560.380897	2033.977556	3857.124493
1914.24864	2193.965774	2930.634804	1877.121605	3193.254664	3317.161941	2855.752333	2414.322078	3935.311971
3685.848738	3830.533319	4727.6291	3935.370453	6079.611811	5945.178133	3714.678531	4783.719941	3816.734368
931.3103939	1440.347682	1200.127802	940.5052326	1742.025977	1453.241166	1035.127663	1406.131628	1924.277708
336.0665235	393.1483276	344.3832022	513.1532347	521.8568222	693.0785569	509.0615944	351.8929672	542.996028
442.1435729	281.5273685	517.0610566	464.2092991	585.3327647	622.3099685	482.6142465	397.3309142	490.2271708
381.2647594	283.9259407	383.8686397	416.4804122	434.6737818	356.127431	251.5508478	224.8198738	477.994857
3497.911387	3347.81157	3020.83753	2989.095931	3165.87181	3177.171411	3191.802218	2335.278804	3249.154042
970.2306761	968.5791235	1027.238066	910.1110484	859.5898153	812.2534172	453.1367295	539.7379186	741.6294512
999.608357	1244.408456	1775.471821	1606.447406	2809.940777	1562.599677	996.1546094	1412.197831	1342.553862
2155.982404	2354.049057	2455.854545	597.5165756	408.7785348	682.9265111	0.001403199	0.001403199	0.001403199
70598.89157	76885.70676	91015.40329	88793.19593	121829.1015	104546.6196	76227.38709	81840.12392	92828.55685
5420.398066	6378.154002	6708.730144	0.001403199	25.75687159	28.82810898	0.001403199	22.56232699	156.9431843
16615.98515	16035.6136	15277.16397	5451.788935	5817.784324	5182.075811	16949.60024	14302.01122	18223.59321
4370.333135	3172.993885	3997.190413	46.08325718	24.07203626	133.1516985	73.39949734	51.599017	192.1266227
1929.825726	2095.666317	2574.328782	2176.833403	2283.957153	2435.036794	2150.612604	2001.32806	2463.312631
6186.538619	6430.912712	6431.334669	6134.410622	6611.117238	6668.172705	7148.556186	7836.534354	8372.017608
2547.794153	2798.853798	3181.04623	2905.025392	3082.799679	2570.625641	2555.197341	2819.61983	2741.96921
2802.44734	3298.276265	3515.042407	3152.636386	2876.422971	2607.375033	2813.236956	3728.782999	3734.753593
426.0427159	669.6289586	805.7357453	655.9873938	510.0900148	686.0665716	360.6904521	756.2076554	785.0276439
1058.635712	587.7752887	1084.923603	215.817036	1943.606668	2343.46088	681.9756356	1415.436643	1532.037374
4421.568648	4385.04725	4739.979647	1153.079054	1078.065943	1275.133245	3522.01216	3852.656985	5016.103727
1097.620805	960.7775306	795.2327339	704.551548	930.4089713	766.0686494	940.744732	1429.057533	1276.016629
2239.11356	2515.878122	2926.840782	704.9382251	789.1413641	869.5632268	2373.611041	2322.815689	3331.852762
2473.334786	2316.87149	1996.459614	842.9818943	661.8812225	1217.024855	1497.385739	2022.785743	3465.318614
29654.71787	30272.6257	30392.52625	11841.56682	11683.27486	11739.5074	31198.82846	28254.63951	33242.1973
1783.721672	1712.573315	1875.662014	1391.119182	1811.790506	991.224833	1030.662126	1144.227054	927.4503536
1132.737024	1644.688299	1677.561402	467.8527338	821.2867211	699.8774302	1569.589211	973.6818085	1389.772618
9246.74196	8759.819163	10427.3847	2447.391588	3682.884798	3230.703679	10324.36281	7933.480708	10699.32851
35576.94465	35352.45105	37270.44496	4399.913342	4621.159374	46359.16466	39572.09829	3991.2	3886.41523
444.4203688	469.5665721	426.8503634	432.6715574	257.9328404	296.0390094	585.9590074	650.9950925	458.3070305
3473.721892	3532.385941	3218.666946	5017.616795	5844.780298	5761.645654	4098.816048	3534.317114	4037.973784
1872.067927	2085.936843	1828.817323	3461.107774	3348.763374	3440.241942	2129.197252	2688.546093	2532.939629
4440.687368	5018.35071	3941.411499	3485.144869	3505.142544	3950.442368	4424.257806	3757.882487	4543.696268
3566.070373	4010.023926	4004.744579	4712.849896	5322.851667	5014.92265	4052.538701	4380.005886	4582.140878
1518.187685	2039.286655	1831.571229	3112.648415	3696.326611	3561.193029	2785.756818	2625.791501	2424.284827
743.4522311	867.1874399	1235.107073	846.4139602	1033.879416	984.0500784	0.001403199	125.1597885	93.07703375
4260.675043	4979.917236	4614.577951	6032.53414	6381.09306	6231.489388	4639.56535	4157.309339	4350.154866
671.6375443	1261.182511	1216.530519	1199.92028	1658.240109	1353.201306	861.7412634	1097.978424	711.1722718
178.4587708	249.1755037	347.1547174	393.8377008	0.001403199	450.9119465	0.001403199	0.001403199	0.001403199
854.8653993	1735.697921	1729.029321	1121.157639	1071.632138	852.2035734	1053.59777	1452.140884	1228.43556
211.908533	220.8484179	230.792603	457.0428101	408.6544023	327.1139704	306.47484	325.121851	263.2599364
1229.398161	1488.268978	1314.859041	2636.241332	2766.379737	2700.976047	1823.797431	2000.85413	1486.468985
121.8945356	106.0194194	217.0788647	439.3060611	395.8094113	326.3377781	404.3987435	204.3517268	84.5475665
250251.8093	290307.1074	275811.1934	268385.6138	495568.3641	493962.2543	375533.3043	401353.8913	313554.9123
1604.603093	1830.259189	1710.168127	412.9504233	389.9279587	369.1847331	1151.63311	948.4889469	1110.846531
510.1871487	838.9281918	710.4585545	1235.568485	1115.534428	1137.763758	867.8724776	884.4152794	743.9860688
187.726004	216.0238883	225.4401403	508.9516332	459.5851666	277.0063588	429.5899584	452.1699219	392.9020318
14390.17034	15905.58235	16538.10783	17716.85787	16870.84042	18076.73434	18352.53778	18979.71286	17498.87317
1862.422877	2280.103992	2542.19972	4028.012877	3891.964785	3506.21758	3014.564508	3021.510889	2557.729513
309.5318737	148.6434465	178.6181895	0.001403199	403.7780333	0.001403199	0.001403199	217.0337524	174.3485185
4147.220467	5028.188897	4727.939095	8903.193487	9723.378723	8650.646734	6979.295037	6928.785649	5382.382803
1603.532525	1403.858348	1557.019426	1935.534624	1651.537792	1430.819838	1625.312677	1694.950111	1848.269359
3217.590924	3234.358001	2503.375872	5329.267184	5265.037221	4545.053517	3998.368772	4083.390749	3383.111646
621.8349868	412.7405558	613.9016952	1347.813964	1554.81286	1083.243473	1213.089262	888.9275665	839.8439124
133725.5818	150836.7513	151248.77	153624.7887	164301.9527	161089.8359	163043.5435	163863.6048	148700.9281
1222.470837	1376.259295	1494.844512	2795.759536	2764.040599	2846.909049	2423.373254	2214.794655	1785.320419
2702.349676	4072.873887	3533.450549	13321.41235	11165.68479	11132.27949	4907.072134	5320.250979	3556.303115
1757.053506	2441.037167	1809.564157	2870.192408	2959.414473	2598.388581	2204.084687	1971.853658	1444.073814
3844.749298	3885.234116	4400.684526	6001.210337	4938.623604	5402.785945	4163.544099	5463.838074	2784.279769
2158.556083	1920.381129	2568.444161	4076.439982	4488.5006	2954.853977	2676.228358	3037.176354	2553.918573
2938.494113	3141.677016	3283.650442	2500.263859	2099.273881	1349.893576	3757.968484	3223.378906	2685.645782
2844.487643	2624.631129	2947.42363	4382.504665	3621.311109	2863.828293	2509.931445	3399.113261	2149.288949
7503.232201	8379.689556	6847.215733	15047.59004	15012.26614	14125.75823	12049.98346	10704.41948	9922.307944
720.4804058	1087.971625	493.843382	3249.042723	2286.562556	2393.028646	977.7047966	1556.112198	1166.916201
6816.55916	5011.853662	5429.757739	12336.94547	10489.37985	10016.09597	9513.400875	9125.095634	6914.753863
4649.61274	5814.729073	4963.371649	5807.130995	7070.920468	5193.614614	5497.835608	5482.206169	5363.156871
1182.841317	1856.605905	1637.363077	1573.435656	1570.223241	1765.260238	893.833888	1917.299229	849.8877336
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12262.86777	11684.94274	12549.58993	16327.49516	18007.31925	17295.43709	15508.37936	15736.89348	15577.6333
2234.974225	2977.197006	2736.230084	1733.624247	1788.463488	1799.389037	2442.785166	2274.863862	1901.125719
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605.2761526	776.0707029	524.6516621	290.4570011	529.9475849	280.4662798	504.088046	241.06147	518.9799336
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6597.47561	6840.51601	6798.145707	4931.438747	4615.04262	4505.325964	6257.93148	6769.371081	5228.256881
38814.75222	42187.01165	41407.33029	29502.60684	29606.12491	29456.44436	37705.49434	37815.23044	30512.36607
3849.773027	3166.13657	3277.040708	4714.086629	5059.792959	5330.049182	3580.453388	3103.914268	3597.51616
1558.0582	1096.525714	829.3277017	611.7196131	314.5786908	383.4577558	369.0617166	845.4715424	701.5969159
6025.330007	6566.500801	6817.309401	4571.720392	4554.725175	4789.415869	6887.080561	6722.593139	6226.054902
4420.503539	4474.663839	4370.909142	2543.539762	3431.56304	2594.204113	3814.222903	4234.389791	3170.46248
428.8959599	459.1528655	455.5272223	133.2944767	268.8241739	253.2926051	329.5538453	562.7394829	572.074109
9368.927478	8565.732888	10071.13738	13403.45637	11764.38636	10910.53338	8158.503917	11117.16094	8969.073345
1721.638206	1669.256377	1383.472357	1018.142664	892.8332014	783.3867239	1514.871382	1368.194878	801.1453071
29620.38158	31437.93618	31158.76074	21301.55377	21711.80483	21621.19848	29545.65071	29869.16757	22793.62903
2065.32321	1951.071223	1930.901938	3752.878257	3881.180277	3887.616645	1483.174979	1849.450344	1940.095637
3492.208137	3226.219597	3098.379673	2508.541247	2380.679414	2141.347923	3091.155988	3527.735271	2207.283614
11101.3853	12735.13711	13044.12419	5731.549389	4436.154253	5832.907397	5083.324712	8530.610967	6835.83028
1033.05331	1411.214194	887.1857969	770.2934204	889.4853892	668.5458376	826.5177378	945.8126989	641.6439885
21387.82039	23247.21257	22405.89914	15427.347	15054.46155	15602.98739	21882.19347	21195.59796	16345.32139
2683.144898	1971.516609	1900.648729	606.7643796	663.8444046	872.8543674	1341.602712	1572.440636	1071.866631
2685.527656	2847.058304	2733.050359	1481.685437	1857.1924	1887.971004	2589.856772	2648.742478	1772.005424
1786.503148	1707.964919	1674.566652	730.7739744	485.4753876	950.4381209	650.9677166	862.8548737	660.9918773

5.43_509.1360m/z	509.1360345	5.428733333	neg
5.43_534.1550m/z	534.1549942	5.428733333	neg
5.43_538.9885m/z	538.9884755	5.428733333	neg
5.43_549.0171m/z	549.0170834	5.428733333	neg
5.43_554.2193m/z	554.2192991	5.428733333	neg
5.43_577.1238m/z	577.1237505	5.428733333	neg
5.43_602.1425m/z	602.1425092	5.428733333	neg
5.43_606.9759m/z	606.9758536	5.428733333	neg
5.43_617.0044m/z	617.0044101	5.428733333	neg
5.43_651.1009m/z	651.1009289	5.428733333	neg
5.43_674.9634m/z	674.9634067	5.428733333	neg
5.43_684.9918m/z	684.9918108	5.428733333	neg
5.43_752.9791m/z	752.9790997	5.428733333	neg
5.43_781.0864m/z	781.0863705	5.428733333	neg
5.43_820.9658m/z	820.9658238	5.428733333	neg
5.45_292.0360m/z	292.036044	5.451166667	neg
5.45_438.0397m/z	438.0396754	5.451166667	neg
5.45_448.1619m/z	448.1618541	5.451166667	neg
5.45_477.2345m/z	477.2344704	5.451166667	neg
5.45_505.0794m/z	505.0794003	5.451166667	neg
5.45_619.0744m/z	619.0743842	5.451166667	neg
5.47_210.9838m/z	210.9838074	5.471616667	neg
5.47_262.1484m/z	262.1483592	5.471616667	neg
5.47_273.0441m/z	273.0441391	5.471616667	neg
5.47_294.9536m/z	294.9536077	5.471616667	neg
5.47_295.1300m/z	295.1299836	5.471616667	neg
5.47_311.1616m/z	311.161564	5.471616667	neg
5.47_312.1279m/z	312.1278865	5.471616667	neg
5.47_386.1906m/z	386.1906346	5.471616667	neg
5.47_509.0741m/z	509.0741239	5.471616667	neg
5.47_550.9211m/z	550.9211016	5.471616667	neg
5.49_179.9365m/z	179.9364929	5.489016667	neg
5.49_286.6171m/z	286.6170618	5.489016667	neg
5.49_430.2278m/z	430.22781	5.489016667	neg
5.49_441.0869m/z	441.086938	5.489016667	neg
5.49_457.2086m/z	457.2085966	5.489016667	neg
5.49_505.1926m/z	505.1926362	5.489016667	neg
5.49_826.8537m/z	826.8537322	5.489016667	neg
5.50_264.9344m/z	264.9344166	5.497816667	neg
5.50_287.0514m/z	287.0514738	5.497816667	neg
5.50_338.0707m/z	338.0707392	5.497816667	neg
5.50_355.0390m/z	355.0390109	5.497816667	neg
5.50_423.0266m/z	423.0265796	5.497816667	neg
5.50_544.2846m/z	544.2845966	5.497816667	neg
5.50_570.8373m/z	570.8373772	5.497816667	neg
5.50_589.1500m/z	589.1499601	5.497816667	neg
5.50_654.8700m/z	654.8700384	5.497816667	neg
5.50_704.8156m/z	704.8156257	5.497816667	neg
5.52_361.1507m/z	361.150741	5.516816667	neg
5.52_410.1042m/z	410.1041849	5.516816667	neg
5.52_453.1745m/z	453.1744588	5.516816667	neg
5.52_497.1263m/z	497.1262968	5.516816667	neg
5.52_696.0357m/z	696.0357106	5.516816667	neg
5.52_837.1800m/z	837.179966	5.516816667	neg
5.52_950.9948m/z	950.9947956	5.516816667	neg
5.53_290.0529m/z	290.052926	5.525416667	neg
5.53_363.1666m/z	363.1665692	5.525416667	neg
5.53_384.1424n	383.1351134	5.525416667	neg
5.53_397.0674m/z	397.0673983	5.525416667	neg
5.53_399.0645m/z	399.0644516	5.525416667	neg
5.53_424.0865m/z	424.086488	5.525416667	neg
5.53_443.1750m/z	443.1749634	5.525416667	neg
5.53_459.2239m/z	459.223922	5.525416667	neg
5.53_465.0545m/z	465.0545427	5.525416667	neg
5.53_477.1344m/z	477.1343528	5.525416667	neg
5.53_480.2968m/z	480.2968249	5.525416667	neg
5.53_482.0157m/z	482.0156963	5.525416667	neg
5.53_533.0421m/z	533.0421014	5.525416667	neg
5.53_540.2535m/z	540.2535471	5.525416667	neg
5.53_543.0710m/z	543.0709773	5.525416667	neg
5.53_550.0033m/z	550.0033351	5.525416667	neg
5.53_560.0612m/z	560.0611891	5.525416667	neg
5.53_568.2436m/z	568.2436337	5.525416667	neg
5.53_601.0294m/z	601.029421	5.525416667	neg
5.53_628.0485m/z	628.0484783	5.525416667	neg
5.53_669.0175m/z	669.0174634	5.525416667	neg
5.53_679.0457m/z	679.0457115	5.525416667	neg
5.53_737.0051m/z	737.0051057	5.525416667	neg
5.53_747.0331m/z	747.0331357	5.525416667	neg
5.53_815.0205m/z	815.0205238	5.525416667	neg
5.53_883.0082m/z	883.0082019	5.525416667	neg
5.55_288.1066m/z	288.106591	5.547916667	neg
5.55_320.1539m/z	320.1539025	5.547916667	neg
5.55_329.1973m/z	329.1973049	5.547916667	neg
5.55_443.1923m/z	443.1923242	5.547916667	neg
5.55_453.0863m/z	453.0863278	5.547916667	neg
5.55_481.2056m/z	481.2055921	5.547916667	neg
5.55_521.1255m/z	521.1254582	5.547916667	neg
5.55_537.2347m/z	537.2346793	5.547916667	neg
5.56_427.1608m/z	427.1608001	5.56185	neg
5.56_454.8489m/z	454.8489441	5.56185	neg
5.56_533.2342m/z	533.2341932	5.56185	neg
5.56_667.2124m/z	667.212418	5.56185	neg
5.56_694.2312m/z	694.2311762	5.56185	neg
5.56_762.2182m/z	762.2182087	5.56185	neg
5.56_881.2031m/z	881.2030726	5.56185	neg
5.57_1017.1772m/z	1017.177198	5.57225	neg
5.57_267.0850m/z	267.0849602	5.57225	neg
5.57_313.1273m/z	313.1272958	5.57225	neg
5.57_403.1975m/z	403.1974732	5.57225	neg
5.57_428.9619m/z	428.9618809	5.57225	neg
5.57_491.2135m/z	491.2135087	5.57225	neg
5.57_535.0559m/z	535.0559134	5.57225	neg
5.57_604.2620m/z	604.2619948	5.57225	neg
5.57_745.2286m/z	745.2285935	5.57225	neg
5.57_871.1737m/z	871.1736834	5.57225	neg
5.58_273.9031m/z	273.9030931	5.584533333	neg
5.58_274.1485m/z	274.1484888	5.584533333	neg
5.58_289.0671m/z	289.0670958	5.584533333	neg
5.58_295.1166m/z	295.1165755	5.584533333	neg

5042.697543	6003.842971	6085.050383	2160.375575	2554.715201	1992.820709	2362.52171	3224.14778	2755.263175
1494.598246	1556.884935	1798.070621	4117.184636	4690.960994	4334.119412	3327.979705	3108.394223	2537.94065
4272.992341	4110.819461	4290.650189	2955.07828	2632.623374	2614.494352	3890.402742	3586.073338	3011.941576
19123.16484	19092.81614	17910.34002	12691.80793	12684.2155	11712.31819	17091.90704	17589.32642	13840.10922
694.1072298	449.8021884	652.7436496	1277.1528	1342.539211	1452.510401	270.0706911	259.0714119	642.1517562
3080.448227	4462.198305	5024.879446	2028.484824	1389.669582	1351.402174	2338.565008	2704.625697	1778.479419
920.27515	1343.265171	1120.77426	2627.652029	2860.804394	2611.922956	2219.847318	2033.517223	1319.692699
2822.366145	2681.498884	2733.935637	2055.479604	2074.805341	1600.353736	1620.248501	2620.060928	2122.750954
14435.54073	15446.43045	14955.63914	8867.974733	10440.94747	10000.26031	13908.64885	13287.25742	11305.86461
2126.930633	1617.821063	1765.422631	1492.566221	1636.211329	1522.826572	0.001403199	0.001403199	0.001403199
3443.095829	3106.72776	3205.827285	2009.532192	1890.221545	1870.549985	3539.673436	2398.007204	2674.172448
12422.6923	13194.26973	13184.18147	8530.136329	8881.94491	8367.927309	14164.70572	11945.93078	8344.119368
7323.211102	7864.743041	6931.509449	4648.882856	5964.101856	4187.723754	8019.254115	7414.624121	5890.69826
2583.769542	2567.837375	2412.28609	985.7713759	737.0072214	627.6263088	620.3848649	1597.521521	693.0182473
3552.656344	3573.897826	4707.221786	2772.286671	2520.922721	3070.128663	3265.910695	3218.581263	2769.446866
660.2512148	628.3384929	728.8863078	299.3382793	299.8944738	133.8019388	429.3334189	526.6566238	530.5366349
1193.248962	1189.359785	1347.303948	483.7997113	469.6654765	271.0274948	1074.406687	950.6650797	927.7939169
443.5784698	353.8541275	601.1202986	690.4074803	668.8940385	419.8341606	1117.256738	839.0077734	885.4015631
15127.26385	13327.17632	13921.85485	15258.43255	13971.6931	11309.47764	22729.25109	20851.48948	20278.2419
1084.370833	1106.882436	1024.704127	1138.931574	1175.816488	1661.29998	85.51436068	0.001403199	193.4303087
4597.722869	4196.407236	4618.335126	3616.581234	3984.614429	3406.950121	438.621333	145.3792533	325.636086
391.8439966	231.2206159	297.9083193	327.5018339	370.7647574	415.4862846	487.5581278	373.398174	366.944475
318.1100462	345.6597334	337.8660372	371.5876347	477.8045344	466.3711822	723.0969081	420.5967626	361.9893562
699.8712824	516.0393327	499.7391058	356.8496376	268.4094424	263.043368	634.5635976	616.1988182	320.8351333
644.6894365	526.0094264	513.0499942	581.6847595	697.8870621	710.2656972	692.8020046	703.6711841	662.9223238
1544.74303	1417.41282	1250.393597	1513.003107	1471.7856	1483.014651	1364.551	1056.621834	1146.808488
3110.623535	2795.616956	2416.85957	3538.988955	3740.27956	3787.013909	3384.572358	2278.772767	2693.605989
330.8513433	502.0410479	509.7069994	145.9029186	59.79840808	153.1041373	535.6320252	462.6895365	547.5198435
291.8851564	262.0608611	255.6462978	0.001403199	97.78872803	0.001403199	288.7937692	323.1760178	205.5931782
891.9090278	836.9497806	836.8737004	758.3654484	601.4404583	786.7634107	549.0829765	371.3968003	267.1166058
1559.341183	1265.342163	1201.482816	1226.167767	1872.854281	1923.501071	2582.102199	787.6681631	1732.053976
390.4890607	232.1874968	259.1470989	208.1856593	371.6045427	277.8285867	534.5052501	401.4286899	268.7951685
197.5860545	162.982101	151.5767405	288.3802234	308.3672083	298.9914039	204.1190971	201.5171829	138.0556268
2383.851073	2154.134919	2174.436215	1529.210364	1138.684448	1668.314685	2769.676573	2359.772432	2424.903674
1370.985916	1032.809731	971.6086778	1032.397708	780.5152633	947.6307208	404.8861196	488.166687	449.611954
2165.055468	2853.862358	2018.910283	3217.109823	3230.25979	3313.906089	2160.434541	2497.697919	2384.052062
1184.801117	1180.390744	1104.293081	406.8466276	498.6554248	800.120811	1163.605593	1212.973121	1052.100472
2371.403236	1307.761981	1164.324764	1207.482861	3292.985307	2361.962957	3021.18589	1977.781219	2357.573246
3084.36544	2390.119029	2211.251875	2676.366747	3289.811055	2874.587759	3403.374993	2803.636383	3054.264881
3211.664856	2689.342145	2588.888841	2901.421149	3450.82129	3491.724675	3262.899505	2533.502472	3400.295877
3178.955242	2326.869299	2483.600594	2623.443029	3002.921029	3529.928931	3625.429783	3927.10404	4609.040078
2419.911067	2231.575787	1881.904602	2044.073449	2225.979411	2366.732391	2030.658466	1894.863737	2186.975914
1169.999712	903.0593442	1042.502307	789.8659145	1558.53866	1012.801177	1172.180005	1116.884914	1086.382381
1232.245286	1572.558243	1674.83642	946.0515659	2591.59619	1494.833631	1243.318789	1406.162283	1035.732151
11904.4191	9524.03468	8499.331084	9271.047708	11313.90346	9399.432595	15670.92425	11129.56545	13964.13972
938.5652921	867.8023444	326.616891	446.8796983	416.4956464	445.5850748	250.2571854	506.3733311	538.4046718
8484.275042	7937.778383	6486.080758	7644.344243	10643.89327	9168.826346	12468.77423	7929.09826	9357.394699
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23302.46838	19621.08992	18142.2734	16440.87949	19749.46793	18371.70573	20656.2184	18960.00974	22710.44774
302.8907701	96.34310164	187.7530471	0.001403199	75.14801448	94.4839054	101.0016175	187.3831821	170.5699889
6272.07058	5451.633688	5756.851316	5557.578086	7182.214975	6409.042663	5166.287473	5811.513724	6424.141804
2505.102323	1821.851674	1352.466393	1298.009822	2043.765094	1454.103451	2180.796807	1376.533666	1934.956684
1388.44767	2244.837338	1732.494877	508.228453	223.8016701	526.5311623	1024.732588	1682.834619	1701.450337
834.2039018	1510.781497	1154.940008	0.001403199	0.001403199	0.001403199	622.3421005	800.5568386	950.7013442
3606.285092	3307.466672	3289.874119	912.8899561	1452.113844	746.2729108	3206.321665	2487.692917	3169.016314
1816.827963	1376.132179	1455.707515	784.5003883	959.6671005	821.6753128	549.4530836	526.0740967	611.8065686
7003.168391	5781.884154	6036.377596	6582.992099	8461.205684	7440.960275	6300.854262	5400.242142	6399.896783
23640.91743	20010.69282	20030.40292	24623.04842	27686.40052	24490.77195	24670.43861	23212.39474	24238.01516
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41012.2939	36986.90312	39381.96424	45989.72465	56665.64735	44486.13246	37010.55114	37616.64805	37125.12674
6551.53898	6021.333826	5241.184627	5883.343681	6716.37367	5732.054883	4190.6821	4417.527562	4120.967091
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8257.231459	7817.888929	6905.297918	2428.216264	4021.449989	2578.014338	6355.99161	6057.438321	7561.950117
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42346.08494	37560.0858	34987.414	13830.15179	17288.88083	14974.79067	31342.78856	29622.22728	38660.86023
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3367.612166	2749.401659	2477.047883	998.6448352	1487.562118	872.2981782	2693.090092	2035.687225	3158.148284
152.4292605	0.001403199	0.001403199	1316.497883	1608.38514	1149.401048	729.9046949	269.5026054	1099.189084
6314.281513	4807.684544	4884.793889	2051.040767	2658.093785	2215.532782	4797.206353	3940.219278	6229.010734
2645.403756	2416.798297	2231.030974	566.6213345	902.4652488	562.6971777	1644.561454	1758.19696	2452.993425
4790.507101	4118.659456	4286.333768	1080.680688	1844.83958	953.4999444	4130.933365	3145.76288	4416.798114
19721.0341	16646.82042	15434.91213	5947.507665	7628.835092	6509.492601	13938.86191	12268.54372	17475.006
3480.245079	3506.292931	3546.898692	394.4543861	1643.139334	537.2779666	3523.734152	2588.973948	3655.116878
13082.4927	12088.39825	11244.87581	4916.495156	5646.101845	4974.11255	9391.575484	8160.76536	11714.03435
9923.226228	8863.526169	8853.037867	3184.884198	3623.641013	2763.307776	7054.336265	7488.687231	9450.609641
7389.210416	6654.993695	4993.500381	2006.145564	2197.897087	1991.896869	5197.489453	4812.485389	6653.889394
1163.835459	948.121328	1186.947964	810.1338302	1366.151197	952.881557	778.5858319	1061.561518	1032.513724
7780.907357	6134.935723	6662.045513	7759.06218	10020.45744	8819.715927	8289.308409	8423.579666	7572.671318
1675.075016	1581.458812	1393.40167	1615.304595	2355.74291	1568.604012	1720.677495	2120.705268	1939.003671
8655.007475	6612.656313	7270.778372	5033.066383	6129.65162	4703.346932	6662.026013	6728.459804	6787.637566
1041.625337	1075.987612	1259.9076	1747.436979	2219.581996	1966.005791	1079.217541	1359.403923	865.5786847
1173.41775	988.3619047	1164.893517	659.4431408	1171.553482	749.2137748	846.8081559	445.6245918	767.4685628
9679.707238	7834.284449	9551.414278	10154.58284	12189.39559	9945.808153	7897.088526	8212.590922	7792.665143
4931.450505	4163.033534	4942.069466	4864.983375	5790.007938	4921.679012	4615.772265	4676.124843	4143.961133
1948.662157	1304.159654	1582.968043	999.8423309	1219.354425	1282.569652	1710.128995	1610.146872	1516.087506
2496.745315	1630.267002	1322.083501	1355.247722	1463.830449	1080.639327	2081.233194	1386.924766	1477.442729
964.5506142	429.7183843	0.001403199	1266.615096	1556.478447	1593.266596	775.7972698	968.5040092	442.363415
8523.958267	7722.293641	7860.460474	10186.15108	13607.91927	11583.88262	6686.683155	7417.755482	5210.826358
3133.362376	2451.583686	2966.621636	3376.55236	4916.332363	4728.614615	3465.958578	2834.288537	2495.745839
1896.958988	2377.462355	2036.993096	3368.136588	3868.60048	4319.520203	1728.963261	2031.458953	1937.375838
15936.05081	12041.37953	12913.13679	20968.55185	24473.3542	18194.95595	13113.94008	15077.8971	11578.0052
4543.190802	3718.511074	2510.638784	6343.451174	7582.919802	7111.385987	3603.278481	5295.654054	4247.822632
994.0145799	614.6519978	644.8935622	920.9032986	717.5838447	958.5780097	639.1211472	524.4470749	574.2624605
2003.798211	1883.425566	1867.796477	1410.697901	1783.213331	1236.620263	2483.058227	2043.451312	1710.850301
338.2066756	168.6325402	154.5806948	527.9854309	403.0838137	409.412224	1749.875296	1635.33971	1122.958817
6225.769775	4624.474668	4403.715885	4988.764452	6013.398586	5020.781443	7584.098851	5351.993866	6069.754098
2922.910374	2931.481823	2683.481476	411.356662	389.2942342	408.2375945	1389.592185	1597.278679	1073.382983
11591.13079	9404.760991	11199.55878	13616.2837	14708.76574	13665.58273	12398.89269	13883.35752	12348.19508
3075.191391	1903.284919	2326.854581	3888.983775	3902.723563	3899.080946	2241.37991	2273.554886	2047.200079
38383.20142	33434.73705	34781.23301	51197.39934	59789.25099	50965.44688	36370.98909	35647.15336	28760.60578
1996.496483	1562.157423	2212.908697	2933.755234	3740.828297	4245.407957	1673.124173	1789.062897	1905.299697
1162.8924	745.0268212	981.0173504	989.0631911	1277.572309	1075.217179	1531.663728	933.0565491	1144.345714
2820.190657	2286.3402	2235.804743	3724.278121	4429.796372	4749.017264	2813.549683	2838.212997	2504.871148
2159.590157	1858.041928	1701.563126	3194.418787	3874.764976	3919.954594	1996.688933	2120.695802	1684.485737
1475.291706	1360.436301	1617.548271	1554.645752	2011.554919	1608.764312	1481.69827	1274.967959	1533.532828

| | | |

5.76_148.0530m/z	148.053003	5.7632	neg
5.76_328.0111m/z	328.0110832	5.7632	neg
5.76_368.9795m/z	368.9794667	5.7632	neg
5.76_373.1298m/z	373.1297573	5.7632	neg
5.76_436.9666m/z	436.9666352	5.7632	neg
5.76_446.9959m/z	446.9958944	5.7632	neg
5.76_463.9856m/z	463.9856143	5.7632	neg
5.76_572.9422m/z	572.9422416	5.7632	neg
5.76_575.1361m/z	575.1360591	5.7632	neg
5.76_582.9708m/z	582.9707687	5.7632	neg
5.76_650.9585m/z	650.9585147	5.7632	neg
5.76_718.9458m/z	718.9458345	5.7632	neg
5.76_786.9332m/z	786.9332248	5.7632	neg
5.76_826.8525m/z	826.8524806	5.7632	neg
5.79_257.9908n	514.9831875	5.785316667	neg
5.79_355.0108m/z	355.0107696	5.785316667	neg
5.79_395.9983m/z	395.9982872	5.785316667	neg
5.79_504.9539m/z	504.953916	5.785316667	neg
5.79_691.1232m/z	691.1232182	5.785316667	neg
5.79_793.0373m/z	793.0373247	5.785316667	neg
5.81_272.1238n	317.1242645	5.806016667	neg
5.81_320.1538m/z	320.153815	5.806016667	neg
5.81_402.1017m/z	402.1016883	5.806016667	neg
5.81_437.0551m/z	437.0550819	5.806016667	neg
5.81_443.0706m/z	443.0705569	5.806016667	neg
5.81_521.0869m/z	521.0868842	5.806016667	neg
5.81_558.1549m/z	558.1549446	5.806016667	neg
5.81_589.0744m/z	589.0743795	5.806016667	neg
5.81_598.1524m/z	598.1524165	5.806016667	neg
5.81_599.1083m/z	599.1082751	5.806016667	neg
5.81_622.0974n	621.0900946	5.806016667	neg
5.81_626.1426m/z	626.1426028	5.806016667	neg
5.81_689.0774m/z	689.077359	5.806016667	neg
5.81_725.0495m/z	725.0494888	5.806016667	neg
5.83_182.9886m/z	182.988646	5.825	neg
5.83_214.0262m/z	214.0261855	5.825	neg
5.83_222.0869n	221.0795795	5.825	neg
5.83_274.1484m/z	274.1484015	5.825	neg
5.83_289.0671m/z	289.0671474	5.825	neg
5.83_316.1953m/z	316.1953131	5.825	neg
5.83_357.0547m/z	357.054656	5.825	neg
5.83_374.0448m/z	374.0447598	5.825	neg
5.83_408.0997m/z	408.0996931	5.825	neg
5.83_415.0133m/z	415.0132842	5.825	neg
5.83_425.0422m/z	425.0422106	5.825	neg
5.83_429.1381m/z	429.1380757	5.825	neg
5.83_483.0007m/z	483.0006691	5.825	neg
5.83_493.0296m/z	493.0296412	5.825	neg
5.83_629.0045m/z	629.0045428	5.825	neg
5.83_696.9919m/z	696.9918938	5.825	neg
5.85_273.9031m/z	273.9031241	5.84575	neg
5.85_276.0433m/z	276.0432892	5.84575	neg
5.85_385.1693m/z	385.1693006	5.84575	neg
5.85_427.1976m/z	427.1975537	5.84575	neg
5.85_491.0634m/z	491.0633942	5.84575	neg
5.85_513.1484m/z	513.1483684	5.84575	neg
5.85_550.9213m/z	550.9212909	5.84575	neg
5.85_551.2480m/z	551.2479983	5.84575	neg
5.85_558.1053m/z	558.1053321	5.84575	neg
5.85_581.1364m/z	581.1364237	5.84575	neg
5.85_649.1240m/z	649.1239706	5.84575	neg
5.85_651.1216m/z	651.1215806	5.84575	neg
5.85_659.1526m/z	659.1525548	5.84575	neg
5.85_727.1397m/z	727.1397129	5.84575	neg
5.85_764.9794m/z	764.9794364	5.84575	neg
5.85_931.1023m/z	931.1023446	5.84575	neg
5.87_295.1167m/z	295.1167347	5.866533333	neg
5.87_300.2182m/z	300.2181813	5.866533333	neg
5.87_344.2080m/z	344.2080401	5.866533333	neg
5.87_360.1041m/z	360.1040849	5.866533333	neg
5.87_428.0915m/z	428.0915248	5.866533333	neg
5.87_436.2164m/z	436.2164455	5.866533333	neg
5.87_480.1827m/z	480.1827133	5.866533333	neg
5.87_490.1180m/z	490.1180368	5.866533333	neg
5.87_509.2759m/z	509.2758617	5.866533333	neg
5.87_518.1859m/z	518.1858993	5.866533333	neg
5.87_540.1679m/z	540.1679405	5.866533333	neg
5.87_548.1704m/z	548.1704401	5.866533333	neg
5.87_583.1339m/z	583.1339178	5.866533333	neg
5.87_602.3009m/z	602.3009234	5.866533333	neg
5.87_863.1148m/z	863.1148408	5.866533333	neg
5.88_289.1350n	577.2636749	5.88025	neg
5.88_292.9870m/z	292.9869775	5.88025	neg
5.88_302.1434m/z	302.1433789	5.88025	neg
5.88_342.1657n	387.1663709	5.88025	neg
5.88_370.1310m/z	370.1309649	5.88025	neg
5.88_454.1142m/z	454.1141721	5.88025	neg
5.89_135.0314m/z	135.0313868	5.894166667	neg
5.89_288.1641m/z	288.1640595	5.894166667	neg
5.89_455.1550m/z	455.154984	5.894166667	neg
5.89_481.2445m/z	481.2444898	5.894166667	neg
5.89_523.1423m/z	523.1422537	5.894166667	neg
5.91_338.0707m/z	338.0706583	5.908066667	neg
5.91_386.1154m/z	386.1154402	5.908066667	neg
5.91_402.2499m/z	402.2499012	5.908066667	neg
5.91_537.1205m/z	537.1204787	5.908066667	neg
5.91_540.1245n	539.1172399	5.908066667	neg
5.91_605.1082m/z	605.1082002	5.908066667	neg
5.91_608.1124n	607.1050749	5.908066667	neg
5.91_673.0956m/z	673.0956145	5.908066667	neg
5.92_217.9890m/z	217.9890303	5.9168	neg
5.92_218.9863m/z	218.9863237	5.9168	neg
5.92_294.9535m/z	294.9534956	5.9168	neg
5.92_368.8720m/z	368.8720239	5.9168	neg
5.92_675.0923m/z	675.0922932	5.9168	neg
5.93_269.1506m/z	269.1505726	5.927283333	neg
5.93_277.0329m/z	277.0329088	5.927283333	neg
5.93_291.1217m/z	291.1216625	5.927283333	neg
5.93_428.1274m/z	428.1273969	5.927283333	neg
5.93_497.2010m/z	497.2009612	5.927283333	neg

2405.624815	2889.452	2746.976088	1632.638047	1722.216602	1502.241962	3568.085423	3359.36119	2890.06864
12083.06967	13202.69129	13079.0391	7616.220058	8089.711731	7540.188058	16515.07674	15078.0514	13044.69451
2173.743337	2197.186479	2546.06611	1158.323505	1495.362957	1045.145512	3347.494687	3314.0561	2782.174534
756.4078091	838.8138794	833.5108629	157.934695	300.5711012	373.0201629	958.756326	1060.829117	864.9704721
4026.683162	4099.246837	4860.891868	1882.989649	2413.459859	1878.723888	6526.533229	5983.432548	4756.865587
25818.04456	27121.30735	26727.3873	13905.82734	16884.76712	14080.11612	35323.43132	32069.69517	28135.03635
949.7023994	1050.753341	1180.144705	398.6773756	711.1351371	725.279621	1733.245655	1442.527751	1432.082298
1566.698792	1611.422903	1517.571386	591.1781114	1325.152021	1297.473633	2447.385071	3035.893527	1849.223877
1228.820579	1275.262824	1452.945859	1539.954142	2089.019338	1829.309648	1646.471797	1401.874592	1333.467004
11779.48573	12779.57919	11179.21333	6295.136146	8194.753786	6691.798171	18256.2893	15233.75582	13628.27844
7412.941447	7694.809343	7707.126627	4736.681248	5413.229624	4622.886639	11661.23137	9191.69094	8528.195123
4626.962057	5916.876688	6241.118474	3372.539289	3848.632224	2385.060639	7692.156465	7843.192112	5976.578398
2862.695855	2350.614022	2396.563126	1286.280579	1527.071722	1729.138836	5094.253289	4116.87661	3841.710662
2449.753907	2521.091511	1092.186632	1680.868784	2437.639853	2219.74965	3752.347202	3007.312784	2988.38843
20333.48227	22545.90387	21209.47303	10075.4637	13615.63797	11542.86908	29151.45455	26093.83731	23569.97727
653.4529781	485.5143456	345.3747109	165.1292724	477.8764069	492.1335279	980.026239	842.8176136	818.779009
1138.154763	1174.88823	1394.293148	397.6157243	652.3702165	601.6254548	1452.463237	1463.172318	1250.954408
2640.073493	3279.215549	3445.401705	1527.276367	1836.886403	1841.415928	4641.510609	4229.494437	3305.700816
837.3826358	887.4042757	1267.129745	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199
1071.488771	622.3989779	719.4176075	3354.196941	2487.724561	3067.326102	1637.244778	1430.741425	1311.777383
72437.5979	78002.57945	77949.86933	19214.47201	16760.9808	16610.72994	107102.536	103028.0222	103527.5317
1413.907991	1363.899221	1387.230478	2393.866206	1765.828421	1551.217307	1751.432751	1650.23971	1935.088172
672.5333363	347.2630497	418.2951103	1712.960017	1675.383647	1614.484054	1052.924322	1187.585561	952.0312713
36927.32091	38490.43344	39983.50719	21567.61328	19764.27587	20830.34782	2158.032876	2094.979319	1881.098905
573.2316616	768.7761992	578.7147182	2575.889588	1820.31328	1966.922592	1618.75334	1312.942532	1193.294208
4980.484241	5418.126701	5535.333372	17342.11992	14413.65392	12861.22876	11349.11067	9510.319157	8583.214367
2468.742901	2530.244258	2206.707845	7673.073769	6433.411533	6175.654138	4163.133383	4052.326847	3549.38858
2642.31474	3374.864265	3269.639059	12376.74322	9779.781524	8877.377601	6690.703147	6144.511976	5868.513669
600.8038781	576.8902629	514.4398576	2430.502019	1715.456719	2077.305288	1922.640795	2154.618564	1670.791083
6876.606207	5887.771037	7100.983362	8650.480241	6383.029188	6904.451632	4800.477033	4111.254389	4586.564869
8814.205157	9008.527012	7975.25945	11653.41781	12435.32318	11541.58791	12435.32318	984.8532002	270.3632893
1389.362722	900.7837453	1018.565427	4380.788777	3709.600862	3640.882819	2340.206034	1758.965767	2261.152026
1735.683795	1307.911	1780.210019	3846.938098	2229.740142	2304.530375	198.2826444	0.001403199	149.6571388
1480.129983	1383.288099	957.3630074	4680.602265	3932.849469	3660.497652	2638.98626	2125.665158	2103.402524
1332.087568	1269.439635	1438.843983	1355.924925	1713.620578	1526.41087	1857.414828	1511.982403	1622.884403
74.39215591	35.05929876	75.55829357	60.44011007	24.16761683	102.0554606	118.7316883	87.6739875	0.001403199
42773.68576	41126.30263	44508.37744	57228.92873	43758.62976	44825.54252	36382.26344	35486.40232	34521.91226
314.2567556	354.1327529	422.0893985	966.1678961	674.1876499	610.8431749	621.6047596	458.0701166	510.7470784
23258.50177	23484.61278	25491.25083	31558.00509	23220.27424	23544.76569	20142.05496	19868.4366	19313.54653
1047.446388	1034.535065	1013.922675	1593.183276	1490.12447	1424.759081	1376.078812	1385.768428	1159.127994
16264.57895	15543.38661	17379.22057	21538.24223	17040.06015	17067.11469	14312.03141	14124.15315	12747.81626
1256.403694	999.4329806	1215.18517	1861.587223	1185.593123	1273.246227	1093.955814	878.8892396	838.0729707
293.3125238	175.3039946	472.1864084	71.37327087	51.64811807	0.001403199	176.1342604	162.1493454	358.8750842
2642.945439	2445.599392	2928.514347	3560.328134	2266.667599	1985.820395	2306.739567	1509.056625	1739.18928
12063.94483	12143.17068	12910.8827	8873.722285	12146.72206	11644.0841	11012.06303	10273.39734	9389.156303
1023.844619	993.6152452	1335.388006	1826.151194	1478.423393	1318.384102	1436.484484	1222.520775	1420.302681
1666.482083	1499.743858	1675.112122	2511.009746	1715.754277	1173.731068	1183.154611	1177.655945	1203.263112
8308.765006	7372.892962	8723.51462	10982.62908	7720.970679	7705.916183	6582.905867	6533.312332	6359.978229
5132.630282	5090.621991	5810.905606	7779.862609	4820.692913	4420.557119	4171.550579	4346.179194	3053.734036
4736.640824	3900.652898	5159.938972	6753.913146	4348.077145	4303.083195	4083.031305	3781.908731	3389.021599
629.5285155	546.1647779	604.1801187	796.2519569	765.8022515	867.2174117	1137.99097	880.6063843	968.832566
0.001403199	0.001403199	0.001403199	635.746695	523.7151428	568.5053777	0.001403199	0.001403199	0.001403199
4532.44105	4515.787922	5459.747332	9573.380291	8263.794509	9044.42793	5815.500511	6703.157592	6942.509358
4728.619691	4214.43976	5256.02648	1485.66423	1046.421112	1041.619779	4563.903916	5273.820824	4450.712982
1900.760992	1885.842753	2474.109437	238.9524248	246.5894188	0.001403199	0.001403199	0.001403199	0.001403199
8264.602896	10290.17812	9776.377392	7836.922439	7871.206531	7186.076007	13984.38143	12628.70575	13248.0481
4235.898583	3791.924908	3699.13961	3484.406471	4533.664486	4765.361423	5959.725722	4794.642879	5981.761329
750.6677155	710.3723732	959.8323282	1304.57914	859.6281655	995.8078595	784.2359702	1159.23544	735.399881
900.5302191	891.9005032	700.3624856	1061.694812	937.3595656	838.1383114	1217.54648	737.3931355	1013.673151
3673.575755	4087.852822	5012.054973	3532.914467	3184.314782	3472.850174	5565.235477	5405.555312	6501.791527
1810.234351	1918.788705	2417.700573	1886.093923	1176.163775	1450.817333	2948.868539	2699.440537	2433.377222
422.7613261	406.1184439	182.5671557	211.5737334	231.4971606	175.5975108	520.8804405	773.9126004	872.9629251
23180.16974	23879.38769	25222.62323	21951.56236	21138.80483	19504.70806	32003.0262	29960.7429	31794.6655
13531.40146	14100.42399	16274.46902	13199.67267	12721.95175	12243.91115	21915.6379	19147.02812	22283.9684
2553.921746	2038.631989	2838.977157	2548.194664	2276.039629	2325.25607	1656.754948	972.6645432	1331.803592
2160.74846	2131.782489	2772.25741	2290.405038	1420.711754	1546.479616	4403.53528	3354.848354	3928.915704
1123.132653	1155.144574	1310.633635	999.2523353	1080.295423	1052.64324	914.9811791	1132.624512	1154.257471
442.8789377	329.9816735	314.4269208	325.2494011	231.4310657	274.9539375	248.2335203	252.0782242	309.7673006
1229.629942	1797.617283	2026.231505	1265.584075	1242.173241	1321.486057	1882.48226	1472.645679	1919.064777
620.4936446	732.4253934	972.2890444	792.0037938	663.6159994	700.9089358	936.8242461	865.9646235	1067.125387
231.4366645	456.7390758	374.7583917	89.06892871	162.8875241	493.4097512	102.9603566	289.1677738	340.6175017
1544.400766	1597.563732	2076.654578	1249.94644	1155.678021	1321.873198	1855.485113	2017.81332	2194.609938
2524.818851	2847.835706	3656.897853	2433.927212	2536.116715	2025.058055	3145.85837	2550.337848	2483.603915
4589.908588	4517.617834	4869.182788	4008.516632	3535.850438	4083.238317	5573.780962	4397.884538	4587.663166
15946.5399	19314.37492	19167.30985	21736.70194	19512.48847	20646.64886	18995.04825	15970.14238	21435.95982
2074.658	2184.579715	2070.8777	2028.05451	1273.290346	1376.365623	3070.393955	2729.747319	2528.920378
2565.611198	2978.933279	3432.531085	2550.78899	2072.419305	1922.002425	4952.990362	3848.552794	3833.352799
2176.163102	2095.61195	2839.801353	2060.460914	1873.173108	1756.581662	3045.266122	2429.199206	2770.988933
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3519.473695	3891.289166	4377.224891	4614.01614	3584.427301	3027.014121	7266.218811	5092.950908	5301.026745
4611.105302	5664.087605	5717.518723	6464.877186	5807.244806	5851.129066	5236.994783	4704.211495	6158.467538
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1559.665259	1333.179261	1733.474308	1023.090574	1140.054222	1281.441218	971.4783521	1824.376959	2478.42259
200.971693	203.42176	213.1956429	145.03976	221.362769	231.9419132	180.4857647	218.4865524	318.3921234
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2107.136149	3197.425065	3090.746157	3536.52275	3945.495841	3849.285428	2582.203541	2530.162641	2892.361734
4365.110832	4536.955271	4690.723354	5648.564578	5644.114396	6097.992056	2920.49616	3365.373377	3651.746599
1891.759654	2391.344844	2277.712496	2223.415695	2353.200776	2034.518149	2314.353498	2721.482717	3453.546854
1630.863546	1627.852031	1653.735746	2561.757773	2985.340374	3216.367078	1260.948254	2249.263267	1724.813835
633.453546	566.5441724	617.7212022	918.7475849	1216.827675	1167.711136	321.0153939	736.5914814	789.3283021
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783.9562795	903.4920105	758.5352294	750.4047754	1136.935187	911.8752481	934.721385	819.8980952	865.5802228
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1862.641673	1763.648258	2178.29672	1694.548442	1703.270975	1751.336957	1732.395902	2329.470621	2366.397531
1767.874559	2044.649535	2386.650769	904.9968801	1050.360687	871.5458928	1844.402942	2001.948436	1621.62369

5.94_179.9364m/z	179.9364114	5.937716667	neg
5.94_241.1084m/z	241.1084258	5.937716667	neg
5.94_283.1551m/z	283.1551026	5.937716667	neg
5.94_427.1225m/z	427.1224584	5.937716667	neg
5.94_541.2657m/z	541.2657024	5.937716667	neg
5.94_599.2247m/z	599.2246823	5.937716667	neg
5.94_609.2532m/z	609.2532135	5.937716667	neg
5.94_667.2124m/z	667.2124182	5.937716667	neg
5.94_745.2283m/z	745.228319	5.937716667	neg
5.94_813.2154m/z	813.2154453	5.937716667	neg
5.94_881.2026m/z	881.2025788	5.937716667	neg
5.95_267.0850m/z	267.0849876	5.95155	neg
5.95_481.2059m/z	481.2059221	5.95155	neg
5.97_281.0102m/z	281.0101695	5.965483333	neg
5.97_333.0932m/z	333.0931683	5.965483333	neg
5.97_401.0804m/z	401.0804361	5.965483333	neg
5.97_480.9179m/z	480.917925	5.965483333	neg
5.97_497.1260m/z	497.1259794	5.965483333	neg
5.98_406.1802m/z	406.1802437	5.9829	neg
5.98_429.1381m/z	429.1381341	5.9829	neg
5.98_499.1813m/z	499.1812541	5.9829	neg
5.98_518.2609m/z	518.260939	5.9829	neg
5.98_541.1523m/z	541.1522572	5.9829	neg
5.98_609.1398m/z	609.1397738	5.9829	neg
5.99_258.0692m/z	258.0692359	5.9916	neg
5.99_283.0912m/z	283.091211	5.9916	neg
5.99_288.1640m/z	288.16402	5.9916	neg
5.99_334.0887m/z	334.0887366	5.9916	neg
5.99_385.1691m/z	385.1691246	5.9916	neg
5.99_402.0760m/z	402.0760369	5.9916	neg
5.99_470.0634m/z	470.0634808	5.9916	neg
5.99_525.2709m/z	525.2708736	5.9916	neg
5.99_538.0514m/z	538.0513635	5.9916	neg
5.99_743.2128m/z	743.2128278	5.9916	neg
6.01_214.1451m/z	214.1450803	6.007266667	neg
6.01_215.0388m/z	215.0387706	6.007266667	neg
6.01_291.0829m/z	291.0828936	6.007266667	neg
6.01_665.1963m/z	665.1963013	6.007266667	neg
6.02_676.3375m/z	676.3374516	6.01945	neg
6.03_271.1664m/z	271.1664455	6.028183333	neg
6.03_289.0674m/z	289.0673604	6.028183333	neg
6.03_294.9535m/z	294.9535335	6.028183333	neg
6.03_421.0215m/z	421.0215439	6.028183333	neg
6.03_422.0896m/z	422.0895931	6.028183333	neg
6.03_521.1626m/z	521.1626102	6.028183333	neg
6.04_293.1377m/z	293.1377337	6.040433333	neg
6.04_453.1744m/z	453.1743968	6.040433333	neg
6.04_526.2492m/z	526.2492202	6.040433333	neg
6.04_606.2127m/z	606.212689	6.040433333	neg
6.04_674.1998m/z	674.1998275	6.040433333	neg
6.04_722.8574m/z	722.8574344	6.040433333	neg
6.06_402.2500m/z	402.2499799	6.056116667	neg
6.06_447.1409m/z	447.1409272	6.056116667	neg
6.06_470.1646m/z	470.1645549	6.056116667	neg
6.06_470.2375m/z	470.2375123	6.056116667	neg
6.06_491.2137m/z	491.2136812	6.056116667	neg
6.06_558.1551m/z	558.1551121	6.056116667	neg
6.06_583.3128m/z	583.3128018	6.056116667	neg
6.07_389.1822m/z	389.1821742	6.07	neg
6.07_416.2010m/z	416.2010486	6.07	neg
6.07_445.1720m/z	445.1720154	6.07	neg
6.07_478.1420n	523.141502	6.07	neg
6.07_626.1428m/z	626.14279	6.07	neg
6.07_661.1321m/z	661.1321785	6.07	neg
6.09_167.1078m/z	167.1078027	6.087383333	neg
6.09_311.1502m/z	311.1501888	6.087383333	neg
6.09_327.0158m/z	327.0158282	6.087383333	neg
6.09_450.0496n	449.0423396	6.087383333	neg
6.09_599.0955m/z	599.0955352	6.087383333	neg
6.10_214.1450m/z	214.1450454	6.101316667	neg
6.10_259.0282m/z	259.0282317	6.101316667	neg
6.10_329.0624m/z	329.0624065	6.101316667	neg
6.10_337.0884m/z	337.0884186	6.101316667	neg
6.10_381.0547m/z	381.0547063	6.101316667	neg
6.10_405.0759m/z	405.0758995	6.101316667	neg
6.10_428.0651n	473.0630454	6.101316667	neg
6.10_523.1776m/z	523.1776322	6.101316667	neg
6.10_683.1916m/z	683.191626	6.101316667	neg
6.11_413.1821m/z	413.1821282	6.113516667	neg
6.11_521.1257m/z	521.1256815	6.113516667	neg
6.11_591.1650m/z	591.1650467	6.113516667	neg
6.12_283.1664m/z	283.1663928	6.123483333	neg
6.12_301.0671m/z	301.0670961	6.123483333	neg
6.12_312.1255m/z	312.125548	6.123483333	neg
6.12_481.1697m/z	481.1697224	6.123483333	neg
6.13_155.0715m/z	155.0714776	6.133983333	neg
6.14_176.9623m/z	176.9623026	6.143466667	neg
6.14_445.2446m/z	445.2446109	6.143466667	neg
6.14_457.2085m/z	457.2084719	6.143466667	neg
6.14_481.2070m/z	481.2070353	6.143466667	neg
6.14_918.8061m/z	918.8060567	6.143466667	neg
6.15_385.1692m/z	385.169161	6.154666667	neg
6.15_601.0770m/z	601.0770407	6.154666667	neg
6.15_669.0648m/z	669.0648711	6.154666667	neg
6.16_344.2078m/z	344.2078334	6.161866667	neg
6.16_477.0994m/z	477.0994222	6.161866667	neg
6.16_611.0586m/z	611.0586153	6.161866667	neg
6.16_845.7978m/z	845.7977525	6.161866667	neg
6.17_399.0830m/z	399.0830139	6.171316667	neg
6.17_543.0713m/z	543.0713132	6.171316667	neg
6.17_545.0872m/z	545.0872004	6.171316667	neg
6.17_613.0742m/z	613.0741535	6.171316667	neg
6.18_360.9745m/z	360.9744799	6.181866667	neg
6.18_459.2240m/z	459.2240175	6.181866667	neg
6.18_505.2662m/z	505.2662108	6.181866667	neg
6.18_698.3763m/z	698.3762823	6.181866667	neg
6.18_698.8707m/z	698.8706969	6.181866667	neg
6.18_722.8578m/z	722.8578019	6.181866667	neg
6.20_320.0729m/z	320.0729063	6.195716667	neg
6.20_343.1302m/z	343.1302397	6.195716667	neg

669.937042	512.2938722	570.5061078	417.6459371	639.0463444	737.0843059	532.880025	671.7919794	674.8723791	
902.4716538	884.1211377	1077.973521	583.6792269	993.6359236	799.8199948	517.0716232	794.3152947	691.2690879	
719.5041791	747.7459147	843.2200119	858.0829164	1276.56535	1024.876874	545.7935612	715.5000777	810.9333164	
5169.621047	5197.131289	5264.209942	6761.250816	7928.849391	7752.388331	5917.366367	6360.187954	6842.309463	
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4180.852091	3490.020122	4355.92298	5228.795039	5778.542901	5773.078959	3518.822127	3912.733533	3735.567485	
45415.35406	50170.81731	50498.22745	54453.70776	68455.51724	64982.83395	42925.06128	49176.39729	46698.93338	
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4672.315593	3756.791662	4565.664509	5693.784009	6192.732241	6014.675731	3260.925356	3681.779318	3410.419068	
1549.883317	1875.964587	1836.860973	1143.50308	1449.133396	1542.093276	1352.635607	1556.0169	1660.59171	
3313.790805	3756.594429	3931.175836	1385.823705	2135.936868	1940.455765	2041.712262	2678.106347	3529.143064	
992.4377983	847.056968	1198.058953	759.7971082	835.9119186	930.034239	1013.757082	1055.60577	1079.198754	
2783.961678	2690.197718	3078.914768	1266.700923	1959.0364	1715.393447	1077.390793	1349.690931	1330.944301	
947.2852703	1436.04915	1203.860453	453.9180453	524.670751	487.3892994	294.5075775	462.4798271	395.3602059	
2847.373204	2323.614169	2410.573838	1859.336544	2938.448797	2515.212596	3023.440681	2875.770315	2590.499342	
1871.798276	1640.857407	1942.006806	2071.482108	2253.561765	2000.751894	1498.075029	1825.95268	1839.089115	
5118.405275	6395.649118	6150.460801	5152.458537	6365.200842	7050.362215	4256.084922	4233.582071	3927.306972	
4120.493882	5024.474047	5381.899854	4302.018119	5449.734494	5966.018239	3909.415053	4708.450979	4047.92744	
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3887.415393	3781.532435	3925.273731	3320.944379	3482.882551	3870.423533	2617.355065	1896.30788	2194.116796	
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4261.133739	4503.545841	5015.971756	5584.096167	5722.139024	6163.963156	3394.722824	4551.587707	4425.724707	
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46891.87324	51187.91989	53960.32171	61492.74763	66238.94745	70798.09334	41628.93281	45087.88017	44574.13778	
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147.6859049	74.80672905	182.338698	54.51751907	111.1834493	130.5184951	163.5236032	30.75808907	102.3154182	
186.6363942	198.6207884	267.8607359	350.5418727	443.647614	403.1534161	527.7073117	479.7825892	539.7473679	
7161.948172	7977.073296	8112.634239	6927.704213	7603.999288	6977.753243	6432.88244	6555.899469	6809.373316	
1393.459265	1431.614389	1968.834593	1077.599769	1026.441402	1255.046516	1104.331865	1058.245039	975.6418424	
1783.558596	2090.083492	1765.655765	0.001403199	0.001403199	0.001403199	1126.240314	884.4407374	1240.049341	
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463.0090877	386.5792908	492.1090024	502.9090349	487.9249921	462.6036321	429.1801619	331.1557007	391.7080056	
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1247.766505	1344.349499	1813.534394	0.001403199	0.001403199	0.001403199	0.001403199	58.8485527	0.001403199	
1418.30499	1393.67781	1829.379017	492.4062466	469.8690278	536.5830129	892.6738222	693.048893	1104.009999	
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1758.846946	1768.431929	2449.38836	2319.182162	2096.679908	1624.282721	1599.398827	1836.834522	2034.19909	
782.5621399	1043.142536	1194.217417	1588.24232	960.1313391	1028.234086	1059.961783	1249.485368	852.0730001	
0.001403199	522.1559415	338.3512117	2037.906319	391.3815446	699.9745478	173.4540832	639.1741018	462.3878533	
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964.7276736	1053.457911	1251.874527	1023.681349	1154.005402	783.3777739	430.4897267	607.7859764	566.8493747	
175.1352949	364.6831598	493.6749097	624.1253848	921.6782419	590.2785575	223.0718744	95.64540863	447.0623073	
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7186.406598	8753.722131	9466.079124	0.001403199	0.001403199	113.9251672	2901.397814	3919.259598	3238.629872	
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325.6064608	455.1434976	491.7554725	844.5076328	686.7816588	586.3589071	0.001403199	0.001403199	240.2711895	
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4262.282774	4962.100926	4854.200733	3032.000503	3165.286564	3773.16814	2531.744699	2963.610901	3235.522516	
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6.20_352.1592m/z	352.1591983	6.195716667	neg
6.20_361.0416m/z	361.0415581	6.195716667	neg
6.20_455.1152m/z	455.1151775	6.195716667	neg
6.20_462.2867m/z	462.2867481	6.195716667	neg
6.20_521.1631m/z	521.1630765	6.195716667	neg
6.20_575.0329m/z	575.0328587	6.195716667	neg
6.20_643.0202m/z	643.0202497	6.195716667	neg
6.21_266.0857m/z	266.085741	6.206233333	neg
6.21_334.0735m/z	334.0734783	6.206233333	neg
6.21_454.1790m/z	454.1789512	6.206233333	neg
6.21_507.0452m/z	507.0452188	6.206233333	neg
6.22_232.0595m/z	232.059488	6.215	neg
6.22_341.1583m/z	341.1582987	6.215	neg
6.22_409.1459m/z	409.1459416	6.215	neg
6.22_413.2006m/z	413.200589	6.215	neg
6.22_477.1336m/z	477.1335747	6.215	neg
6.23_283.1665m/z	283.1665121	6.230633333	neg
6.23_351.1541m/z	351.1541139	6.230633333	neg
6.23_532.2895m/z	532.2895288	6.230633333	neg
6.23_541.2654m/z	541.2654249	6.230633333	neg
6.25_323.0041m/z	323.0040641	6.248083333	neg
6.25_325.0018m/z	325.0018045	6.248083333	neg
6.25_337.0884m/z	337.0883961	6.248083333	neg
6.25_430.2165m/z	430.2164504	6.248083333	neg
6.25_472.2311n	471.2238102	6.248083333	neg
6.25_521.0936m/z	521.093593	6.248083333	neg
6.25_544.2401m/z	544.2400842	6.248083333	neg
6.25_566.2223m/z	566.2222769	6.248083333	neg
6.25_705.0729m/z	705.0728878	6.248083333	neg
6.25_821.1821m/z	821.1820816	6.248083333	neg
6.25_889.1693m/z	889.1692733	6.248083333	neg
6.26_231.0334m/z	231.0333848	6.261966667	neg
6.26_363.1664m/z	363.1663632	6.261966667	neg
6.26_506.1623m/z	506.1622603	6.261966667	neg
6.26_574.1495m/z	574.149493	6.261966667	neg
6.26_579.2092m/z	579.2092186	6.261966667	neg
6.26_634.2101m/z	634.210057	6.261966667	neg
6.26_637.0855m/z	637.0854679	6.261966667	neg
6.26_957.1569m/z	957.1568984	6.261966667	neg
6.27_215.0386m/z	215.0386345	6.272366667	neg
6.27_346.9588m/z	346.9587596	6.272366667	neg
6.27_375.0756n	420.0738747	6.272366667	neg
6.27_385.1121m/z	385.1121001	6.272366667	neg
6.27_458.2591m/z	458.2591087	6.272366667	neg
6.27_479.1157m/z	479.1156957	6.272366667	neg
6.27_525.2707m/z	525.2707347	6.272366667	neg
6.28_339.1426m/z	339.1426499	6.2811	neg
6.28_442.0559m/z	442.055886	6.2811	neg
6.28_481.1698m/z	481.1698535	6.2811	neg
6.28_510.0429m/z	510.042944	6.2811	neg
6.28_587.1339m/z	587.1338836	6.2811	neg
6.28_704.8160m/z	704.8159564	6.2811	neg
6.30_329.1973m/z	329.1973363	6.302033333	neg
6.30_465.2499m/z	465.2498506	6.302033333	neg
6.30_487.2556m/z	487.2555781	6.302033333	neg
6.30_513.1487m/z	513.1486845	6.302033333	neg
6.30_519.1464m/z	519.1463954	6.302033333	neg
6.30_525.1573m/z	525.1573176	6.302033333	neg
6.30_659.1527m/z	659.1527204	6.302033333	neg
6.30_772.8029m/z	772.802884	6.302033333	neg
6.30_795.1271m/z	795.1271416	6.302033333	neg
6.32_210.9838m/z	210.9837902	6.320716667	neg
6.32_227.0387m/z	227.0386574	6.320716667	neg
6.32_277.0330m/z	277.0330139	6.320716667	neg
6.32_350.1646m/z	350.1645769	6.320716667	neg
6.32_361.1508m/z	361.1508032	6.320716667	neg
6.32_391.1356m/z	391.1355667	6.320716667	neg
6.32_402.1771m/z	402.1770994	6.320716667	neg
6.32_429.1382m/z	429.1381704	6.320716667	neg
6.32_545.8536m/z	545.8535713	6.320716667	neg
6.32_565.1132m/z	565.113242	6.320716667	neg
6.32_727.1404m/z	727.1403745	6.320716667	neg
6.33_285.1346m/z	285.1346018	6.331216667	neg
6.33_318.8743m/z	318.8742555	6.331216667	neg
6.33_397.1484m/z	397.1484033	6.331216667	neg
6.33_477.2133m/z	477.2133306	6.331216667	neg
6.33_505.1498m/z	505.1497706	6.331216667	neg
6.33_527.2866m/z	527.2866216	6.331216667	neg
6.33_646.3213m/z	646.3213182	6.331216667	neg
6.34_404.1753m/z	404.1753014	6.339983333	neg
6.34_427.1604m/z	427.1604349	6.339983333	neg
6.34_477.8658m/z	477.865808	6.339983333	neg
6.34_527.2473m/z	527.2472835	6.339983333	neg
6.35_138.8602m/z	138.860225	6.348783333	neg
6.35_288.1277m/z	288.1277183	6.348783333	neg
6.35_403.1612m/z	403.1612468	6.348783333	neg
6.35_444.2607m/z	444.2607081	6.348783333	neg
6.35_545.0868m/z	545.0867925	6.348783333	neg
6.37_341.1586m/z	341.1585588	6.373833333	neg
6.37_440.8787m/z	440.8787054	6.373833333	neg
6.37_442.0560m/z	442.055964	6.373833333	neg
6.37_467.1152m/z	467.1151612	6.373833333	neg
6.37_617.1820m/z	617.1820327	6.373833333	neg
6.39_208.9680m/z	208.9680296	6.380666667	neg
6.39_289.0672m/z	289.0671667	6.380666667	neg
6.39_366.2231m/z	366.2230962	6.380666667	neg
6.39_371.0702m/z	371.0701909	6.380666667	neg
6.39_374.2551m/z	374.2550932	6.380666667	neg
6.39_389.1822m/z	389.1821723	6.380666667	neg
6.39_413.2007m/z	413.2007105	6.380666667	neg
6.39_439.0580m/z	439.0579696	6.380666667	neg
6.39_618.9087m/z	618.9086504	6.380666667	neg
6.39_707.1551m/z	707.1551266	6.380666667	neg
6.40_228.1606m/z	228.1606042	6.39835	neg
6.40_248.9498m/z	248.9498512	6.39835	neg
6.40_303.0829m/z	303.0828502	6.39835	neg
6.40_525.1571m/z	525.1571254	6.39835	neg
6.40_790.8451m/z	790.8450941	6.39835	neg
6.41_244.0049m/z	244.004881	6.408833333	neg
6.41_358.1309m/z	358.1309318	6.408833333	neg

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1181.811954	860.1408626	1191.207571	1071.407718	976.9017882	1015.25529	1807.09335	1676.156554	1773.16245
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150.151494	285.2538192	414.6841294	565.2331737	168.3345059	237.5744623	429.0336629	563.1468201	388.8997292
2400.313856	2420.03056	2664.932428	4572.412359	4109.98136	4427.826206	3085.670829	3263.214761	3197.007234
361.4893934	294.4251863	671.9281614	553.8677989	526.2556986	628.6135216	433.146239	460.7478533	701.6030964
15307.91688	13451.99031	15243.98623	12835.07246	12085.48305	13354.16623	11839.79151	12624.88595	13385.25084
8287.678554	7464.35395	8600.541557	7590.727086	6837.313692	7581.56098	7018.035701	7054.429761	7593.683369
15417.553	12846.14488	16204.75549	18274.3066	17530.07729	18038.96193	14856.58957	14373.42129	15196.02777
4759.747419	4299.718608	5157.15768	3876.551571	3777.975008	4722.517873	3929.699836	4277.55637	4297.196798
5394.660505	3891.368664	5221.96809	8454.038071	6980.509127	8259.261762	4724.324049	4495.107949	4760.078759
1713.543549	1114.231257	1733.929725	2313.376409	1685.240182	1950.23346	1396.644056	1245.234696	1627.678553
5659.560974	4383.571582	5819.015853	3548.217857	3310.414433	2996.488605	3949.937907	4484.297622	4859.676922
1362.644191	1182.006242	1269.918382	665.9501134	377.7265715	477.375742	843.9944016	831.8053677	1285.744823
930.4982222	679.1938491	1008.422768	1165.00404	1045.79531	1295.085014	1017.933499	1055.975189	1066.279703
909.6999748	777.6071849	1128.445657	1360.88152	1033.048945	1320.294098	1304.63267	1150.800308	1031.010841
1022.924418	824.3917598	1169.488142	661.1711124	566.0905922	708.6773215	1200.534488	1060.811001	1002.605028
253.9644595	212.4810654	404.3851395	0.001403199	0.001403199	161.2204824	88.48866709	78.31346512	361.5378008
30487.43164	24047.49649	29510.05279	11894.47785	10842.52932	12125.40576	21458.8862	24116.00379	23113.18934
424.437913	237.1345624	225.3604322	599.9609978	118.3685057	402.3746741	555.6438383	594.6296305	423.4891807
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3753.74997	2784.620655	3880.159865	4463.407783	3307.330919	3739.790412	3129.409333	3383.015724	3429.745153
4264.144679	3273.637352	3147.206817	4048.182389	3079.91809	4719.978318	2930.770534	3109.516121	2646.024368
8840.71654	6422.640873	8615.74183	8058.62242	7637.291612	10019.7441	7751.850543	8202.282669	8096.057288
5619.972776	4161.865648	4352.671838	5528.634594	3928.924963	5502.150822	4889.609005	4984.251262	5942.519176
697.2600037	574.0217591	792.9662028	341.5641863	211.8289418	237.3958799	559.4053211	685.4135945	628.6930483
4293.400456	3183.947325	4584.452327	5951.821771	4570.140057	5595.625804	3614.130026	4452.257195	4271.123513
1931.632406	1249.567424	2206.243163	2329.732952	1952.918778	2360.389674	2003.472566	2106.443466	2006.41222
2141.547472	1789.568836	1957.449545	2097.062974	2077.213752	2409.099832	1675.836207	2244.38073	2235.580216
883.9017618	1250.094724	930.6567952	105.5688457	255.306727	156.0436437	722.5563929	584.5680161	684.5586172
1703.109923	613.2412723	1515.521153	1989.152524	688.0400625	1333.712445	921.7476401	1427.805786	1012.442166
16489.67379	15648.72575	17353.54275	20118.13781	16985.39341	20842.61244	12693.09001	13627.51009	12547.95139
3039.331295	3672.112995	3883.394446	3668.339869	2341.343512	4075.464182	3676.506949	3153.601705	3799.664401
328.6769138	242.1396277	261.3313293	277.6620277	306.0281911	240.9253072	332.4840136	451.5878505	403.1923734
3185.997247	2439.297978	3200.14717	3161.830019	3237.582119	2739.969559	3478.715994	2677.292557	4115.959752
4839.475171	4465.233154	4977.260329	7373.667158	7770.458226	7469.272586	8464.876359	10283.91044	11070.43294
523.6632032	444.9038588	365.5927175	538.7291293	541.3927627	647.668653	337.1049587	342.8372675	300.0968457
1392.382589	1050.740855	1281.414718	1947.375414	1797.59714	1687.690511	1200.884018	1707.525749	1610.74172
2340.542987	1725.43957	2326.276392	1427.750444	1406.204345	1019.236231	1999.801095	1931.599944	2210.099752
2298.516779	1357.555731	2007.952526	1237.319514	1090.079785	1147.761748	2090.008284	2726.382441	2789.725377
1176.578418	1707.243966	1268.08747	982.2641125	1202.618865	1033.297855	971.7774877	980.735616	1314.14425
2470.037011	2118.971846	2463.827082	3640.365489	4129.817978	3477.082346	4082.843997	5191.752279	5422.033708
1083.545572	1341.08298	1028.266851	2092.268871	1857.15647	1645.568968	636.3887306	1277.653733	1021.381745
1395.314526	1276.188529	1427.330038	2130.403467	2427.777546	2369.910439	2527.098864	2670.555931	3585.561782
532.7693064	872.2799725	772.9974376	643.8358207	673.7520753	624.353628	478.0879966	226.7571969	528.8600291
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1402.899401	1590.907171	1626.636738	2024.974587	2041.853565	1444.891049	1119.531781	1747.629213	1861.275671
2478.179548	3785.219064	2997.889129	3021.725261	3223.71525	3248.543572	1615.643525	1826.429066	2367.422104
1764.174874	2559.181751	1530.990008	2208.598193	2027.414208	1989.217631	1953.888653	2174.358265	3364.523131
1485.023552	1669.86952	1845.928231	1881.666303	1353.885912	1206.527539	1107.118533	1205.532181	1539.11593
3245.05321	2851.878674	3991.177369	4801.014515	3840.059654	4161.059274	2474.759152	2450.709916	2915.343279
5815.187746	6942.937417	6487.805799	6617.248978	5631.345307	5435.613931	7128.997921	6019.292452	7747.604361
2992.712144	3244.249748	4072.261809	3378.628531	2708.965014	3706.411865	3838.436966	3198.320254	3341.449533
1590.245771	2708.634958	2601.899179	2164.766511	2815.923178	2139.52936	3086.74847	2064.864517	3306.142321
501.8410738	599.6063618	488.8473924	642.2517903	645.521189	497.7932032	610.26881	491.0926746	642.9609375
1091.251611	1526.745197	1685.377459	900.4730494	824.9246259	773.2872116	1820.698309	1855.022418	2407.712909
976.5353132	1039.436665	916.5239416	984.9233342	1375.668987	1070.691591	1219.342536	987.1613054	1304.301271
43.92552792	189.9117577	50.13574058	1942.242211	975.5466785	801.0424672	263.3720705	102.331459	302.9417267
55835.04176	64491.72058	65831.61438	80742.19112	80253.03994	72413.85933	51473.57883	51374.38542	58691.08918
467.9779796	352.2493036	471.820678	820.5994413	697.6844286	679.424927	226.9862937	179.3150463	330.1950388
490.6852718	710.6717222	714.9947833	1012.662575	749.0101389	534.4741825	256.5676551	268.1096878	437.3999305
19728.86146	22416.61471	22863.5197	26884.9807	26461.71981	25083.61081	17729.01405	17328.60633	20341.75961
3694.091833	3859.370197	3172.67575	3834.543918	3962.342304	3472.366082	4146.904947	3193.288764	4516.244576
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2749.140612	3677.913101	3758.310835	3423.919871	3245.765497	2554.08223	2736.35461	2625.8564	3058.023381
2531.984912	3395.920421	2920.012079	3856.313715	3565.192735	4008.940065	2105.671042	2515.458745	3134.874234
1390.906322	1612.276959	826.1441351	452.2668956	471.3822569	441.0154481	896.9193028	1371.600472	1820.814538
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2782.66902	2728.79246	2549.820934	4128.224036	3927.200938	3862.938568	2643.300935	2373.182794	3025.23964
4180.197423	4620.040151	4242.880399	4758.256098	5360.124101	4776.439591	3846.467236	4171.384527	5037.132689
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1910.293686	1517.037048	1611.934441	1909.65718	2060.608597	1876.686335	2262.975568	1542.41489	1866.982897
2275.790912	2671.548667	2718.432193	4199.933942	4908.338821	4204.349453	4729.656046	4686.365431	5269.661822
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933.7787788	999.6155003	867.4387285	1159.668639	1235.531636	1116.829545	1124.445716	904.0770149	1077.28769
573.6006815	403.0084248	369.0146007	935.7165497	1088.061175	1017.016463	358.434057	455.281256	342.054066
1383.122744	1209.425623	1400.238703	1169.077462	1587.274699	1271.265938	1630.972006	1297.657491	1371.863784
1384.533886	1397.614632	1712.752671	2388.434799	2667.141179	2622.248373	1653.864996	1504.812762	1425.709992
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72131.02758	74063.16689	84300.24682	101753.0812	97045.3945	97188.25882	69921.67019	71777.90972	72696.17565
134097.1759	144779.5882	156040.4739	154988.7954	153824.6502	157178.7134	120400.1831	124852.8723	123736.9357
620.1488272	573.7157614	840.5573336	1393.577158	1304.868618	1334.468386	671.0957118	802.2351837	678.3892905
1807.142497	1573.417321	1413.446879	1908.053325	2428.171235	1886.704716	1674.934026	1724.89784	1472.101987
2092.327433	1828.059165	1461.250413	351.1808625	393.780636	460.3776185	1282.263483	1936.584337	1084.767004
1424.770224	1342.221835	1371.53908	1312.803108	1339.942075	1412.019697	1512.333517	1259.617375	1281.342932
38.89413034	35.97036964	46.12752281	21.22927357	34.73890488	25.14874466	85.98050669	110.9454799	89.35173499
2301.894064	2412.366368	2773.302512	3716.513377	4446.348461	4175.285694	2413.273479	2583.766035	2408.363807
636.5453011	895.5951215	824.6432113	1242.979465	861.2046414	1271.745999	652.3677481	329.1982918	734.6368462
2620.078474	1747.850432	2401.308266	2899.561809	3516.681741	3344.966586	3219.789155	1834.718132	2662.058121
655.5661805	878.7334427	974.0239616	1147.401291	739.8515511	982.0119773	32.43221958	102.9550436	141.3566494
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6.41_458.1732m/z	458.1732097	6.408833333	neg
6.41_539.2503m/z	539.2502788	6.408833333	neg
6.42_170.0016m/z	170.0015927	6.41995	neg
6.42_527.2869m/z	527.2869435	6.41995	neg
6.43_246.1535m/z	246.1534532	6.433933333	neg
6.43_518.1026m/z	518.102857	6.433933333	neg
6.43_525.2710m/z	525.2709777	6.433933333	neg
6.43_918.8061m/z	918.8061039	6.433933333	neg
6.44_301.2254n	346.2238375	6.442716667	neg
6.44_411.1278m/z	411.1277577	6.442716667	neg
6.44_429.1768m/z	429.1767873	6.442716667	neg
6.44_453.0500m/z	453.0500467	6.442716667	neg
6.44_465.2502m/z	465.2502357	6.442716667	neg
6.44_497.2011m/z	497.2010665	6.442716667	neg
6.44_547.1030m/z	547.1029575	6.442716667	neg
6.44_550.1861m/z	550.1860614	6.442716667	neg
6.44_565.1518m/z	565.1517592	6.442716667	neg
6.44_615.0902m/z	615.0902364	6.442716667	neg
6.46_455.1547m/z	455.1546515	6.458366667	neg
6.46_457.2074m/z	457.2073656	6.458366667	neg
6.46_525.1942m/z	525.1941586	6.458366667	neg
6.46_543.2559m/z	543.2558865	6.458366667	neg
6.46_618.1733m/z	618.1732998	6.458366667	neg
6.48_208.9681m/z	208.9680781	6.477433333	neg
6.48_268.1168m/z	268.1168068	6.477433333	neg
6.48_313.1119m/z	313.1119075	6.477433333	neg
6.48_336.1045m/z	336.1044937	6.477433333	neg
6.48_373.1871m/z	373.1870654	6.477433333	neg
6.48_385.1509m/z	385.1508642	6.477433333	neg
6.48_391.1979m/z	391.1979144	6.477433333	neg
6.48_505.2662m/z	505.2661987	6.477433333	neg
6.48_523.1779m/z	523.177859	6.477433333	neg
6.48_540.0670m/z	540.0669873	6.477433333	neg
6.48_551.2485m/z	551.2484528	6.477433333	neg
6.48_605.1828m/z	605.1828485	6.477433333	neg
6.48_659.1527m/z	659.1526522	6.477433333	neg
6.49_302.1434m/z	302.1434275	6.494283333	neg
6.49_345.0934m/z	345.0933785	6.494283333	neg
6.49_357.1299m/z	357.1299492	6.494283333	neg
6.49_368.1169n	368.11696	6.494283333	neg
6.49_465.1358m/z	465.1357567	6.494283333	neg
6.49_472.0793m/z	472.0793149	6.494283333	neg
6.49_481.2049m/z	481.2049081	6.494283333	neg
6.49_519.1464m/z	519.1463502	6.494283333	neg
6.49_527.2480m/z	527.2479812	6.494283333	neg
6.49_601.1113m/z	601.1112956	6.494283333	neg
6.49_669.0984m/z	669.0983508	6.494283333	neg
6.51_188.1011m/z	188.1011288	6.509966667	neg
6.51_224.5637m/z	224.5637303	6.509966667	neg
6.51_271.1553m/z	271.1552646	6.509966667	neg
6.51_318.8745m/z	318.8744708	6.509966667	neg
6.51_339.1430m/z	339.1429941	6.509966667	neg
6.51_483.2606m/z	483.2605814	6.509966667	neg
6.51_547.1773m/z	547.1773401	6.509966667	neg
6.51_615.1647m/z	615.1647249	6.509966667	neg
6.51_683.1520m/z	683.1520364	6.509966667	neg
6.52_288.0873m/z	288.0872663	6.520516667	neg
6.52_356.0754m/z	356.0754248	6.520516667	neg
6.52_646.3214m/z	646.3214181	6.520516667	neg
6.52_845.7974m/z	845.7973919	6.520516667	neg
6.53_193.0795n	238.0776635	6.531066667	neg
6.53_501.0961m/z	501.0961072	6.531066667	neg
6.53_528.2173m/z	528.2172648	6.531066667	neg
6.54_344.9430m/z	344.9429709	6.539816667	neg
6.54_530.2974m/z	530.297359	6.539816667	neg
6.54_683.1215m/z	683.1214767	6.539816667	neg
6.54_704.8160m/z	704.8159659	6.539816667	neg
6.55_483.1856m/z	483.1855828	6.548566667	neg
6.56_389.1821m/z	389.1820901	6.55905	neg
6.56_526.2487m/z	526.2486934	6.55905	neg
6.56_661.1317m/z	661.1316523	6.55905	neg
6.56_729.1195m/z	729.119487	6.55905	neg
6.57_295.1664m/z	295.1664452	6.570233333	neg
6.57_367.9068m/z	367.9067888	6.570233333	neg
6.57_371.0702m/z	371.0702187	6.570233333	neg
6.57_391.1872m/z	391.1872493	6.570233333	neg
6.57_507.0450m/z	507.0449997	6.570233333	neg
6.57_575.0329m/z	575.0328781	6.570233333	neg
6.57_585.0868m/z	585.0868348	6.570233333	neg
6.57_787.8455m/z	787.8454752	6.570233333	neg
6.58_532.2895m/z	532.2894823	6.582416667	neg
6.58_613.0747m/z	613.0746842	6.582416667	neg
6.59_238.5793m/z	238.5793169	6.592933333	neg
6.59_290.1798m/z	290.1798036	6.592933333	neg
6.59_300.1277m/z	300.127666	6.592933333	neg
6.59_363.1663m/z	363.166324	6.592933333	neg
6.59_673.1710m/z	673.1709903	6.592933333	neg
6.62_244.0049m/z	244.0049374	6.61635	neg
6.62_316.1588m/z	316.1588674	6.61635	neg
6.62_481.2445m/z	481.2445085	6.61635	neg
6.62_545.0872m/z	545.0871665	6.61635	neg
6.62_549.2323m/z	549.2323343	6.61635	neg
6.62_603.0899m/z	603.0899146	6.61635	neg
6.63_276.9554m/z	276.9554093	6.63275	neg
6.63_442.0557m/z	442.0557225	6.63275	neg
6.63_455.1154m/z	455.115394	6.63275	neg
6.63_481.2054m/z	481.2054471	6.63275	neg
6.63_503.0636m/z	503.0635721	6.63275	neg
6.63_523.1026m/z	523.1026643	6.63275	neg
6.64_207.9188m/z	207.9188075	6.644916667	neg
6.64_297.0416m/z	297.0415622	6.644916667	neg
6.64_420.0738m/z	420.0737902	6.644916667	neg
6.64_749.0926m/z	749.0926421	6.644916667	neg
6.65_694.3409m/z	694.3408643	6.653683333	neg
6.65_762.3288m/z	762.3287725	6.653683333	neg
6.66_225.0745m/z	225.074527	6.663683333	neg
6.66_329.1973m/z	329.1972611	6.663683333	neg
6.66_345.0933m/z	345.0933225	6.663683333	neg
6.66_362.9534m/z	362.9534471	6.663683333	neg
6.66_487.2553m/z	487.2553437	6.663683333	neg

384.7511626	145.8857881	294.8117758	565.2714725	728.0633339	566.5831701	162.419474	88.53961182	77.76104355
2731.942839	3366.526956	3077.501543	762.4952362	693.0427367	1041.29671	2213.740108	2219.843678	2441.331952
843.4475907	775.0983656	811.5208775	931.8767067	921.3636605	889.761663	1258.740735	1020.272422	982.9567064
2754.329828	2632.838122	2751.519419	0.001403199	0.001403199	79.43506118	1874.606471	2055.370946	1911.948718
4556.200569	4250.577121	3799.073264	7023.047307	6482.273427	6966.115599	4856.097607	4363.466604	4190.511395
4751.274243	4115.54177	4359.184779	6086.776656	5148.042463	5273.700922	6098.783101	4517.074706	5937.807623
4583.544245	5102.830391	5116.215626	6965.993549	5905.509987	6654.57193	4702.8522	4581.369422	4024.637422
8595.363984	8169.727108	7032.595561	8694.880964	8552.349665	9636.602582	11777.23568	9450.633319	10142.71351
2237.682806	1612.382661	1852.462904	2161.541415	1915.891853	2262.957517	2829.867689	2380.329345	2230.003537
42724.05029	45810.54582	47533.46467	53355.82733	50946.34785	52172.79282	47558.48717	50412.97574	49976.64021
27866.9334	28021.42347	29272.89036	34330.96882	32628.42265	32464.24477	27538.51896	29134.09589	28373.25411
1352.123694	1058.657582	959.9372717	995.9372505	992.4589063	674.4805325	789.9337198	913.5247787	647.1689861
755.4026345	701.6387192	607.2220248	1678.634698	1594.171909	1678.90563	1290.76264	1114.097224	1164.09292
2389.017835	2278.776525	2440.904063	1832.443048	1795.687283	1884.219086	1813.080357	2329.882877	2357.201623
10771.69936	10596.83574	12334.79599	13232.75284	12982.25421	13015.79244	11948.54188	12944.93416	11984.85698
2596.404696	2458.79549	2220.972548	2843.251674	2531.056257	2554.161006	3293.808182	3231.580597	2904.199376
1424.492213	1177.250871	1250.726073	781.737148	1149.375724	949.3463844	1088.204848	977.2068405	1196.439935
5643.330109	6050.446386	6486.594139	7120.874564	5621.478741	6139.143158	6671.587796	6460.140719	6921.220607
775.9016723	964.8111031	1191.083738	2302.10172	1779.030798	1657.616106	977.2210413	1227.118523	1174.270423
9057.379492	9436.122189	9874.476456	10949.73381	10107.70251	9863.107371	9743.249051	10344.35893	9668.326334
1760.80829	1726.387641	2319.889537	1668.684898	1427.788914	1673.574172	2043.145184	2414.743704	2465.481469
5801.222053	5761.754356	6787.808462	2572.221854	1372.420074	1793.529111	5329.028531	6049.909817	5299.14036
1208.187948	1100.1743	1345.860116	1406.887062	1282.66171	1546.27885	1934.001805	2143.624742	1866.473651
497.6728828	490.66942	471.0895622	561.3782471	441.0264457	508.9861845	863.9718836	826.8603223	861.5790656
9346.156039	9884.456759	11688.05582	18548.90097	17374.11684	16673.10484	13891.74477	15480.08449	15445.21653
1090.558596	1032.810799	1193.507625	517.6105057	377.4990607	374.5085114	1182.617166	1277.396188	1145.172673
4440.380667	4522.376703	5272.006715	8414.386186	7633.333665	7456.607908	6226.75207	7299.907865	6600.957887
1457.977961	1524.982414	1699.598354	2194.218783	2203.488801	2036.293511	1769.232938	2155.425097	2228.842561
6784.764128	7620.098922	8071.567002	11428.69049	10712.55703	11022.27653	7958.148337	9016.846554	9046.023339
611.8476391	721.1609455	910.6484347	417.0516938	260.4939479	385.0458126	773.6719496	744.962204	775.8303313
13795.48625	14115.72214	15236.74325	16017.35742	14905.46628	15436.89964	18473.13975	19359.74977	19359.74977
4153.111967	4171.352921	5185.722143	5887.320116	4784.516119	4476.424795	8522.610968	9577.50918	8815.735294
1639.126603	1477.15101	1872.012722	3344.346687	3135.240413	3721.435081	2715.084096	3067.551485	2549.12187
222.9104834	512.0376218	532.723469	488.453749	0.001403199	409.0276422	470.0621235	492.0600433	294.4351122
2707.606765	2384.757265	2797.207348	710.9380501	555.8641467	831.1011576	1974.813475	2036.361045	2170.728548
1012.184181	1090.807744	1118.291533	1258.154882	1100.618911	1126.220083	3047.854204	3548.699182	2776.244492
810.3779969	739.3317715	1078.062534	832.3563868	676.2114461	544.3483447	1127.362693	1269.541024	1093.013452
989.4986701	1340.926135	1216.95363	663.1572774	577.1193017	639.2450965	543.7018055	629.9657402	598.7839141
483.3049267	596.8031698	631.5768235	478.2700213	495.7091241	666.486158	463.6364352	358.8317805	517.4378196
1065.479995	1207.27099	1331.673101	1022.168446	750.0329467	1021.423154	909.1183781	1248.032289	1397.548456
6534.732917	7630.546226	7431.006121	3023.357181	2393.283426	2487.112814	7253.834289	8352.615005	7793.34677
2523.279255	2131.331582	2710.359987	4691.972903	3733.976164	3873.899111	3568.409052	3642.136398	3896.531444
5374.297259	5745.956146	5750.401931	2669.409492	2685.497308	2880.524366	4733.353995	5815.682241	5201.207076
272.6052177	84.2235357	618.5447182	496.8597372	527.784979	489.8035465	0.001403199	427.7218437	452.0652399
3508.882598	3128.045233	3036.165777	3049.416672	3133.73125	3246.754983	4043.019266	3952.837286	4758.091087
2683.852556	2638.336546	2818.116545	594.4405064	744.5282371	506.3998581	2632.086397	3076.49271	2718.40538
1303.896081	1982.387903	1466.602673	279.8348094	199.0101041	173.0573435	1035.135443	1862.834857	913.4113139
59.05020115	82.08187485	93.88270012	58.23948643	79.24978167	163.5655666	20.79321856	42.40243466	76.17079136
5438.154772	6139.787916	6032.199965	7231.603265	7155.952156	6709.401196	5837.1814	7016.634704	6061.096141
5097.010794	5388.51392	5837.584739	5169.083476	4950.044458	5168.344943	4152.683942	4687.536498	4314.610301
3742.611553	3281.498517	2823.701323	2799.863856	3314.960245	3332.064255	4266.949375	3209.753162	3319.048222
1011.955804	1068.818983	1013.162033	808.0959485	1041.274675	1172.679282	793.5218189	899.0056776	949.6459372
1877.802726	2384.557186	2696.716092	2225.166788	1836.520458	1928.642207	1356.786525	2093.07366	2179.056649
8232.706734	8511.975034	9087.735875	3253.714242	2784.297768	2823.630783	6772.597518	8658.655584	9184.362323
4158.956957	5479.299367	5624.852448	1418.549315	1014.473419	1634.141713	4045.437065	4229.757641	5749.348729
2756.830291	3280.640461	3831.554559	1058.079876	1180.396155	1291.900787	2308.131089	2945.434378	3545.078353
6186.900583	6421.416746	6426.322422	8624.947405	9160.09631	8906.850823	7947.399146	8335.070061	8546.351686
1128.912781	1533.706198	1154.044053	1899.593595	1665.940114	1964.463541	1619.154026	1427.999731	1736.772093
2242.989214	2565.524146	2593.9764	653.2473163	274.2484107	614.2423738	1778.485966	2194.470158	1914.060399
5180.406599	3693.590886	3940.908962	3041.430982	3479.038829	3380.892391	4850.764021	4512.572498	4971.875558
114798.9767	120689.5953	124380.128	139330.9163	136330.7129	133865.8998	113935.0326	126895.6143	122860.6633
1081.991482	1062.349384	850.0100176	835.1373524	936.4129901	873.5014516	1265.934378	1336.535526	1285.229001
333.6623603	537.9693811	599.0910146	354.4732669	327.1862374	0.001403199	349.7674469	514.3093378	678.6323142
2444.940948	1937.237712	1966.705498	1720.460591	2505.917727	2312.936757	2285.562478	2531.880629	2301.099092
1662.989612	1720.190462	1717.68149	1243.979902	1518.538016	1231.825639	2987.140269	3021.283684	2699.636913
2622.286702	2971.224855	3182.923245	5414.118105	5520.338508	5764.975536	1828.12387	1894.841093	1776.599291
21529.19264	20398.99816	16267.79255	17741.34572	21666.75754	20501.99509	27092.91157	22302.13599	22890.81091
1541.401708	1947.736245	1604.550004	1457.349101	1379.67754	1825.227693	863.3843072	918.7073054	1014.367988
89039.4241	96869.20933	101752.6088	120503.8483	124158.8768	120866.739	78413.44251	90918.53989	82692.69426
1086.847588	546.2795212	682.1539795	886.3936108	854.8166872	786.8954364	364.3662085	585.0305724	696.0149378
3242.961765	3330.145162	4087.218734	4546.08804	5562.219628	5852.636677	2947.031677	3630.447101	2731.208595
1810.81459	2301.900116	1719.908811	2990.173428	3280.003248	2487.244583	1293.031749	1812.92141	1512.568412
4133.59937	5133.600462	4894.719232	9986.880643	9707.408752	9357.839569	4003.555198	4825.416889	4523.702272
2154.597336	1641.261075	1339.50032	1299.914996	1584.6304	1602.670687	1772.135778	1583.959031	1335.7206
3684.938714	4802.169375	4520.656882	3647.597681	3481.01198	3431.50932	2323.261501	2798.411476	2282.970876
1902.519955	2049.710813	2115.495712	2361.722192	2851.858868	2371.502176	1142.233949	1581.50524	1492.661316
1862.985211	2062.363851	2052.962895	1834.121327	1846.660479	1667.354972	919.0992264	1446.522328	798.1306332
1172.464929	1534.150321	1532.97809	1421.724436	1484.554238	1317.721022	740.9357464	838.2090843	844.2394857
3787.320088	3381.548717	3251.32403	3087.290405	3626.849273	3058.586063	3676.6669	3482.868367	3760.897347
4437.241165	3092.456673	3408.076737	3808.333743	5356.000222	5624.46532	5249.596551	3923.792999	5341.768236
1614.709787	2129.847704	2214.065703	303.8312653	149.7014506	132.4604414	1977.080723	2409.710001	2194.646449
1286.410911	1227.541676	1625.317221	3738.426263	2947.395347	3240.647139	2075.109612	2271.040062	1637.724923
1484.268285	1430.826318	1201.340687	1684.436831	1700.651776	1676.248386	1169.049175	1515.584936	1268.002978
1165.038737	1099.402289	1282.67964	1939.979996	1332.647842	1243.349925	612.1733983	1015.2893979	876.8102226
167.9364306	258.6784151	71.03646422	2565.550666	2756.80904	2847.437894	620.2788025	694.0003642	685.3279018
5436.624085	4919.892801	4803.404226	9352.258406	8964.209854	8500.31684	4369.569492	5215.256458	5080.245468
2741.128126	3224.423672	2750.27097	283.0163166	360.3657536	324.841022	1535.890974	2778.721924	1894.694252
404.3588624	310.2578982	386.0130903	504.3296477	355.8616241	412.7526752	47.45457483	78.83433985	35.70468071
494.3521136	400.8146218	529.4075521	565.5161883	300.3075251	627.3969994	651.4294183	976.578735	612.4505112
9073.592947	9100.968263	8644.01538	11892.55969	11745.38005	12083.15223	8786.339351	9638.607294	10074.02009
2876.041644	3017.24725	2667.475596	6650.421945	6265.315839	6662.559479	3889.015466	4715.314508	4635.994638
873.8380235	886.8020635	1233.794356	1701.081451	1995.908853	2008.36502	1101.891789	1580.832067	743.6121988
3570.073865	3964.390595	3674.084532	5234.426047	5384.123068	5069.728014	3244.75822	4073.649649	3670.312579
2382.831979	2248.557516	2348.531926	2252.124473	2829.335428	2447.211221	3230.726909	2800.459753	3071.753605
721.2218313	1100.921881	508.3292532	2175.098528	1559.955119	1454.024818	1651.934889	1733.446502	1610.568307
2978.514911	2662.063663	2662.505011	1027.693689	1026.825273	1053.441725	2858.037473	3430.443001	3752.046507
4268.86529	4334.821724	4052.575874	4480.84464	3893.860323	3534.739473	5085.763551	5824.392117	6096.318612
3237.883795	4033.855602	2897.325896	4563.56976	3832.677127	3800.178841	228.6818988	350.9473763	271.7155435
1329.386421	1111.202077	851.24613	603.5620852	297.9595331	596.9443662	1774.235264	1753.777082	1399.160709
767.8195792	576.9730948	422.9603716	301.6268655	361.1458032	253.5081125	756.8092112	481.3987047	417.6968796
932.8302683	824.9336343	748.4798888	392.7792491	307.200514	327.5437158	1020.660448	1047.363483	954.420029
1467.846739	1300.442711	802.3628985	1474.187139	2130.667036	1744.439792	1620.154765	2063.390805	2865.637933
3871.449	4749.805737	4555.92659	2751.762807	1479.104667	2720.863471	0.001403199	0.001403199	0.001403199
6092.55075	6551.233239	7205.657356	372.2729465	362.9850732	224.8275847	3318.048943	3564.478369	4580.04188
1517.169109	2346.472897	2082.548154	177.1642549	694.1253309	0.001403199	1414.784314	1158.445518	1298.707065
3088.295007	2847.572116	3010.251107	4899.5698	4603.251116	3629.226988	3508.219613	4138.313511	4301.449521
2771.981107	3317.887691	3265.848753	2761.800567	2588.377396	2469.872999	1926.256666	2451.794494	2795.055978
1505.457347	1555.874246	1715.82273	1000.026067	659.8275374	770.7905603	250.9111816	424.5859833	561.945042
1698.413147	1692.733948	1685.745802	1892.516167	2351.397684	1538.463405	2612.291888	2106.571837	2154.718348
14315.72537	14604.67495	14302.53208	15377.92037	13749.6562	13508.37184	8171.209362	9625.381847	10195.86032

6.66_501.0988m/z	501.0988137	6.663683333	neg
6.66_514.8937m/z	514.8937201	6.663683333	neg
6.66_545.8535m/z	545.8534563	6.663683333	neg
6.68_266.1011m/z	266.1010638	6.680966667	neg
6.68_751.1077m/z	751.107706	6.680966667	neg
6.69_210.9837m/z	210.9837407	6.69475	neg
6.69_479.0188m/z	479.0188101	6.69475	neg
6.69_506.0379m/z	506.0378764	6.69475	neg
6.69_512.0366n	557.0351455	6.69475	neg
6.69_523.1778m/z	523.1778494	6.69475	neg
6.69_526.2483m/z	526.2483403	6.69475	neg
6.69_568.9882m/z	568.9881747	6.69475	neg
6.69_570.9858m/z	570.9858132	6.69475	neg
6.69_579.0171m/z	579.0171244	6.69475	neg
6.69_647.0047m/z	647.0047296	6.69475	neg
6.69_714.9921m/z	714.9921373	6.69475	neg
6.69_782.9794m/z	782.9794478	6.69475	neg
6.71_183.0048m/z	183.0047888	6.70695	neg
6.71_421.0371m/z	421.0370733	6.70695	neg
6.71_444.0485n	489.0477254	6.70695	neg
6.71_505.1676m/z	505.1675927	6.70695	neg
6.72_397.1482m/z	397.1481794	6.717366667	neg
6.72_456.1941m/z	456.1940803	6.717366667	neg
6.72_465.1359m/z	465.1358702	6.717366667	neg
6.72_996.8230m/z	996.8230169	6.717366667	neg
6.73_260.0484m/z	260.0484499	6.72945	neg
6.73_465.2499m/z	465.2498751	6.72945	neg
6.73_533.1234m/z	533.1234062	6.72945	neg
6.74_446.9064m/z	446.9064161	6.739333333	neg
6.74_448.2016m/z	448.2015736	6.739333333	neg
6.74_654.8698m/z	654.8698701	6.739333333	neg
6.76_291.0829m/z	291.0829139	6.759433333	neg
6.76_350.0707m/z	350.0706943	6.759433333	neg
6.76_355.1383m/z	355.1383153	6.759433333	neg
6.78_202.1167m/z	202.1167233	6.776866667	neg
6.78_413.1821m/z	413.1820787	6.776866667	neg
6.78_519.1463m/z	519.1463192	6.776866667	neg
6.78_871.3106m/z	871.3105562	6.776866667	neg
6.78_881.3409m/z	881.3409195	6.776866667	neg
6.78_949.3277m/z	949.3277705	6.776866667	neg
6.79_210.9837m/z	210.983691	6.7874	neg
6.79_339.9118m/z	339.91182	6.7874	neg
6.79_367.9069m/z	367.9069447	6.7874	neg
6.79_481.1697m/z	481.1697024	6.7874	neg
6.79_525.2709m/z	525.2709079	6.7874	neg
6.79_813.3535m/z	813.3535417	6.7874	neg
6.80_381.1196m/z	381.1196073	6.799583333	neg
6.80_571.1025m/z	571.1025236	6.799583333	neg
6.80_579.1109m/z	579.1109075	6.799583333	neg
6.80_803.3246m/z	803.3246039	6.799583333	neg
6.81_523.1415m/z	523.1415324	6.809016667	neg
6.81_532.3130m/z	532.3129792	6.809016667	neg
6.82_367.1576m/z	367.1575671	6.817666667	neg
6.82_551.1729m/z	551.17289	6.817666667	neg
6.82_588.8247m/z	588.824754	6.817666667	neg
6.82_600.3006m/z	600.300562	6.817666667	neg
6.83_171.0201m/z	171.0201284	6.832183333	neg
6.83_179.9365m/z	179.9364696	6.832183333	neg
6.83_213.0573n	425.1073238	6.825	neg
6.83_390.2501m/z	390.2500621	6.832183333	neg
6.83_446.2762m/z	446.2761623	6.825	neg
6.83_561.0817m/z	561.0816987	6.832183333	neg
6.83_593.2587m/z	593.2586561	6.832183333	neg
6.84_251.0902m/z	251.0901806	6.842166667	neg
6.84_432.1959m/z	432.1958763	6.842166667	neg
6.84_661.1685m/z	661.168508	6.842166667	neg
6.86_316.1225m/z	316.1224969	6.86375	neg
6.86_330.1643m/z	330.1642854	6.86375	neg
6.86_343.1228m/z	343.1228452	6.86375	neg
6.86_496.9494m/z	496.9493611	6.86375	neg
6.86_537.0739m/z	537.0738861	6.86375	neg
6.86_605.0617m/z	605.0616752	6.86375	neg
6.86_683.0775m/z	683.0775191	6.86375	neg
6.88_271.1553m/z	271.1552729	6.8759	neg
6.88_428.1175m/z	428.1175124	6.8759	neg
6.88_469.0864m/z	469.0864207	6.8759	neg
6.88_496.1055m/z	496.1055017	6.8759	neg
6.88_562.1861m/z	562.1860502	6.884583333	neg
6.88_751.0651m/z	751.0650811	6.8759	neg
6.90_314.1798m/z	314.1798474	6.896766667	neg
6.90_449.2091n	494.1987421	6.896766667	neg
6.90_450.1546m/z	450.1546228	6.896766667	neg
6.90_509.2759m/z	509.2759184	6.896766667	neg
6.90_639.0898m/z	639.0898091	6.896766667	neg
6.90_772.8025m/z	772.8025404	6.896766667	neg
6.91_277.0330m/z	277.0330473	6.9072	neg
6.91_350.0705m/z	350.0705497	6.9072	neg
6.91_363.1665m/z	363.1665489	6.9072	neg
6.91_426.2114m/z	426.2114298	6.9072	neg
6.91_518.1419m/z	518.141875	6.9072	neg
6.91_519.1462m/z	519.1462372	6.9072	neg
6.91_793.1248m/z	793.1248309	6.9072	neg
6.92_443.1587m/z	443.158674	6.915966667	neg
6.92_470.1776m/z	470.1775514	6.915966667	neg
6.92_521.1751m/z	521.1750644	6.915966667	neg
6.92_538.1654m/z	538.1653756	6.915966667	neg
6.92_725.1374m/z	725.1374463	6.915966667	neg
6.92_861.1122m/z	861.1122197	6.915966667	neg
6.92_997.0863m/z	997.0862908	6.915966667	neg
6.93_606.1536m/z	606.1535953	6.926366667	neg
6.94_362.1224m/z	362.1223946	6.939266667	neg
6.94_427.1978m/z	427.1977554	6.939266667	neg
6.94_430.9405m/z	430.9405498	6.939266667	neg
6.94_480.9181m/z	480.9181082	6.939266667	neg
6.95_329.1971m/z	329.1971255	6.951516667	neg
6.95_583.3130m/z	583.3129678	6.951516667	neg
6.95_605.2948m/z	605.2948354	6.951516667	neg
6.96_226.9661m/z	226.9661213	6.96195	neg
6.96_292.9870m/z	292.9869754	6.96195	neg
6.96_388.2343m/z	388.2343004	6.96195	neg

526.7038093	405.3366961	454.5679927	1482.828262	1316.020917	1302.825356	949.3097209	1107.928719	1158.772226	
10348.7239	10252.52269	9569.229143	9763.586446	10295.77019	10005.9675	10840.18984	10924.80592	10488.6255	
5330.07107	5893.228112	4701.961067	6332.432975	6597.769774	5319.835293	7963.077715	6846.698265	6946.191519	
840.3664504	1099.038608	937.7051925	2284.425395	2404.929326	2055.67308	814.6062112	1009.058588	1147.999374	
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800.3294672	845.0331701	745.5150657	812.8770201	1117.219843	898.6859211	930.8733771	942.403875	1159.105494	
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63563.79794	73884.58354	67547.60328	76791.82808	75406.17505	72803.95607	8294.036006	9733.255699	10430.32456	
1473.765466	1072.067965	1568.971322	1269.247354	1281.8476	1630.764598	1601.124937	2543.087852	2118.208832	
5247.514864	6331.239425	6293.618234	6026.100533	5676.631941	5301.41185	3947.599187	5413.815618	5566.868208	
2553.817756	3806.922867	2894.01763	3299.149822	3849.895193	2437.484824	92.90061458	351.8818665	236.2914048	
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16316.45826	19146.23726	16742.37458	20382.14186	18831.43556	19325.34992	1498.853828	1964.105225	1944.712566	
7570.461939	9334.86885	8853.328165	10094.64429	9877.639022	10188.05104	683.1790508	710.2130394	729.5507859	
3428.593856	5197.35149	3890.151061	4963.389191	5641.921321	4425.887728	0.001403199	0.001403199	199.9007123	
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454.8828497	349.3715133	660.5937873	675.5253462	712.1142416	645.9284406	0.001403199	0.001403199	0.001403199	
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3497.000314	4353.026841	4211.884355	4671.841695	4538.715994	4061.205492	2927.668628	4395.032804	4379.034341	
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6613.965759	8488.192966	7766.479147	7566.020763	7490.075088	8263.676985	8047.619101	6803.780731	8307.361849	
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2847.375608	2805.837113	3049.932277	1522.91725	1125.13435	1442.86287	2405.189316	3354.06301	3166.146367	
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1750.040725	1799.830221	1653.677225	3059.818911	2873.209122	2791.246509	808.1381227	1226.117741	1270.096007	
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906.4751389	918.2322827	1079.261754	1523.761571	1291.196648	1512.818865	1070.708784	1123.539828	1108.769464	
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383.9461982	385.2602481	463.8702465	820.1925885	638.0906655	740.3680688	561.2748063	582.4525344	443.2614055	
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254.8974015	502.462525	634.0074612	560.1766862	576.155817	495.1272923	426.7018388	447.6384273	197.4236756	
3272.176395	2152.241642	3136.165138	212.5099879	0.001403199	440.5473252	1198.850343	2421.066245	2037.435401	
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785.0890063	463.0718742	583.128332	597.416082	716.1973836	669.1420986	1011.238077	641.9496584	695.1797892	
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5411.20613	4680.788572	4978.877974	2967.317095	2580.138409	3238.292328	4981.989507	4660.891831	4118.352452	
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543.6562777	489.9044248	604.4053715	118.1112448	192.1420466	0.001403199	517.6505918	276.7006817	399.2293069	
6814.238061	6050.476861	7877.972417	925.5982649	542.4999051	1595.653296	3266.591029	4795.678723	3692.314056	
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768.4902857	591.3885356	615.5668808	469.6398704	602.0920503	327.1611391	796.2634943	204.4591866	235.1594556	
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6220.950546	6958.844305	6415.966509	7092.969056	5730.615499	5259.80462	5748.218091	6851.247	7168.904302	
2245.074993	1776.469467	1749.884595	2127.140256	2275.806366	2057.705146	2457.305864	2423.866362	2383.003796	
879.841691	1112.149827	1049.800028	645.3538408	1053.333863	805.1799106	828.7644786	1060.442359	844.4047524	
794.3793065	836.2916862	1146.593905	1188.94599	798.2191426	799.7538595	391.3705931	650.1082328	731.9742242	
76211.17159	73513.52078	77638.68331	33210.95397	30411.16481	32835.29879	43614.55748	55061.3342	55672.32366	
19248.10593	19789.26732	19141.96606	8496.733024	6963.134488	8954.687852	12013.44101	14526.1004	14639.27208	
1402.52318	1486.032545	1318.148157	1176.797017	1354.034908	1279.125976	1553.187782	1501.761293	1489.408943	
1599.243335	1624.39192	1781.043287	1840.390391	1596.346337	1846.874248	1751.592743	2042.607118	2003.055821	
6836.774739	6585.445345	5464.890982	6046.82641	6075.06841	5667.902671	7539.379685	6607.848007	6175.266969	

6.96_722.8574m/z	722.8573621	6.96195	neg
6.97_487.2555m/z	487.2554661	6.970716667	neg
6.97_569.1319m/z	569.1319268	6.970716667	neg
6.98_330.1384m/z	330.1383943	6.981183333	neg
6.98_413.1821m/z	413.1820743	6.981183333	neg
6.98_481.1696m/z	481.1696415	6.981183333	neg
6.98_537.2144m/z	537.214371	6.981183333	neg
6.98_549.1570m/z	549.1570304	6.981183333	neg
6.98_784.8297m/z	784.8297137	6.981183333	neg
6.99_367.9067m/z	367.9067314	6.993516667	neg
6.99_437.1799m/z	437.1799004	6.993516667	neg
6.99_562.9159m/z	562.9158556	6.993516667	neg
7.00_156.9876m/z	156.9876242	7.0023	neg
7.00_179.9769n	358.9526651	7.0023	neg
7.00_212.9493m/z	212.9493034	7.0023	neg
7.00_214.9463m/z	214.946349	7.0023	neg
7.00_239.9683m/z	239.9683134	7.0023	neg
7.00_290.9653m/z	290.9652504	7.0023	neg
7.01_365.1279m/z	365.1278603	7.01105	neg
7.01_433.1153m/z	433.1153109	7.01105	neg
7.01_494.9284m/z	494.9284064	7.01105	neg
7.01_630.9047m/z	630.9046526	7.01105	neg
7.02_239.0902m/z	239.0902424	7.018266667	neg
7.02_343.1223m/z	343.1223178	7.018266667	neg
7.03_418.9163m/z	418.9162698	7.02545	neg
7.03_525.2708m/z	525.2708037	7.02545	neg
7.04_171.0201m/z	171.0201052	7.035966667	neg
7.04_360.9744m/z	360.9744037	7.044716667	neg
7.04_367.1583m/z	367.1583258	7.044716667	neg
7.04_477.2346m/z	477.2345665	7.044716667	neg
7.04_918.8066m/z	918.806599	7.044716667	neg
7.06_372.1488m/z	372.148754	7.055233333	neg
7.07_302.1434m/z	302.1434182	7.0658	neg
7.07_362.9417m/z	362.9417078	7.0658	neg
7.07_430.9393m/z	430.9393207	7.0658	neg
7.08_358.2603m/z	358.2602907	7.076316667	neg
7.08_402.2499m/z	402.2498924	7.076316667	neg
7.08_470.2376m/z	470.237646	7.076316667	neg
7.08_606.2126m/z	606.2125814	7.076316667	neg
7.08_674.1999m/z	674.1999285	7.076316667	neg
7.08_742.1874m/z	742.1874313	7.076316667	neg
7.09_401.1433m/z	401.1432778	7.086816667	neg
7.09_523.1414m/z	523.1413961	7.086816667	neg
7.09_638.3549m/z	638.3549111	7.086816667	neg
7.09_639.0900m/z	639.0899581	7.086816667	neg
7.09_753.8511m/z	753.8511167	7.086816667	neg
7.10_278.9711m/z	278.9711276	7.097333333	neg
7.10_318.1382m/z	318.1381932	7.097333333	neg
7.10_418.2169m/z	418.2169056	7.097333333	neg
7.10_431.2295m/z	431.2295044	7.097333333	neg
7.10_472.2453m/z	472.2453071	7.097333333	neg
7.10_532.3129m/z	532.3129293	7.097333333	neg
7.10_595.3720n	640.3707835	7.097333333	neg
7.10_662.3527m/z	662.3527222	7.097333333	neg
7.11_298.1855m/z	298.1854923	7.107783333	neg
7.11_329.1973m/z	329.1972553	7.114116667	neg
7.11_427.1806m/z	427.18058	7.114116667	neg
7.11_536.0483m/z	536.0482743	7.107783333	neg
7.13_362.9538m/z	362.9537535	7.1264	neg
7.13_445.1696m/z	445.1694665	7.1264	neg
7.13_453.1359m/z	453.1358566	7.1264	neg
7.14_318.8750m/z	318.8750467	7.138633333	neg
7.14_319.0776m/z	319.0776443	7.138633333	neg
7.14_331.9228m/z	331.9227532	7.138633333	neg
7.14_366.2230m/z	366.2230123	7.138633333	neg
7.14_389.1816m/z	389.1815885	7.138633333	neg
7.15_241.1060m/z	241.1059526	7.147366667	neg
7.15_285.1709m/z	285.1709489	7.147366667	neg
7.15_374.2551m/z	374.2550844	7.147366667	neg
7.15_413.1434m/z	413.1434254	7.147366667	neg
7.15_426.0763m/z	426.0762973	7.147366667	neg
7.15_481.1308m/z	481.1308289	7.147366667	neg
7.15_494.0636m/z	494.0636234	7.147366667	neg
7.15_549.1182m/z	549.1182134	7.147366667	neg
7.15_562.0512m/z	562.0512381	7.147366667	neg
7.15_630.0391m/z	630.039145	7.147366667	neg
7.16_345.1557m/z	345.1557069	7.1647	neg
7.16_464.3021m/z	464.3021499	7.1647	neg
7.16_519.1463m/z	519.1463945	7.1647	neg
7.16_544.1191m/z	544.1190929	7.1647	neg
7.16_562.2872m/z	562.2872186	7.1647	neg
7.16_570.3409n	569.3335852	7.1647	neg
7.16_587.1340m/z	587.133981	7.1647	neg
7.16_603.1268m/z	603.1268174	7.1647	neg
7.18_272.1692m/z	272.1691681	7.178516667	neg
7.18_332.1541m/z	332.1540578	7.178516667	neg
7.18_402.2500m/z	402.2499818	7.178516667	neg
7.18_425.1172m/z	425.1172371	7.178516667	neg
7.18_476.1314m/z	476.1314135	7.178516667	neg
7.18_479.1772m/z	479.1772135	7.178516667	neg
7.18_493.1047m/z	493.1046593	7.178516667	neg
7.18_503.1335m/z	503.133549	7.178516667	neg
7.18_509.1074m/z	509.1074341	7.178516667	neg
7.18_520.1238m/z	520.1238059	7.178516667	neg
7.18_536.0480m/z	536.0479995	7.178516667	neg
7.18_538.2251m/z	538.225062	7.178516667	neg
7.18_561.0918m/z	561.0918421	7.178516667	neg
7.18_587.0460m/z	587.046021	7.178516667	neg
7.18_606.2128m/z	606.2127827	7.178516667	neg
7.18_633.1394m/z	633.1394049	7.178516667	neg
7.18_639.1097m/z	639.1096714	7.178516667	neg
7.18_655.0339m/z	655.0338787	7.178516667	neg
7.18_674.1997m/z	674.1997014	7.178516667	neg
7.18_742.1872m/z	742.187214	7.178516667	neg
7.18_809.8507m/z	809.8506647	7.178516667	neg
7.18_810.1745m/z	810.1744691	7.178516667	neg
7.20_164.9571m/z	164.9570508	7.201166667	neg
7.20_295.1163m/z	295.1162755	7.201166667	neg
7.20_358.2604m/z	358.2604075	7.201166667	neg
7.20_492.2583m/z	492.2583314	7.201166667	neg

10156.97779	8110.752896	8315.06874	10663.49341	7665.986575	8897.88702	11417.66554	9879.089836	10739.95935
6117.36634	5413.657789	6956.367429	7257.109115	6025.387997	6863.776492	3286.39666	4776.772063	4372.690742
1031.220147	888.8981147	727.6549807	2242.534793	2057.461044	2010.300379	857.2016997	971.1054039	1166.847192
10676.11291	10506.23016	12290.37714	17997.26709	14313.47198	17092.03609	10523.22376	11969.93505	11848.02417
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6937.917182	6748.53239	7056.211998	8292.486075	6377.459423	7584.0534	5797.114167	6610.560281	6311.087095
480.2095175	245.4326982	215.1602005	288.3356253	412.1710018	205.4993446	377.8030314	351.4717519	425.7388029
2256.337081	2039.981174	2603.880972	2530.311604	2577.667445	2620.212766	2133.287225	2598.596376	2011.674818
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4010.336729	3255.303725	3243.880863	3063.176972	3566.571601	3537.067329	3604.935135	2884.142536	3126.500795
1637.623039	1699.920613	1493.693492	2329.208778	1932.243627	2030.972201	1966.814333	2123.759175	1913.171176
7570.028422	5902.447576	5860.218416	6244.436592	6189.700004	6516.752147	7851.959088	7889.441861	6847.684447
6507.864029	5665.267681	5812.766925	6029.331762	6032.254248	6485.911042	7549.548958	6439.492044	6573.28778
15964.47994	13587.59325	13426.46417	14142.83902	14092.0582	14801.27059	18222.56369	15681.9857	16130.83432
1022.59699	963.5713682	914.621729	1069.97094	868.8903952	1115.476755	1299.85781	1110.418737	1136.270029
640.496215	603.5205488	567.5838376	612.9405301	634.7320231	642.6279027	680.5575802	569.7425537	716.0743513
2760.99818	2092.242806	2263.664337	2497.520551	2301.121717	2594.306967	2698.010348	2560.160425	2467.433371
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5353.495335	5069.6831	5017.745756	2209.225503	1553.194661	1924.893412	4319.159114	4553.561732	3799.277809
1437.076009	1264.287964	1224.255198	354.1962203	161.6228416	135.8435236	956.900306	1145.108818	913.6253987
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3167.427012	2601.849011	2729.016122	3017.103736	3103.552843	3892.425532	4146.103139	4119.705073	3410.32084
645.1209485	520.0209098	416.7279096	471.54129	441.1368478	551.344784	558.2888126	534.7442727	455.2015132
0.001403199	109.875597	193.4857549	255.8402031	57.11016332	265.7498324	75.41210066	125.930517	177.7662383
8510.389029	7909.093715	7163.983757	7831.894652	8348.238275	8589.310745	9870.238668	9661.062416	8427.633963
4915.34199	4816.228809	4474.592211	5531.185	5249.184372	5394.901538	4138.896924	4230.273365	3869.305299
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972.7390147	1127.744861	1277.686739	1190.540202	1100.125746	1060.632453	1170.446087	1421.218474	975.410709
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338.2444877	241.8722722	262.8716901	232.0440924	202.7479511	89.01778903	94.18789073	355.0324993	292.1027931
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11592.82571	12108.35949	11725.62904	5270.824663	5038.054226	4474.884202	8548.693243	10159.55538	10152.64312
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4203.505688	4228.493321	4455.838689	2907.95351	3162.328241	3316.968133	5496.677433	5950.589938	5267.531557
26504.47494	26457.323	26783.78006	4100.727323	4415.946644	3649.546762	15537.6306	19841.12905	17585.36192
5602.862226	5521.824015	5838.411486	428.9633714	272.8543777	422.6753052	2712.485147	4135.072161	3797.404234
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1067.947403	1032.076347	1351.038614	366.5702781	752.0200415	524.248496	767.1159409	361.7162701	285.997469
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1692.111421	2342.58813	2407.764988	3969.410493	3931.691393	3614.658321	2639.946984	3046.905125	3067.302394
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927.2830732	1514.558789	1319.13229	1355.003931	1135.894678	1234.48309	1103.487229	1391.487846	1297.168358
625.0140521	1169.370495	920.5156087	1765.265798	1436.819679	1682.650199	543.1731762	880.2770936	957.6183915
2971.630196	3243.478599	3139.418265	1120.239751	1665.222496	1502.833839	2279.38737	2674.883795	2471.692132
2927.801833	4071.363381	5046.456437	104.4016489	251.9179579	283.5992278	1584.687199	2562.03459	1079.344291
888.6778787	580.0195475	765.6028186	306.6778821	644.8731363	643.3125649	436.9335261	557.8797302	786.6625046
1605.475841	1874.331044	2030.475046	2385.016109	2425.266749	1684.356658	2849.461174	1563.018295	
5167.133437	6681.316463	6528.190089	9669.416993	10162.27429	10750.39313	4837.656226	6376.246307	5592.509814
503.0369816	401.3895757	632.1799849	855.2775304	558.106676	795.5704671	611.3903845	658.892612	441.4391793
9009.782522	10811.21432	10343.91515	15076.51773	14697.55025	14976.03094	9169.638605	11604.52571	10118.52948
3493.714538	3781.43154	4041.657688	4931.026805	4582.793259	5295.520603	3502.11839	4628.298895	4001.118684
1155.490493	1882.530176	1467.117099	1992.437998	1959.645116	2444.348117	987.0801013	1391.401126	1101.075334
636.6569	694.2248082	524.6214477	0.001403199	15.69207228	8.736138235	118.8002408	366.7522379	446.8513171
1920.551198	2003.719046	1761.381634	2300.460579	2029.919748	2788.07737	2078.78823	2185.287707	1712.764923
39406.76094	46060.16011	42928.03036	55021.28692	54568.73467	55005.97012	39481.51476	46436.37452	43120.88301
2213.385629	2483.52018	2035.701964	652.9677742	415.4199875	481.6396877	1276.43252	2116.712621	1511.105151
721.7400537	1419.027846	1297.7744	1047.135182	803.7941645	1442.516812	1121.563886	1100.867313	1082.833151
1487.552069	1714.664783	1570.092575	1479.879513	1448.618266	1243.254992	1147.662461	939.6919631	1134.504695
5297.756856	6140.268433	6281.264515	9602.492094	8550.016811	9493.672308	5737.006294	7221.877428	5525.533869
1364.280802	1409.169227	1339.134577	1449.148022	1126.814969	1376.092633	1163.022801	1445.542984	993.9608962
11478.28293	13700.98826	12980.64591	10599.53547	11237.86745	11458.77675	6867.695177	8798.30605	7928.389269
5345.157006	5610.146598	5345.961441	8516.881929	8252.904059	8000.74625	4889.059378	6297.715899	5064.982931
1390.895945	2401.039789	1891.434061	2267.162439	1452.584707	1748.962088	1294.688778	2380.671471	1810.506165
7568.783965	9166.873117	8394.736478	9969.586851	9469.74006	11340.67699	8026.425828	10502.65228	8438.86038
2929.114906	3425.270014	3579.96997	2590.839706	2422.599481	2883.591395	1836.836128	2405.056566	2136.360428
2323.493397	2804.495584	2513.361184	4353.901578	4234.967086	4302.854153	1849.485633	3157.873916	2544.442923
1528.84652	1540.995764	1551.786509	2401.730798	2314.099035	2894.041549	1558.377364	2270.256057	1633.510355
27429.20174	25821.35581	23420.21671	25415.01759	29048.27892	28395.12891	32829.87694	31657.88394	28463.0144
621.5483237	673.0484777	1365.836894	2211.29968	1456.13037	2239.721683	1187.432598	1107.25001	385.1193647
243.9626113	318.0338116	263.6030354	353.8258462	425.125962	399.4637305	366.1614525	322.7954474	287.6002519
553.2919367	729.8967834	723.4926736	859.3683278	859.4514327	842.0878883	591.4887668	891.3004055	603.4222868
1131.560021	1057.6386	1337.390974	1772.966323	1737.353553	1902.288167	888.5105095	1338.887281	960.5256858
1349.989193	1120.905131	1761.713346	982.3864016	946.5632297	865.4482421	728.3932376	767.8552094	650.5143249

7.20_509.2759m/z	509.2759495	7.201166667	neg
7.20_533.3163m/z	533.3162935	7.201166667	neg
7.20_560.2459m/z	560.2458858	7.201166667	neg
7.20_747.2182m/z	747.2181578	7.201166667	neg
7.20_815.2055m/z	815.2054667	7.201166667	neg
7.21_372.1470m/z	372.1469676	7.211683333	neg
7.21_663.8473m/z	663.847303	7.211683333	neg
7.23_496.1724m/z	496.1724064	7.225666667	neg
7.23_506.2011m/z	506.201068	7.225666667	neg
7.23_537.2144m/z	537.2144321	7.225666667	neg
7.23_574.1886m/z	574.1885837	7.225666667	neg
7.23_642.1762m/z	642.1762133	7.225666667	neg
7.23_710.1637m/z	710.1636898	7.225666667	neg
7.23_778.1510m/z	778.1509928	7.225666667	neg
7.24_316.1952m/z	316.1952412	7.237866667	neg
7.24_339.9118m/z	339.9117875	7.237866667	neg
7.24_412.9305m/z	412.9305182	7.237866667	neg
7.24_427.1976m/z	427.1975948	7.237866667	neg
7.24_546.2928m/z	546.2927724	7.237866667	neg
7.24_647.1942m/z	647.1941701	7.237866667	neg
7.25_221.9562m/z	221.9561862	7.248333333	neg
7.25_334.1591m/z	334.1591302	7.248333333	neg
7.25_449.0552m/z	449.055204	7.248333333	neg
7.25_579.2063m/z	579.2062764	7.248333333	neg
7.25_845.7977m/z	845.7977345	7.248333333	neg
7.26_223.9541m/z	223.9540967	7.262266667	neg
7.26_330.1383m/z	330.1383327	7.262266667	neg
7.26_416.2195m/z	416.219547	7.262266667	neg
7.26_619.1968m/z	619.1967909	7.262266667	neg
7.28_214.1451m/z	214.1450552	7.2779	neg
7.28_389.1821m/z	389.1820946	7.2779	neg
7.28_505.2659m/z	505.2658749	7.2779	neg
7.28_687.1843m/z	687.1842533	7.2779	neg
7.28_755.1711m/z	755.1711462	7.2779	neg
7.29_304.1591m/z	304.159058	7.286583333	neg
7.29_345.1557m/z	345.1556779	7.286583333	neg
7.29_413.1433m/z	413.1433104	7.286583333	neg
7.29_415.1489m/z	415.1488727	7.286583333	neg
7.29_549.1183m/z	549.118328	7.286583333	neg
7.29_570.3409n	615.3391609	7.286583333	neg
7.29_617.1056m/z	617.1056037	7.286583333	neg
7.29_753.0802m/z	753.0802103	7.286583333	neg
7.29_819.3011m/z	819.3011162	7.286583333	neg
7.30_374.2551m/z	374.2550665	7.303966667	neg
7.30_385.1507m/z	385.1507493	7.303966667	neg
7.30_437.0304m/z	437.0304124	7.303966667	neg
7.30_437.0551m/z	437.0550519	7.303966667	neg
7.30_437.1794m/z	437.1793731	7.29525	neg
7.30_481.1308m/z	481.1307881	7.29525	neg
7.30_481.2065m/z	481.2064513	7.303966667	neg
7.30_495.0139m/z	495.0139124	7.303966667	neg
7.30_522.0329m/z	522.0329033	7.303966667	neg
7.30_528.0314n	573.0300431	7.303966667	neg
7.30_563.0012m/z	563.0011893	7.29525	neg
7.30_584.9832m/z	584.9832134	7.303966667	neg
7.30_595.0119m/z	595.0119262	7.303966667	neg
7.30_632.3292m/z	632.3291562	7.29525	neg
7.30_662.9998m/z	662.9997626	7.303966667	neg
7.30_683.3269m/z	683.3268774	7.29525	neg
7.30_730.9870m/z	730.9869689	7.303966667	neg
7.30_798.9749m/z	798.9749381	7.29525	neg
7.31_272.1691m/z	272.169141	7.314366667	neg
7.31_618.9087m/z	618.9086915	7.314366667	neg
7.31_996.8233m/z	996.8233199	7.314366667	neg
7.32_441.2124m/z	441.212048	7.324733333	neg
7.34_575.1706m/z	575.1705868	7.33585	neg
7.35_378.1019m/z	378.1019343	7.346316667	neg
7.35_439.2167m/z	439.2166945	7.346316667	neg
7.35_459.0474m/z	459.0473858	7.346316667	neg
7.35_465.2502m/z	465.2502306	7.353466667	neg
7.35_486.0658m/z	486.0657839	7.346316667	neg
7.35_537.0634m/z	537.0634435	7.353466667	neg
7.35_587.0461m/z	587.0461176	7.346316667	neg
7.35_605.0508m/z	605.0508099	7.346316667	neg
7.35_635.3054m/z	635.3054009	7.346316667	neg
7.35_673.0385m/z	673.038543	7.346316667	neg
7.35_703.2924m/z	703.2924238	7.353466667	neg
7.36_226.9660m/z	226.9660445	7.36395	neg
7.36_918.8064m/z	918.8063524	7.36395	neg
7.37_210.9836m/z	210.983617	7.372733333	neg
7.37_487.2555m/z	487.2554513	7.372733333	neg
7.37_663.8472m/z	663.8471955	7.372733333	neg
7.37_817.3229m/z	817.3228976	7.372733333	neg
7.37_845.7986m/z	845.7985684	7.372733333	neg
7.38_296.1691m/z	296.169147	7.381583333	neg
7.38_343.1222m/z	343.1222333	7.381583333	neg
7.38_683.3531m/z	683.3530536	7.381583333	neg
7.39_339.9118m/z	339.9117571	7.3938	neg
7.40_292.9870m/z	292.9870125	7.404266667	neg
7.40_388.2341m/z	388.2340944	7.404266667	neg
7.43_1059.2237m/z	1059.223734	7.426916667	neg
7.43_297.1821m/z	297.1820934	7.426916667	neg
7.43_316.1954m/z	316.1953587	7.426916667	neg
7.43_384.1833m/z	384.1833377	7.426916667	neg
7.43_736.2791m/z	736.2790597	7.426916667	neg
7.44_583.3130m/z	583.3129713	7.440866667	neg
7.44_641.2717m/z	641.2716834	7.440866667	neg
7.44_668.2911m/z	668.2910762	7.440866667	neg
7.44_855.2624m/z	855.2624397	7.440866667	neg
7.45_618.9088m/z	618.9088161	7.453016667	neg
7.47_413.1819m/z	413.1818811	7.473983333	neg
7.47_505.1310m/z	505.1309661	7.473983333	neg
7.47_550.2462m/z	550.2461957	7.46525	neg
7.47_618.2337m/z	618.2337286	7.46525	neg
7.47_624.3394m/z	624.3393904	7.46525	neg
7.47_641.1052m/z	641.1052114	7.473983333	neg
7.47_646.3215m/z	646.321491	7.46525	neg
7.47_686.2205m/z	686.2205008	7.46525	neg
7.49_481.0918m/z	481.0917751	7.4852	neg
7.49_508.8658m/z	508.8658205	7.4852	neg

5550.318441	7427.970333	6231.404499	7184.791261	7533.279445	7612.673489	6225.00736	8289.625913	7198.785054
288.5519693	208.7856722	117.6472564	557.4734967	225.4844461	545.0398283	686.3956278	711.3592193	509.2564604
699.4015665	795.0128566	936.4325851	324.0252032	554.2045348	762.9885491	544.3088239	348.2829097	588.8873151
4003.706607	3979.894711	4806.073243	3509.157242	2702.019725	2941.980169	2474.75678	2776.03589	2907.550761
1649.609088	2341.403192	1953.971832	1971.909165	1455.902316	1949.802089	1455.660626	1492.399384	1530.181195
1439.109912	1450.28732	1703.576095	1781.516356	1580.336862	1455.777128	1232.63257	1749.041882	1506.500018
2962.397334	2289.22071	2357.738363	3081.462244	3528.267326	3227.038808	4132.366683	4441.531117	3303.861479
1033.923988	1013.909294	935.9003048	604.5538396	454.9723164	433.3768391	472.7570646	576.6382637	717.924381
26598.06182	26758.48383	24783.78077	15013.57716	16467.83896	14294.93529	16828.07717	18926.91961	17575.20347
117.0354739	270.0325267	444.5379676	121.6481969	129.1867093	88.81861501	258.9563303	318.4509773	243.8451426
7238.881611	8018.681978	6880.393644	4677.133512	4677.839136	4008.345361	4101.810628	5897.604967	4458.347736
4364.661203	4144.595532	3863.02743	2639.196814	2816.397638	2867.707567	2907.878556	3466.129993	3185.627856
1885.262788	2446.821154	2073.832445	651.1853968	811.9722527	911.2042569	600.8570704	1410.193587	979.4482067
690.5834733	608.018002	660.7651372	0.001403199	180.9483513	212.5809469	215.2736896	993.4230272	510.4305862
888.9541963	1282.497952	1125.353234	1410.236825	1610.650676	1294.731714	653.0423739	845.4228512	798.8086557
2946.842085	2903.493739	2467.833623	2571.747169	3119.181842	3009.249869	3002.399022	2504.422333	2655.674317
2602.461568	2576.169489	2582.661949	2526.934546	3252.922103	2771.891302	3354.206272	2940.036468	2748.565053
1612.151364	1853.089254	1903.861962	1987.919385	1800.077245	1549.818641	2348.289777	2266.903968	2238.960103
389.3901405	355.2448895	457.299996	978.8180503	538.5148512	467.2481253	543.1016577	1405.195131	1173.792508
275.9478521	374.6890338	254.762194	0.001403199	553.7364233	302.9321884	134.8344519	531.8948441	397.9976028
571.1072957	561.4661829	613.7292987	675.2287007	619.7297537	598.5498173	510.3239937	766.6197513	569.0767101
95.55868441	53.03986816	194.1155914	101.8009163	151.639038	164.1849286	0.001403199	43.46591759	49.25502018
10934.57374	12436.28464	12000.06806	17968.70297	17337.27282	16922.27379	108.5278836	0.001403199	76.84834094
1478.533277	1480.557	1617.409385	2050.002218	2056.899871	2064.310107	1096.800442	1320.266988	1587.187135
2880.104006	2744.382913	3156.968729	3662.727297	3578.794464	3370.309047	5639.335437	4054.977	4441.273707
460.2210069	308.8527593	367.2460382	482.5751169	393.0904195	356.1408164	400.5769228	365.5262356	512.7410169
3622.91861	3986.635437	3884.368213	5895.558589	5588.580871	5195.924066	3587.87533	4007.119131	4437.702378
0.001403199	0.001403199	388.8029743	99.53069429	98.41171016	140.4453149	0.001403199	0.001403199	312.9329136
5178.275767	5452.720401	5279.373143	5679.929629	5691.354175	5681.953462	7865.157215	8112.848766	8050.179233
125.204266	70.47696011	91.49687801	104.4120305	30.71104619	136.8818079	196.6799766	59.55816639	133.8763741
15487.62481	18242.86741	17601.33499	25735.35022	24708.84028	23904.32995	17006.94679	17861.56077	19416.24618
1696.123474	1789.851418	2026.222367	2484.777527	2302.908196	1770.771418	2390.992079	2678.196061	2522.742825
2319.824597	2634.933803	2688.622842	3156.699562	2938.666803	2863.85705	4634.630641	4417.571039	5441.449452
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67784.92172	72261.09935	69541.58169	100024.1	94014.49826	91890.54273	54851.84009	63886.40603	61423.11083
22337.43415	24915.13979	23381.39224	32494.74803	31815.07382	30007.73737	18242.58556	18665.54954	20962.79081
419.0188711	155.8502055	367.0641476	606.2248937	273.4241535	355.4589021	0.001403199	141.3231277	238.405443
6647.261504	7239.1578	6543.923717	10067.10796	9783.770635	10072.60064	5652.887286	4876.987018	6801.482776
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3902.015672	4772.003442	3793.791147	6827.223837	5895.649809	5337.56884	2788.16149	3450.316168	3265.895666
610.5365254	865.6070084	1395.756807	1973.814552	2002.985976	1203.469038	784.004233	372.3210347	580.6207109
6318.172652	6885.616471	6436.0925	181.3299277	743.7120718	219.2435383	3322.63086	2867.281097	3891.348249
46022.646	44568.97722	42200.51147	43115.69256	48177.35014	45594.70149	47949.15118	43231.94984	47430.04268
3416.148923	4170.443015	4184.108335	2269.601123	4133.788066	3945.634359	2785.003137	3004.493869	3225.76158
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1385.688588	1313.809781	1713.641511	2034.312213	1745.868758	1503.48228	1306.373061	1252.081921	1383.154351
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7709.382301	8835.772271	8374.928493	7091.454678	6251.049173	6630.434907	5568.918864	6204.046524	7056.663966
5679.575235	6172.796198	5864.834013	4633.016759	4729.637198	3657.520457	3852.995496	4228.351535	4571.806342
62741.29492	67601.43083	66203.37931	52355.80222	51825.17906	51897.46561	45277.40114	48249.19965	52598.32621
2214.914197	2231.749961	2161.852474	1242.221055	1679.166408	1444.347022	1315.729901	1216.365695	1693.831839
2426.676353	2777.806922	2603.888152	2442.021094	2012.058841	1951.097022	2288.464783	1872.972717	2032.899817
36041.38489	38042.23998	36994.46474	29714.06691	30358.03874	29333.00853	26553.39749	28704.83381	30392.80898
3707.01327	4629.165993	4209.870577	145.6793112	116.0495969	365.2690665	1934.030644	2099.72671	2491.943703
14021.54623	16401.96327	15358.50126	13142.03775	12818.50835	12754.68234	10101.43611	11929.91707	12218.18625
48636.77469	56960.12432	57425.52889	10814.4108	8569.880416	9529.342783	29906.05397	29595.00766	34237.9052
7498.508569	8057.59861	8355.821739	7025.007476	6439.230086	5274.491505	5261.285917	4865.272163	5951.696121
3046.133581	2710.671206	3527.795051	2640.221062	3163.444783	1965.784133	1858.442036	1735.752144	1990.513724
1990.474639	2409.527464	2167.627577	2985.405164	2890.105944	2892.006921	1622.168599	1706.56498	2420.305541
1641.54605	1349.702745	1732.56223	1884.527115	1859.740092	1087.343237	1672.957918	1150.846669	2000.086728
20268.01309	22052.37138	18199.75257	21668.78056	25214.29084	21054.13222	24870.36548	21217.2463	21950.44439
3967.465556	4768.13356	5024.561596	6323.979035	5997.14311	5453.374135	3985.738103	3984.593089	4502.016227
1267.969101	1639.943378	2044.77511	2252.629909	1784.872198	1546.282792	1508.927018	1399.396719	1697.42811
5696.949428	6241.633971	5665.62081	7584.695181	7744.990692	6958.19157	6903.224694	7352.024467	7922.325933
415.2275738	459.6788549	1155.240959	323.5611042	154.6999671	0.001403199	590.0726421	285.8925629	531.2900925
1405.727743	1138.680473	1028.972914	1270.248613	1196.104447	1287.96868	1535.934709	1330.061942	1268.790435
3602.889224	4464.377682	3831.178697	5248.22705	5441.720893	5411.476306	3572.467408	4235.351751	4015.339539
3047.267461	2554.941831	2237.984378	2177.189805	2613.603457	2291.378864	2750.986625	2741.462446	2766.341684
12120.36536	11245.50722	10490.60279	10978.64297	12480.95334	11287.47237	13114.9044	12631.27227	13068.72357
11777.76078	12709.96122	10852.59113	8276.083484	8445.90558	8270.212896	6828.485452	7457.881987	8065.683726
6840.668703	6347.875849	5250.139479	5644.943216	6704.862143	6092.141791	6880.883257	7182.733777	7201.18439
8435.890452	9435.986141	7909.790333	458.2359044	222.6300243	415.8966874	2316.73543	3320.43445	3221.161617
2765.766129	3160.72712	2666.793735	2843.110902	3431.93612	3746.557289	4560.895298	3819.362821	3743.945418
2457.316173	2957.749776	2720.534769	145.3950665	0.001403199	0.001403199	0.001403199	596.3040676	838.6325927
882.4746942	676.3290747	737.7277161	864.4959118	914.737055	896.6590047	923.6224481	834.2874392	923.7884719
7055.065334	9281.467084	9429.241801	9905.055194	10632.61143	9045.823738	10162.19574	9934.014832	10523.79639
729.582675	805.3781001	639.5563431	768.1198704	832.5404948	853.7453652	855.2507052	775.8257193	686.4884977
3289.284403	3306.758664	2893.310131	3860.862407	3488.829491	3253.879392	1576.782776	2281.94175	2428.15098
4369.142243	3642.700389	3495.93922	4044.130635	4683.936951	4297.356428	4652.757465	4472.394226	4062.260461
2541.375347	3624.020562	2690.155785	3268.051442	3322.920549	2253.700549	2795.079657	5238.924221	3702.053742
4845.478445	5154.550048	3532.551002	1189.598541	5076.339761	5608.388758	6416.329681	5068.409004	5309.044448
329.0536901	460.6038483	415.1894939	528.9471305	637.9467934	663.1517211	293.9617586	373.7675323	421.1049569
332.5057365	425.5790279	548.7860713	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199
748.4744965	1035.077796	483.6045611	562.6377108	497.1699354	729.7364982	0.001403199	761.7985664	143.4521542
1625.169047	1656.651619	1257.044501	1327.036782	1577.732021	1496.040678	1568.510337	1573.690256	1261.481865
1491.016946	1394.884694	1054.057184	1493.940937	1526.36505	1484.646745	1395.290655	1234.153351	1287.9826
827.3857211	1214.610007	1017.807496	1118.428457	1103.685152	1092.552246	866.3299038	1011.864962	897.1619805
2666.880741	2817.912663	3743.866628	0.001403199	0.001403199	0.001403199	1255.392	1588.949097	1437.524645
9075.131646	8823.910751	9526.227692	19634.72213	17949.73976	18732.85821	7611.744472	7868.799226	7617.368083
2583.934614	2925.263179	2982.726693	2658.009072	2745.528393	3067.217326	1683.017558	2068.697094	1818.398697
1338.234478	1230.831611	1525.350872	1645.329032	1505.300324	1189.034414	1008.761812	1015.706702	901.6973658
1122.930699	1404.862907	1550.318425	0.001403199	0.001403199	0.001403199	422.605913	642.6176987	329.7913309
556844.5866	542818.1113	638862.7131	109422.4528	110274.2296	103983.9388	269396.6551	294452.8922	270893.6833
12998.1791	11506.64837	15419.65477	752.8426167	766.5494183	1105.443572	5331.147017	5247.589622	5727.221409
3434.325901	4374.237079	4512.698503	0.001403199	125.40936	0.001403199	1539.164796	1400.320187	1513.604347
18376.35681	16180.91269	21127.07506	2022.257051	1922.758904	2235.368741	7628.913086	9577.786775	8094.824419
2067.208888	2037.224342	1913.073034	2346.24305	2460.295199	2607.593384	2955.361098	2202.126098	2700.613538
14463.55767	15903.54245	16537.59634	17819.85892	18124.31708	17435.57897	11236.06942	12878.89906	13315.66838
11232.36972	10475.09479	12926.20272	12562.26442	14105.51239	15099.39708	6824.768852	7988.371798	8016.344073
14326.49503	14344.59922	17152.69132	6208.054192	5996.625942	5905.726088	12660.78182	14772.61071	12624.15565
3756.06463	4218.40392	4449.419817	1417.336442	1622.73246	1643.509667	3873.935963	4759.624822	3791.680665
10838.09903	11023.89204	11654.75106	4109.722949	4203.806003	4168.631612	6487.589676	8436.970176	7179.514268
4298.715911	3592.026786	3714.46019	5671.454491	6512.079634	5205.343356	2532.612705	3710.051925	3126.14957
1928.127878	2039.58334	1822.281197	557.087985	782.1087566	676.0435678	1162.090585	1180.268445	1013.522868
1487.736302	1453.908958	1690.820494	564.2125436	156.6759186	517.3468981	1282.019042	1351.846581	1614.81094
6535.788036	6749.237517	6647.458627	6159.790599	6971.289662	6337.960584	7196.645796	7277.29161	7648.654139
1597.68665	1239.021307	1496.70161	1405.917301	1864.647917	1781.688177	1661.843419	1340.954862	1750.456031

7.49_573.1183m/z	573.1182609	7.4852	neg
7.49_590.0375m/z	590.0375281	7.4852	neg
7.49_784.8300m/z	784.8299587	7.4852	neg
7.49_809.8508m/z	809.8507731	7.4852	neg
7.50_171.0201m/z	171.0201071	7.497433333	neg
7.50_432.1958m/z	432.1958455	7.497433333	neg
7.50_617.1058m/z	617.1058111	7.497433333	neg
7.51_430.1331m/z	430.1331062	7.50615	neg
7.51_438.2133m/z	438.2133438	7.50615	neg
7.51_539.0891m/z	539.0891285	7.50615	neg
7.51_549.1184m/z	549.1183799	7.50615	neg
7.51_685.0933m/z	685.0933278	7.50615	neg
7.51_821.0676m/z	821.067633	7.50615	neg
7.52_331.9229m/z	331.9229173	7.5166	neg
7.52_333.1558m/z	333.1557838	7.5166	neg
7.52_669.1006m/z	669.1006562	7.5166	neg
7.53_226.9661m/z	226.966097	7.527033333	neg
7.53_357.1557m/z	357.1557036	7.527033333	neg
7.53_377.1283m/z	377.1283305	7.527033333	neg
7.53_601.1132m/z	601.1131981	7.527033333	neg
7.55_605.2948m/z	605.2948541	7.547766667	neg
7.56_387.1664m/z	387.1664493	7.556516667	neg
7.56_389.1822m/z	389.1821884	7.556516667	neg
7.56_551.2092m/z	551.2091641	7.556516667	neg
7.56_619.1968m/z	619.1967888	7.556516667	neg
7.57_481.2062m/z	481.2061882	7.565266667	neg
7.57_687.1839m/z	687.1838864	7.565266667	neg
7.58_329.1587m/z	329.1587117	7.5758	neg
7.58_627.3755m/z	627.3754576	7.5758	neg
7.59_373.0966m/z	373.0965622	7.58625	neg
7.59_440.2271m/z	440.2270942	7.600283333	neg
7.60_459.2241m/z	459.2240893	7.600283333	neg
7.60_731.8344m/z	731.8344458	7.600283333	neg
7.61_237.0746m/z	237.074616	7.6091	neg
7.61_573.1182m/z	573.1182042	7.6091	neg
7.61_641.1055m/z	641.1054909	7.6091	neg
7.61_654.8698m/z	654.8698411	7.6091	neg
7.62_271.1552m/z	271.1552075	7.621333333	neg
7.62_443.2291m/z	443.2291135	7.621333333	neg
7.62_694.8616m/z	694.8616327	7.621333333	neg
7.63_486.9036m/z	486.9035554	7.631783333	neg
7.65_277.0330m/z	277.0329546	7.6458	neg
7.65_383.1694m/z	383.1693857	7.6458	neg
7.65_412.9306m/z	412.9305667	7.65305	neg
7.65_473.1018m/z	473.1018595	7.65305	neg
7.65_496.9495m/z	496.9495255	7.6458	neg
7.65_532.2896m/z	532.2895889	7.6458	neg
7.65_550.2462m/z	550.2461519	7.6458	neg
7.65_577.2250m/z	577.2249941	7.6458	neg
7.65_996.8233m/z	996.8233067	7.6458	neg
7.66_541.0893m/z	541.0893232	7.659433333	neg
7.67_610.1920m/z	610.1920318	7.66825	neg
7.69_389.2413n	388.2343506	7.687666667	neg
7.70_213.1497m/z	213.1497118	7.699916667	neg
7.70_481.2060m/z	481.2059833	7.699916667	neg
7.70_516.2942m/z	516.294248	7.699916667	neg
7.70_550.9215m/z	550.9215072	7.699916667	neg
7.71_391.1873m/z	391.1873335	7.710433333	neg
7.71_593.1447m/z	593.1446776	7.710433333	neg
7.71_722.8573m/z	722.857278	7.710433333	neg
7.72_411.1641m/z	411.1640943	7.719916667	neg
7.72_525.1571m/z	525.1571062	7.719916667	neg
7.72_918.8068m/z	918.8068272	7.719916667	neg
7.73_184.1425m/z	184.1425024	7.729433333	neg
7.73_463.2554m/z	463.2553634	7.729433333	neg
7.73_641.1054m/z	641.1054441	7.729433333	neg
7.74_362.9418m/z	362.9417704	7.738233333	neg
7.74_418.9161m/z	418.9160862	7.738233333	neg
7.74_505.1309m/z	505.1309409	7.738233333	neg
7.74_573.1185m/z	573.1184718	7.738233333	neg
7.74_731.8339m/z	731.8338552	7.738233333	neg
7.75_255.1244m/z	255.1244295	7.747083333	neg
7.75_288.6170m/z	288.6169856	7.747083333	neg
7.75_294.1325m/z	294.1325183	7.747083333	neg
7.76_187.9419m/z	187.9419253	7.756566667	neg
7.76_188.9128m/z	188.9128049	7.756566667	neg
7.76_255.6303n	510.2536999	7.756566667	neg
7.76_392.1565m/z	392.156465	7.756566667	neg
7.76_413.1822m/z	413.1821754	7.756566667	neg
7.76_553.3023m/z	553.3023089	7.756566667	neg
7.77_468.2583m/z	468.2583217	7.770583333	neg
7.77_523.2082m/z	523.2081618	7.770583333	neg
7.77_550.2283m/z	550.2283138	7.770583333	neg
7.77_737.2000m/z	737.1999513	7.770583333	neg
7.77_873.1746m/z	873.1745697	7.770583333	neg
7.77_941.1610m/z	941.1609915	7.770583333	neg
7.78_299.1977m/z	299.1976875	7.7828	neg
7.78_740.8479m/z	740.8479402	7.7828	neg
7.78_753.8507m/z	753.8507376	7.7828	neg
7.79_641.1258m/z	641.1258038	7.793283333	neg
7.79_657.3875m/z	657.3875456	7.793283333	neg
7.79_709.1129m/z	709.1128731	7.793283333	neg
7.80_481.2059m/z	481.2058977	7.802066667	neg
7.80_547.1777m/z	547.1777188	7.802066667	neg
7.82_226.9661m/z	226.966106	7.82385	neg
7.83_443.2292m/z	443.2291553	7.8311	neg
7.83_550.9215m/z	550.9214723	7.8311	neg
7.83_633.2899m/z	633.2899073	7.8311	neg
7.84_179.9364m/z	179.9363906	7.838516667	neg
7.84_319.1763m/z	319.1763286	7.838516667	neg
7.84_360.9745m/z	360.97446	7.838516667	neg
7.84_412.9304m/z	412.9304498	7.838516667	neg
7.84_570.8371m/z	570.8371131	7.838516667	neg
7.86_171.0201m/z	171.0201125	7.855233333	neg
7.86_389.1823m/z	389.1822638	7.855233333	neg
7.86_440.1620m/z	440.1620447	7.855233333	neg
7.86_731.8343m/z	731.8342665	7.86405	neg
7.86_809.8508m/z	809.8507641	7.86405	neg
7.89_274.1849m/z	274.1849396	7.89215	neg
7.89_575.1340m/z	575.1339983	7.89215	neg
8144.353396	8472.762864	9637.166908	12131.75935	12881.55317	12207.19009	6174.684583	6472.712186	5913.090901
1152.387308	1482.037269	1162.678213	1119.566049	1234.686701	1049.306341	1765.994661	1366.924896	1798.255462
7416.186573	7277.056434	7550.66869	7157.019361	9387.113421	8069.348979	7783.287893	7845.736466	8214.026254
8543.428745	7506.419287	8501.139641	7749.906939	9764.997854	10176.55285	10048.93454	8378.291085	9736.425918
978.4964734	829.8290221	953.9773452	786.2520282	1013.710882	1003.497252	1010.438397	861.9341427	920.2752666
229.732178	314.1852259	574.6448706	1301.836679	1261.32409	1064.763414	173.9738195	318.2455857	570.4740022
12722.13848	12182.32651	13652.07852	16223.68942	16788.46661	14667.52537	11150.66953	13673.97302	13600.29267
1898.843547	2264.643397	2194.488953	1700.922578	2649.007926	2223.891857	1548.559345	2235.869654	2188.206712
1978.647164	1567.947134	1901.637996	393.1496587	642.0025765	412.9773929	753.2819069	1159.999273	948.0271396
1022.604343	1785.959933	1777.56319	1246.165567	1561.808483	1412.835482	1187.236068	1443.271202	1269.683957
20670.16935	20504.35655	21706.93826	25374.4248	26350.97284	22460.47995	19364.81126	21497.52333	22662.83884
8571.61275	8700.145775	8377.946961	8133.077444	9299.041056	8111.22114	7311.679743	7805.620979	8691.527992
2238.575436	2286.998707	2818.420374	2001.192236	2636.022491	2030.575736	1934.59747	1769.993568	2441.854394
670.1729328	435.4832959	765.8648288	492.9672456	709.2116468	599.7747949	571.8662254	627.4680616	692.0598837
2443.524115	2354.180093	2577.701898	1427.622901	1372.86674	1315.96774	1184.765619	1363.759752	1556.236293
2439.374656	2405.115611	2428.338425	4729.19842	4870.975289	4304.409046	2634.178789	3306.599342	3699.575725
1208.763892	1084.404838	1290.822692	866.2137864	1208.797505	1195.013224	1242.752869	1079.109806	1240.371988
1938.685039	1782.344873	2082.301817	1688.261413	1685.900748	1536.804388	994.8329507	1306.438107	1384.465095
2570.561038	2791.776522	3032.655893	2194.548364	2454.949764	1946.02495	1644.746872	1772.268062	1763.742931
2631.803171	2492.14498	2601.677274	5801.033811	5130.254054	4784.102084	4089.787128	4383.516845	4491.438183
21836.81882	226.16.7871	22743.57888	2260.496754	2037.545746	2286.475711	8664.235757	8233.234662	8881.934478
3806.478057	3933.157427	4057.933904	7947.166848	8020.078629	7322.17055	2915.486231	2890.501753	2906.002836
9059.24288	8875.28558	9570.137354	15302.69779	14001.1326	16417.29357	6752.511305	7482.866737	6049.589828
5590.355447	5929.276142	6071.69417	6448.556664	6391.571175	6489.528696	7828.16946	8745.80497	8654.55434
2841.523226	3294.593766	3016.319613	3408.727702	3212.786069	3459.620318	4539.08037	5217.804408	5040.583818
3912.729268	3465.081305	3887.568849	2469.178277	2573.965879	2793.419015	2162.383009	3013.678093	2999.013875
1477.687261	1379.638659	1330.953049	1366.400874	1132.659974	1467.701914	2136.614407	2935.308548	2433.461403
581.9062114	822.5869687	743.7643562	585.4620374	577.683268	360.0522085	480.6392448	573.6221628	463.4775034
5842.805893	7327.215209	8375.402376	8476.744353	7275.105873	7841.185951	5807.527666	8407.683324	6643.649346
2366.392599	2702.134214	2316.975196	2071.499174	1993.334045	1844.294592	1315.791776	1680.060511	1378.736
1715.908563	1733.355421	2290.104485	2347.95662	1903.833842	2429.53261	1374.067502	1774.407538	1729.83972
2722.514998	3341.168591	2922.831301	5537.038943	4317.388245	4620.028565	2081.193784	2819.219588	2267.523689
6160.445125	4499.805164	6305.146236	4916.68709	6105.163153	6070.318219	6039.892592	6814.313185	6051.477151
1934.787715	1959.323321	1669.088805	2118.928979	1931.980627	2236.215544	1949.491805	1919.897241	1939.65441
6524.067216	7459.343198	7750.66865	10080.46365	8772.661058	10182.53692	4369.551888	5880.636996	4894.378188
3890.995049	3642.773305	3807.573126	5154.613949	4409.655036	5169.501182	2584.751634	3299.025003	2144.331978
19717.86817	17793.04875	17040.49374	16488.7448	18479.70879	17468.44409	20128.30391	18902.15772	20389.96684
2315.901153	2506.878688	2534.074086	3875.787068	3617.738776	3822.962067	1563.859844	1964.429063	1964.094861
1850.919357	2741.206956	2118.479669	2820.687093	2838.219561	3350.421912	1245.211128	1912.21569	1441.042754
4182.753687	4502.390995	3225.762081	3395.111897	3457.180655	3016.195678	4553.118832	4240.273538	3469.756166
1177.049272	1195.101239	1103.655797	915.5738636	1237.999632	1029.493735	1066.112138	1142.074098	741.6908473
2115.683371	2220.597012	1726.969092	1863.727198	2153.550536	1970.314418	2235.343691	2021.301124	2238.85377
378.7222929	543.7476963	596.8900333	0.001403199	0.001403199	0.001403199	324.8133348	420.0746136	283.6252386
4686.701095	4694.525187	4313.247185	4546.507704	5119.651116	4899.296014	5216.116119	5042.653368	5081.155791
4942.220752	5506.126671	5356.129426	2740.499838	2545.286207	2438.396793	3854.647864	4593.357765	4238.336896
2422.706354	3196.131557	2241.022131	2262.454657	2271.734347	2633.712383	2846.014222	1918.022141	2706.735147
3883.625855	4772.026626	4792.883289	997.7169256	641.9320821	1358.458547	2429.684163	2071.65129	1945.09199
4610.970912	5948.623735	5258.776028	1470.685357	870.8052075	1109.488345	4683.235214	5541.158735	6419.993583
3438.7471	3757.394347	3661.834084	3945.953598	3329.025646	3797.197665	2622.110753	3176.437135	3278.566888
31474.63613	36377.16316	37451.94491	37021.60811	37657.57918	38414.35765	38305.01917	35864.01052	36849.60876
2597.156911	3164.192323	2698.78732	1275.389085	1472.390763	1161.116135	1618.181226	2669.155975	2581.743758
1823.674508	2034.739098	2449.31683	2839.660792	2555.549306	2589.160695	1563.112154	1272.35944	1445.265321
4236.002336	4445.312066	3985.400343	3973.874431	4414.678473	4129.381441	4159.310712	3984.665832	4377.01411
365.3160187	571.8843174	449.8008702	368.4072139	440.8532718	462.7040614	425.7796374	410.0960296	422.7461541
2323.923246	2829.978419	2434.273595	1243.157083	1559.627735	1555.7328	1578.861592	1899.035558	2404.95434
823.0539005	1342.981289	852.7304528	73.89102623	198.4728339	86.01855218	509.6799301	745.927803	1172.731467
6754.634688	7078.410871	5576.311331	6856.562648	7060.772454	6046.325596	7104.056888	6561.706552	6896.196272
549.5627314	570.4197782	672.8699538	615.0650494	742.6197667	756.9672445	365.253861	440.8151652	468.6760408
2227.99446	2236.411819	2703.573942	2465.276214	2798.727724	2296.442334	1617.044055	1831.152407	1833.066897
3038.471761	2360.2839	2045.617797	3262.573464	3549.566122	2611.896226	3691.203574	3448.464547	3777.731039
2189.079123	2243.193491	2213.614097	777.0464506	695.4759825	553.8286334	697.7590237	1013.113135	1049.154971
4517.068531	5277.269427	4844.778853	4759.591017	6213.101122	5057.802138	3559.699968	4174.484224	3979.388819
24009.40005	23758.97275	23077.6819	22550.5294	25122.67384	25159.31291	29584.56294	22722.0425	25876.46052
15.88693695	67.24398634	33.28063648	86.45834011	44.9591273	42.4458393	19.1698668	16.5150938	14.58493781
5353.15222	6252.158033	4957.869637	6617.402811	6837.170345	6371.693977	5239.637115	5339.119547	6468.036544
3708.84159	3656.11622	4060.695129	5881.031316	7420.484112	6205.329994	2557.956199	3282.509294	3429.403798
4423.525929	4313.11295	3997.360314	4437.440132	4661.987729	4731.687895	5029.429621	4475.555094	5695.263514
5100.818691	4720.15798	5290.695937	4932.814884	6040.61263	5519.676863	6388.297941	5348.251236	6206.05274
14220.74349	14648.11089	15212.23359	21112.02472	22465.66593	20467.64162	10612.58287	11789.31473	13312.11861
7110.995587	8343.566088	7483.66282	11389.49655	12335.43569	10996.54678	5617.665211	6274.724439	7259.138823
2665.146956	2148.366875	2541.913749	2825.109028	3449.052738	2665.585913	3004.781976	3265.092634	3125.991656
392.3924891	634.7980154	547.1351204	399.1284355	592.1618567	485.1829257	375.9451767	558.9218859	468.8836589
712.6672942	747.5244663	750.9225729	741.9619884	780.341745	609.7867804	594.5458803	797.7510238	784.7006236
834.0560301	772.4530949	772.8508848	1227.831504	1245.609563	1053.766298	804.7105834	816.8704253	835.804581
190.170784	213.6763036	171.3108304	180.7956843	235.6698263	416.5370685	296.8878644	180.0084229	238.4948932
2532.59168	2363.692004	2622.808979	2514.87343	2595.258226	2401.03265	2657.357296	2600.665835	2633.371752
30135.99547	31216.55705	33147.81544	28106.85729	28278.38774	25398.66089	26018.1924	28495.79845	28827.0733
1967.558752	2060.597054	2338.4976	1651.57081	1362.676017	1129.91036	1086.17931	1367.529963	1413.460296
4985.839813	5040.021898	5591.941969	5858.243264	6493.458493	6247.589087	3760.827216	4091.01188	4268.189856
1424.628399	1746.78753	1889.422255	410.5843537	643.5911884	422.2508711	1515.512507	1481.493359	1411.373887
683.2939713	908.2086976	781.0127254	1385.422098	1258.898236	1329.235767	1042.2635	985.6482009	941.517746
3793.285531	5675.768048	5163.748207	9086.313721	8036.356275	7773.373213	5788.845805	6261.01801	6748.001589
1779.338894	2199.008926	2119.12335	3209.107643	2801.380627	2310.820385	2784.64603	2442.390224	2675.260488
10072.40157	11601.21262	11871.5457	17453.61774	16612.89925	15898.02193	12004.14716	12005.12798	12304.56574
2461.008314	3701.727431	3775.250948	6859.791671	5161.107961	5720.567704	3612.391574	4198.914738	4676.836417
1587.81749	1625.246239	1388.837966	3256.225167	2815.288908	2837.552058	2364.192612	1639.813538	1504.989658
1735.860893	1793.748509	2176.623117	1386.092052	1431.065382	1288.183059	1576.939129	2164.314749	1913.517291
3070.369888	2779.300683	2660.728707	3349.54597	3342.243143	3083.030396	5443.838058	2962.821532	3085.948886
4919.389723	5553.782413	8010.762096	5632.60227	5810.074014	7216.490977	6511.531272	9375.951464	5759.26785
3996.048946	3967.742029	4329.490436	5028.973587	4778.240439	5189.008517	4623.550015	4718.639433	4830.749881
1099.543228	735.4276699	1375.077218	1119.789452	1026.132771	941.788185	579.1114222	551.1207338	1096.7588
1397.962204	1390.463277	1722.800425	2253.576251	1368.353059	1709.604901	1892.839992	2018.465372	2100.086205
3392.288963	3635.916191	4256.793333	1698.574837	1303.270217	1426.672706	2093.052917	2917.132463	2238.690563
795.9551276	1307.181369	1327.834312	543.2242246	54.05344407	433.4339346	480.4727733	634.002675	1225.805498
970.7738577	810.830895	1155.99643	850.9894838	814.0002037	813.2068002	1034.397652	928.2978916	933.9249081
3107.82315	3085.743083	3280.125012	4032.685661	3799.736587	3662.371046	1546.354252	2329.208736	1952.244812
2370.291018	1751.646729	3112.37265	2160.697737	2124.532526	1978.539596	2366.869828	2104.656955	1988.789292
1540.970049	1660.798157	2539.321689	416.3904403	561.154774	743.0355781	611.6428588	675.0069504	633.7550953
973.1271952	949.8915348	1288.123554	1022.447078	1028.317488	1157.324166	1149.179238	996.0517235	1017.190954
2439.929599	2970.915038	3035.745922	2677.72936	2488.134057	2561.547121	2043.573183	2553.991257	2111.47746
2950.862928	2806.644016	3227.215875	2399.348772	2685.500237	2600.827925	2499.172769	2383.440285	2423.039907
6374.712049	5791.792275	5832.014897	6001.158231	6203.52934	6009.958644	6662.604602	6607.822442	6363.363089
172558.1056	165152.391	156406.9723	160959.6405	179111.8551	168515.3014	197578.6066	175625.8677	185017.7083
666.330892	547.8925274	745.7639041	570.9666337	617.5978548	553.522513	586.9705391	628.9479433	449.5862267
1157.105581	997.7358642	1215.969634	1579.321231	1229.622678	1167.313347	576.3741769	755.4482822	557.8472049
436.648813	625.1787604	848.0550391	1170.950709	1237.577318	754.2489584	344.2725258	378.5568273	369.8564292
4720.956866	4487.568759	4859.619109	4058.275042	6282.326731	5060.617916	4253.242403	4698.550993	4588.39164
8975.115738	9147.378384	7373.106161	9167.62834	10307.3092	9340.739117	8118.904574	9665.926369	9014.895109
2544.815313	2545.164501	2804.254175	3150.572902	3567.598092	3259.666746	1849.751204	2403.960267	2172.997567
739.2212124	1187.24184	850.3558873	1311.485896	1788.015671	1699.204629	551.5192118	972.4273276	204.0711514

7.91_686.2022m/z	686.2022155	7.906766667	neg
7.92_391.1978m/z	391.1978379	7.91555	neg
7.92_468.2581m/z	468.2581201	7.91555	neg
7.92_523.2082m/z	523.2081621	7.91555	neg
7.92_533.2372m/z	533.237161	7.91555	neg
7.92_550.2275m/z	550.2275069	7.91555	neg
7.92_591.1960m/z	591.1959577	7.91555	neg
7.92_618.2153m/z	618.215294	7.91555	neg
7.92_873.1745m/z	873.1744676	7.91555	neg
7.92_941.1614m/z	941.1614477	7.91555	neg
7.93_645.2127m/z	645.2127098	7.9268	neg
7.94_208.9679m/z	208.9679243	7.9373	neg
7.94_469.2266m/z	469.226639	7.9373	neg
7.94_483.1850m/z	483.185042	7.9373	neg
7.95_463.2555m/z	463.2554623	7.949583333	neg
7.96_627.3755m/z	627.375456	7.961816667	neg
7.97_342.2109m/z	342.2108571	7.9723	neg
7.98_318.2108m/z	318.2108066	7.984516667	neg
8.00_740.8474m/z	740.8473914	7.99505	neg
8.01_729.3709m/z	729.370928	8.009683333	neg
8.01_996.8233m/z	996.8233174	8.009683333	neg
8.02_510.2536m/z	510.2536383	8.024383333	neg
8.02_694.3591m/z	694.3591296	8.01695	neg
8.03_208.9680m/z	208.9680405	8.033866667	neg
8.03_722.8569m/z	722.8569492	8.033866667	neg
8.04_758.8668m/z	758.8668101	8.042716667	neg
8.04_918.8066m/z	918.8065857	8.042716667	neg
8.05_298.1847m/z	298.1847329	8.053916667	neg
8.07_177.9207m/z	177.9207072	8.066183333	neg
8.07_371.1712m/z	371.171204	8.066183333	neg
8.07_490.2425m/z	490.2424528	8.074883333	neg
8.07_507.1462m/z	507.1462286	8.066183333	neg
8.07_558.2304m/z	558.2303554	8.074883333	neg
8.07_667.1861m/z	667.1861034	8.074883333	neg
8.07_881.1767m/z	881.1767478	8.074883333	neg
8.09_210.9836m/z	210.9836485	8.087016667	neg
8.09_515.1458m/z	515.1458312	8.087016667	neg
8.09_661.1496m/z	661.1496217	8.087016667	neg
8.09_735.1734m/z	735.1734263	8.087016667	neg
8.10_549.8568m/z	549.8567867	8.101016667	neg
8.11_481.2059m/z	481.2058588	8.110466667	neg
8.12_226.9660m/z	226.9660299	8.11925	neg
8.12_300.9742m/z	300.9742184	8.11925	neg
8.12_617.1810m/z	617.1810387	8.11925	neg
8.13_509.2759m/z	509.2758995	8.129733333	neg
8.15_809.8512m/z	809.8511908	8.147366667	neg
8.16_271.1553m/z	271.1552577	8.156183333	neg
8.16_412.9305m/z	412.9305157	8.156183333	neg
8.16_413.1820m/z	413.1820148	8.156183333	neg
8.16_465.2497m/z	465.2497275	8.16495	neg
8.19_294.9536m/z	294.9535545	8.190666667	neg
8.19_685.8637m/z	685.8637114	8.190666667	neg
8.20_437.0551m/z	437.0550721	8.200183333	neg
8.20_996.8236m/z	996.8236144	8.200183333	neg
8.22_465.2111m/z	465.2110584	8.218516667	neg
8.23_443.2291m/z	443.2291276	8.227316667	neg
8.26_457.2084m/z	457.2084034	8.264766667	neg
8.27_319.0800m/z	319.0799567	8.273616667	neg
8.28_783.2029m/z	783.2029221	8.28415	neg
8.28_845.7979m/z	845.7979057	8.28415	neg
8.29_715.2155m/z	715.2154524	8.294766667	neg
8.31_463.2553m/z	463.2552887	8.305216667	neg
8.32_341.0042m/z	341.004228	8.315783333	neg
8.33_351.0449m/z	351.044897	8.3263	neg
8.33_704.8157m/z	704.8157587	8.3263	neg
8.34_481.2056m/z	481.2056115	8.338466667	neg
8.34_495.1464m/z	495.1463936	8.338466667	neg
8.34_588.8246m/z	588.8246427	8.338466667	neg
8.35_187.9419m/z	187.941788	8.347233333	neg
8.35_809.8508m/z	809.8507684	8.347233333	neg
8.39_371.1713m/z	371.1712567	8.393383333	neg
8.40_699.2591m/z	699.2591212	8.40065	neg
8.42_376.2706m/z	376.2705699	8.421216667	neg
8.43_320.8710m/z	320.8710311	8.430033333	neg
8.45_116.9210m/z	116.9210282	8.446233333	neg
8.45_340.1955m/z	340.195479	8.446233333	neg
8.46_277.0329m/z	277.0329265	8.463816667	neg
8.46_445.2448m/z	445.2448102	8.463816667	neg
8.48_845.7979m/z	845.7977952	8.484433333	neg
8.50_459.2238m/z	459.2238112	8.495033333	neg
8.51_872.8042m/z	872.8041661	8.51265	neg
8.52_356.2447m/z	356.2446766	8.523183333	neg
8.53_370.1775m/z	370.1775217	8.533683333	neg
8.54_271.1553m/z	271.1552529	8.540883333	neg
8.57_164.9273m/z	164.9272675	8.568433333	neg
8.59_918.8068m/z	918.8068156	8.586283333	neg
8.60_362.9417m/z	362.9416651	8.596366667	neg
8.61_783.2026m/z	783.2026454	8.606866667	neg
8.62_321.9824m/z	321.9824111	8.6174	neg
8.62_715.2155m/z	715.2155378	8.6174	neg
8.63_358.2601m/z	358.2600626	8.6262	neg
8.63_373.9534m/z	373.9534224	8.6262	neg
8.63_383.9824m/z	383.9824103	8.6262	neg
8.64_273.9029m/z	273.9029378	8.635	neg
8.64_507.1463m/z	507.1463088	8.635	neg
8.64_784.8296m/z	784.829621	8.635	neg
8.65_171.0200m/z	171.0200436	8.645533333	neg
8.65_333.1687m/z	333.1686888	8.645533333	neg
8.65_722.8579m/z	722.8578539	8.645533333	neg
8.66_635.3054m/z	635.3054021	8.6638	neg
8.67_703.2926m/z	703.2925812	8.67015	neg
8.70_457.2084m/z	457.2084291	8.703333333	neg
8.71_481.8688m/z	481.8687924	8.713883333	neg
8.74_187.9419m/z	187.9419139	8.735716667	neg
8.74_294.9536m/z	294.9535872	8.7445	neg
8.74_345.1921m/z	345.1921216	8.7445	neg
8.74_412.9305m/z	412.930547	8.735716667	neg
8.74_481.2058m/z	481.2057765	8.735716667	neg
8.74_799.8220m/z	799.8219653	8.735716667	neg
8.75_918.8065m/z	918.8064856	8.750783333	neg

1393.430591	2188.516835	1347.446646	2728.174242	2075.526048	2437.112647	1455.292017	1986.741662	1981.894763
2459.763554	2582.407993	2349.19952	2808.113333	2967.688664	3126.18235	1634.958286	2689.833994	2222.38756
1984.916898	1707.036449	1827.49527	2312.831474	2381.030807	2570.587001	1864.849641	2312.55208	1954.450118
10802.57647	10717.75704	12080.9198	14405.92031	15148.35876	15424.23242	11006.7236	14548.96344	13624.71761
116404.1743	113246.3271	119021.6874	148696.2815	150933.1528	157697.6897	114544.2989	144070.8265	131909.4217
5307.11134	5934.647891	6532.510646	7292.888023	7600.292411	7652.628975	5009.61931	6940.000729	6737.777817
7290.326487	6195.903332	7478.296494	8362.382797	8509.576495	9820.149078	6134.668087	8172.273447	8210.029235
1208.200407	1235.291995	1176.197171	1849.27033	2746.247233	2183.866897	1325.344444	2348.331867	1984.013669
9667.735952	8950.372542	8368.158885	11110.28699	11975.27965	11965.93334	8380.922557	11376.56199	12057.66269
4791.226309	6006.607225	7000.416231	9042.0643	9222.770597	8100.29456	5655.812077	8740.118258	7987.71575
2537.963402	2268.372307	3056.32542	3551.269429	3589.506735	3730.642306	2431.663725	3254.604053	3338.268227
856.025085	895.2443345	740.438649	949.6934693	1030.431198	1001.735577	952.3671959	972.4050902	1028.119706
2024.653706	1896.260818	2004.83782	1280.561665	1039.124063	1139.087793	853.4099473	1536.70505	1244.020378
1421.156021	1172.285891	1422.514935	2573.586703	1652.47606	2482.126888	698.7129139	784.5890501	649.7263361
5768.489643	5717.988174	4820.88899	8804.822519	7461.323469	7544.538365	6178.924621	8151.102061	7365.201216
14578.66623	16182.66277	16470.57099	19587.27877	18482.5464	18193.90911	14632.82366	18166.16669	15534.53887
1865.500049	1849.983863	2340.173675	3279.706566	2698.304666	2917.317117	1993.258676	2045.211492	2004.417641
646.4372124	557.9102926	285.3083327	667.6868909	444.6807581	750.0403198	488.2963613	568.3180509	715.7486835
6836.049138	5832.67235	5660.085302	6401.697878	6852.876886	6867.414412	6982.515851	5771.854507	7307.134314
1536.622585	2195.621956	2254.054922	84.57761712	0.001403199	80.11100688	2626.630445	2337.435025	1969.705523
10615.84121	9314.434371	8319.582255	10719.00376	10404.38169	11541.7444	10155.34963	8409.374356	12203.89457
6251.703475	5633.714301	6070.390056	5123.558895	4832.51897	4719.963904	5086.354286	4857.005461	6053.021066
6346.568894	6086.433803	6736.131193	7509.766131	8692.305969	7580.364171	7898.262538	7043.223551	8685.375022
731.7451804	796.1272717	863.3675015	844.2235809	952.5353084	733.9932134	969.1083387	884.0977674	990.7334794
5550.570815	5383.236195	5204.351409	6563.533961	5177.623932	6080.058989	6604.77859	5994.909018	6116.185113
6839.525379	7553.653301	6572.857195	7427.531519	8522.557091	6961.59713	9075.594282	9365.78239	8904.188432
16046.6028	15471.43425	14930.68947	17654.68389	17454.56114	16680.87774	19426.54311	16203.00056	18220.26404
3068.464536	3347.813807	3523.690571	5362.08489	5344.881666	4579.344656	2896.646865	2825.580209	2834.806922
275.9010261	300.2582745	302.6174758	326.202598	376.5137476	262.0604948	415.2218766	433.7482085	396.4177847
35911.25316	39162.25969	37706.29783	54947.86305	54096.44675	52054.09458	23054.28061	25625.78643	26708.18959
4041.218769	4167.082092	2872.733892	5581.858123	5742.101823	579.0619471	1813.442283	1115.01278	2238.043031
3290.505163	3427.568817	3153.992592	5677.190842	5770.226845	4969.690021	1686.730312	2263.550815	2083.349167
2796.748338	2798.567626	2232.227843	197.8419445	194.9613549	109.9323961	1265.617839	1723.840408	1307.391987
3616.351296	4243.6274	3747.841246	0.001403199	124.0130067	244.6099777	1603.617011	2120.754412	1585.859004
6414.960528	5577.103137	5774.200904	247.30314	193.4140601	162.4014233	2492.723585	3241.188942	3296.943481
619.197037	713.1195913	510.8523766	567.4951067	834.7556324	659.3100058	612.4458488	617.9361729	770.4638832
317.8315887	625.7260425	703.962255	0.001403199	166.3954712	0.001403199	341.1651178	414.9194594	243.5059207
2053.473559	2349.554087	2056.480353	401.4488993	423.9415633	445.4382426	1192.028271	1256.096222	1424.426157
2283.120648	2281.714415	2383.553821	125.1473219	0.001403199	0.001403199	552.1297383	1421.585518	687.6438687
1656.682168	1414.858204	1196.381873	1375.552491	2050.90497	1355.999545	1805.32747	2347.829368	1844.761325
15080.99904	15042.23616	15582.95345	7233.040918	7400.92142	7463.611045	10960.70503	12642.87662	12167.25979
918.0614953	728.0925732	756.4606844	699.6134686	949.0870938	888.5918109	888.6628171	1130.223965	874.5446972
888.946198	762.1121158	799.7045589	909.8278734	1006.771141	997.1478232	934.3723757	1177.56769	970.4120779
3049.033644	4112.982226	3558.399374	1066.445647	1303.438659	1260.973993	2231.173147	2737.175437	2466.162842
53959.77348	54627.87901	56579.94251	76686.61126	72381.99778	79181.82355	48598.80805	45786.06224	52591.41626
6265.096383	4530.017269	4357.18761	5069.628427	6790.058222	6258.439995	5521.263736	6315.759291	5884.62528
557.4120067	497.7247613	446.7241174	939.1789386	987.1939271	943.2576372	189.6885213	359.5796692	274.1988071
3121.116807	2764.87761	3025.803192	2353.333754	3061.460704	2935.133246	3081.232736	2543.06086	2543.900785
798.6043091	640.502926	768.0836495	781.4680477	634.6406758	933.1103616	323.0064208	518.5190279	545.8597311
2059.556017	1389.424277	2018.7557	1999.918374	2153.987655	2386.504061	1830.541414	1949.022786	2152.300338
1023.115031	782.8419203	1149.126957	828.5800118	1055.723206	1074.953856	1152.267651	552.6476112	1125.283824
4895.324227	4174.108148	6583.96475	4223.102049	5226.326955	4829.758542	6349.295583	3907.546591	5296.398215
1552.913836	1625.34056	1968.649899	1234.656243	1257.028662	1396.127566	1121.478015	1116.688407	1460.024715
18174.90331	15284.24025	20104.81338	17601.66256	19328.26282	18822.9189	21210.05855	16155.73123	17580.12828
782.5766007	819.243205	1088.051815	856.5992176	1118.689692	901.9258354	1087.233089	947.178381	1415.255579
8303.332997	7781.579694	9472.287436	10056.14502	9045.624509	9673.936043	6950.589822	6995.628492	7681.517473
6320.527501	7543.300465	8001.755085	8540.855855	6974.157725	7215.342764	5274.540606	6451.674963	6188.882137
785.3614737	947.845401	796.0291827	977.2449788	856.1470147	726.5892254	893.0784611	879.9138641	720.2045504
2188.126907	3024.615381	2839.766777	3182.296489	2056.655228	2312.267045	1415.102653	2512.440079	1818.116176
11774.38452	10131.49921	12960.51202	11438.37777	10787.73064	11556.74103	14935.90444	13015.13857	12206.52546
4873.172326	6122.794186	7017.770766	6180.255711	4786.908633	5351.370468	4935.269236	5976.898613	5586.797295
5345.554397	5632.226731	5290.485339	7448.24041	5989.440171	6298.664239	6492.324058	7318.760441	7741.742125
6474.158964	5946.995577	6255.633162	6221.951429	5734.432585	5662.81213	6820.161224	6313.619506	6607.049837
546.6733161	799.9890254	301.7958642	373.9386333	477.4393607	447.6270529	435.1031147	594.2257767	638.0037241
64077.08339	61989.35918	61491.45368	59416.8547	67567.07542	65194.86547	71818.53767	62888.29436	68853.97329
2298.635909	2309.342249	2404.728931	1596.532915	1226.199258	1192.340815	1591.389165	2192.318352	1938.721399
2335.889965	2644.386534	2715.123417	3149.883783	3030.227964	2735.187512	1515.397517	2240.740582	1787.358853
2582.176937	2772.860689	1776.694133	195.4500207	0.001403199	101.4427686	1913.366333	515.8874207	309.0880123
595.1840892	573.3855498	469.6301194	609.8234648	440.9687366	482.7094443	555.8412605	531.7066573	514.1607413
8960.120316	8679.805431	6891.927051	9455.250525	8545.913695	7504.571936	9364.053455	9650.102886	10578.55655
18088.44273	18785.6285	17965.01367	25480.3113	24105.93956	23861.94267	9215.79571	10730.20141	10361.58205
3435.443409	3625.80779	3697.708308	5682.792403	5245.091094	4525.518759	2938.653402	4154.730309	4444.920874
1118.780697	911.0859515	934.9786858	883.9456017	945.4883285	933.840171	774.3275414	1022.050467	1138.507373
1820.286014	1795.704982	1438.828355	1655.950406	2167.172404	1649.814484	2478.349273	1632.467511	1694.006203
38.04164546	0.001403199	44.47561943	91.33779045	49.74826468	107.5896483	51.22883872	45.93205261	51.14362494
933.285246	1213.394583	1080.190731	1152.025439	1261.386616	1082.484756	981.0327665	1089.776457	926.1989594
1021.997666	1137.666686	977.6281668	945.0468238	1281.499557	1033.220297	1480.575907	1212.851097	1267.51681
571.5605749	847.6964123	893.2581407	1370.531115	1668.704294	1487.45322	818.8956475	818.1257191	496.6597325
11464.27388	10842.9939	10490.7583	11798.85308	12771.18719	12517.69654	13953.03493	10255.90992	13243.63686
3363.891494	3334.434414	2839.683638	4698.302505	4225.245072	4197.49198	1722.255462	1560.906149	1713.496276
2918.702763	2412.111169	3259.063085	2998.720547	5164.980814	3347.519977	3444.10853	1805.359894	3814.60092
1963.879787	1945.156325	1497.901394	2025.319026	1920.846752	2119.076817	2030.473075	1518.026454	1791.15494
708.1329419	420.5294005	818.0317786	827.7009947	527.5399804	514.6921042	690.1904011	818.2478779	650.4816685
474.3652207	441.2204332	359.6125146	1112.673249	1065.899188	1200.850326	822.4203993	903.2654037	821.4429115
353.3640034	470.7126546	467.4164704	352.9155744	338.4141973	412.9525793	311.5574307	553.4313269	317.8387199
7806.825138	8235.28073	8026.267645	6813.024938	8296.902168	9258.256221	9627.615253	9730.05117	7468.938716
3910.702777	3581.532507	4030.940079	3089.793703	3212.961041	3410.444774	4269.013627	4166.972989	2999.016114
2514.561397	3408.227685	3365.615614	3202.22356	3642.938719	3892.833608	3720.126396	4132.397596	2698.181978
2185.267201	2178.304416	2115.873535	1690.205209	1904.086061	1528.674506	2348.11051	2274.621081	2193.997141
5663.412711	5992.993955	6257.514054	6947.199997	6680.84847	7163.607742	5111.859059	6194.516806	5864.83628
1649.53284	1261.999974	1064.775494	1162.58517	1005.015578	1313.79611	1789.679632	1325.704773	1141.149328
2347.053808	1716.505568	1795.78988	1494.491252	1218.868508	1306.085052	2110.461247	1851.264137	1815.850323
3649.704664	2943.26112	2763.149631	2085.653821	2106.701981	2334.315462	3371.836858	3283.402342	2514.395472
2559.44041	2395.341425	2579.106146	2701.929962	2333.705546	2865.905311	2924.737439	2613.588169	2501.190322
2711.272233	2414.589093	3027.163562	3846.835771	3577.821518	4147.658442	1882.59753	1821.520996	1565.998759
10982.17598	10236.29664	9814.366685	10644.29042	12816.64758	12317.64618	13191.66447	11004.646	11703.72493
650.6388951	631.7031587	496.7608811	550.5633285	509.8002476	594.8506776	829.2051151	614.7521787	483.494242
38.32356391	397.4850918	318.3605425	1184.414711	860.5847827	786.4069639	51.31425263	148.8581163	141.0445169
2088.995553	1582.34143	1979.981292	1889.545679	1866.313436	2705.438665	4330.378988	3020.275417	2330.681534
12098.01404	13252.98635	13134.08562	843.1148185	983.8030088	599.1952549	4598.412738	5281.291259	5672.215071
4669.91501	5574.86698	3980.614768	136.2202023	116.0648979	0.001403199	1398.653716	1560.175274	1083.229952
1934.578661	2082.968728	2204.63023	3026.449469	2727.728223	2512.841799	1532.532661	1974.568885	2088.908576
1369.385311	1455.53408	1223.140972	2153.144824	2482.094551	1736.753277	1058.469851	1330.877777	1750.729555
485.9905421	390.4869285	357.7587784	440.3464269	623.8964304	439.3756969	373.1833157	319.2635803	467.2752496
1223.596539	1045.097504	1172.212188	1423.679159	1630.303691	1336.000413	939.5636481	1199.783587	1527.065127
1623.989159	1357.277124	1500.776343	1229.978726	1105.358686	1176.155786	1203.360244	1238.020941	1271.589944
1172.551733	1021.071305	1084.039057	1442.95028	1661.959578	1190.256964	837.4686651	925.1483917	1459.769663
8286.708695	7774.583803	9647.667097	5033.058945	4009.173168	4747.760909	6095.857397	7108.275907	7286.071658
1483.211212	1347.937608	1556.941535	2067.951621	2894.929523	2584.117087	1450.905125	1903.807671	2863.799036
7031.156779	6583.031007	5722.725113	7672.175491	9305.000916	7541.499339	5173.80269	6943.953714	7502.687249

8.76_226.9660m/z	226.9660469	8.759533333	neg	1184.426873	1083.017185	1223.868106	1000.151778	1442.40921	1313.104981	1398.545879	1456.123771	1549.806634	
8.77_753.8508m/z	753.8507851	8.768983333	neg	4685.183251	4355.734867	5757.392246	7281.065765	7840.753442	5931.035397	6118.547199	5726.700223	6226.815539	
8.78_362.9417m/z	362.9417186	8.782416667	neg	2413.352894	2093.515939	2619.590121	1456.561917	3571.064469	3145.687046	3626.382484	3467.960495	3084.34428	
8.78_731.8341m/z	731.8340881	8.782416667	neg	2773.916248	1657.646724	2722.414878	1779.218197	3569.010221	3673.836423	4351.328613	3408.008734	4037.405107	
8.79_445.2447m/z	445.2446638	8.791166667	neg	1470.711201	1341.887441	1879.482086	927.3418525	1534.572894	2138.952575	1268.672607	1399.254007	1734.55556	
8.79_481.8689m/z	481.8689275	8.791166667	neg	2357.073546	2658.565861	2406.166675	1724.945158	2003.15006	2427.311833	2899.982504	2224.197968	2261.594353	
8.79_590.8230m/z	590.8229818	8.791166667	neg	3289.392162	3157.963483	2784.503803	2000.020011	2048.11438	3085.452707	3743.450132	2503.59252	2999.660226	
8.80_129.9364m/z	129.9363685	8.803433333	neg	884.990079	756.3963474	775.7175398	450.5753404	546.3919089	571.322053	808.2174506	726.0675917	663.8646977	
8.82_187.9419m/z	187.9419286	8.8245	neg	563.7923297	544.5918286	454.9624408	191.0456493	392.7841352	444.662835	674.2514191	486.5855422	525.2671612	
8.82_248.0800m/z	248.0799852	8.8245	neg	394.7727363	455.0473582	537.5366451	270.3230224	324.0874941	566.2700469	635.0722155	531.9245786	558.3917915	
8.82_373.1870m/z	373.1870026	8.8245	neg	1418.421781	1766.839986	1680.019646	2990.359207	2421.879025	2533.109904	680.7336943	887.3832588	1056.997478	
8.84_273.9030m/z	273.9029724	8.8368	neg	1422.916998	1592.367006	1301.563482	1592.66827	1210.96127	1533.984332	1424.183028	1171.426626	1589.234853	
8.84_599.1703m/z	599.1703225	8.8368	neg	8793.363577	9142.926032	9149.202318	3749.977708	2863.675128	3134.789156	5589.215743	6688.412762	6188.903727	
8.84_599.3445m/z	599.3445429	8.843116667	neg	1628.904351	1613.923271	1681.196507	0.001403199	0.001403199	0.001403199	1168.166893	1466.90576	1482.754863	
8.85_654.8698m/z	654.8698119	8.851966667	neg	7314.621241	6706.497273	6215.268494	7410.831074	5846.179281	6902.718533	7272.043284	7445.255204	7742.691372	
8.86_802.8143m/z	802.8143081	8.860733333	neg	4572.722941	3134.163489	2753.113987	2039.855353	1096.011244	1608.963391	3122.285684	1777.373344	1902.835001	
8.88_164.9273m/z	164.9272799	8.879933333	neg	381.9500712	362.4025715	330.8452176	513.8665957	399.928151	396.0625812	345.3988521	417.6417035	397.927582	
8.88_428.9620m/z	428.9619875	8.879933333	neg	1646.657827	1451.801095	1688.528506	2151.032516	1853.74159	1588.865755	1259.770345	2142.453089	1672.944984	
8.89_206.8977m/z	206.8976965	8.888766667	neg	983.2177502	974.4878239	878.0456361	1145.919055	949.6189958	1045.074194	1086.35576	1046.567003	1149.912158	
8.89_226.9661m/z	226.9660646	8.888766667	neg	1147.191686	747.286396	999.3424561	1326.07023	1108.377544	1254.269182	1146.562528	1439.750748	1218.585403	
8.89_350.9285m/z	350.9284851	8.888766667	neg	1728.884811	1498.845836	1534.062721	2540.308597	1857.55112	1570.256299	1460.402253	1912.324338	1961.474871	
8.92_731.8343m/z	731.8342738	8.915866667	neg	2304.550395	1905.312839	2372.817414	2098.51168	2388.68763	2656.872484	2444.993905	3501.6463	2409.660353	
8.95_996.8234m/z	996.823445	8.953233333	neg	7133.543935	5891.963199	7326.59249	6624.064441	7722.791708	8205.074522	6704.762157	6749.764771	6699.967351	
8.96_273.9030m/z	273.9030187	8.962016667	neg	1208.38994	1268.970184	1456.564393	980.7836298	1349.977537	1282.078135	1313.402682	876.8649675	1409.107786	
8.96_344.9429m/z	344.9428824	8.962016667	neg	2516.825169	1903.892867	2195.176824	1837.234514	2506.639399	2594.41949	2084.684323	2464.454086	2360.578316	
8.98_405.1063m/z	405.1063472	8.979616667	neg	1568.388785	1557.291599	1518.667699	1381.735205	1488.514939	1423.075265	1639.52465	1163.899796	1632.380949	
8.99_209.9191m/z	209.9191401	8.9919	neg	804.0026884	939.595263	719.7911471	564.420048	624.2714074	614.5295393	896.5368964	539.8892019	573.2029052	
8.99_481.2057m/z	481.2056766	8.9919	neg	3844.567989	5098.147732	3349.742962	1261.673818	1469.806741	1634.036372	1739.104602	1953.59135	1940.414546	
9.00_883.1926m/z	883.1926044	9.004166667	neg	7492.226693	9340.670995	9692.577635	0.001403199	184.9472487	247.4924983	3554.705192	2339.012802	2439.607043	
9.02_456.2951m/z	456.2950943	9.01635	neg	658.4463269	832.0197484	789.833631	0.001403199	0.001403199	0.001403199	69.49484865	181.0398998	146.2285237	
9.02_465.2390m/z	465.2389713	9.01635	neg	14330.07861	18772.29461	17583.48718	899.3324222	995.0838036	518.5821676	6316.548355	7578.975705	6707.622953	
9.02_533.2267m/z	533.2266688	9.01635	neg	9520.28053	13425.10927	11756.69684	440.9933912	414.667311	510.679355	4088.4225	5245.300189	3921.736303	
9.02_560.2461m/z	560.2460836	9.01635	neg	3760.452247	4867.328002	4371.782709	9.517665959	103.3755035	120.1207098	1170.705158	1393.009444	1415.151262	
9.02_628.2333m/z	628.233328	9.01635	neg	2392.63603	3097.435869	2485.701371	0.001403199	22.58568263	0.001403199	456.3815847	1034.039785	455.8560333	
9.02_663.8470m/z	663.8470717	9.01635	neg	2141.533066	3587.234286	3267.442777	1847.032566	3412.011192	2739.075047	3067.949302	2491.957214	3099.251181	
9.02_737.1896m/z	737.1896407	9.01635	neg	1845.856903	3639.284932	2799.946154	0.001403199	0.001403199	0.001403199	0.001403199	928.3515448	833.2336022	
9.02_747.2183m/z	747.2183093	9.01635	neg	15216.66666	19778.56475	18560.33345	687.623858	493.1058457	441.1521931	6751.06725	7715.338333	7065.507619	
9.02_838.5570m/z	838.5570295	9.01635	neg	982.6897858	1061.839089	712.8336203	167.912646	0.001403199	215.1829686	0.001403199	0.001403199	182.7578386	
9.04_550.1879m/z	550.1878965	9.039016667	neg	1344.224791	2448.819439	2006.952433	0.001403199	0.001403199	0.001403199	361.31143	701.6824532	443.7418424	
9.05_809.8504m/z	809.8504369	9.047766667	neg	6590.26304	6588.001922	5831.781796	5869.926455	6916.621138	7013.913134	7190.808527	4215.39467	6517.09289	
9.07_356.2447m/z	356.2446592	9.065233333	neg	6331.168854	5547.940431	5683.492879	5759.025521	4882.073963	5548.815905	5993.392083	5096.620816	6252.284486	
9.08_509.1619m/z	509.1618791	9.077466667	neg	3139.796127	2786.663739	3421.111182	1945.369137	1966.428281	2397.266469	1960.066263	1591.522889	2322.167888	
9.08_918.8061m/z	918.8061174	9.077466667	neg	4525.566361	4312.322805	5797.792957	4577.854845	3977.811182	4902.590178	5999.913375	4042.156357	5156.977183	
9.12_182.9000m/z	182.9000044	9.115183333	neg	1489.036383	1300.786547	1275.850731	1421.355124	1276.027798	1210.348914	1547.868419	1174.588291	1413.643882	
9.13_350.9286m/z	350.9286303	9.1257	neg	1285.072906	1258.13845	1211.563507	1329.915309	1309.065247	1272.028641	1320.891784	1633.841224	1058.799037	
9.13_465.2111m/z	465.2111099	9.134483333	neg	1537.268117	1745.305239	1487.615302	424.0001052	175.7150347	82.09765384	595.5794531	1038.854279	800.6233241	
9.13_787.8458m/z	787.8458173	9.134483333	neg	2142.030556	2135.5214	1558.825113	3038.286573	2872.26776	2243.97128	2750.70977	2379.35769	3242.029187	
9.13_809.8508m/z	809.8508181	9.134483333	neg	13875.50583	15493.64855	14244.71696	15929.88486	17796.05635	15164.30566	17788.24835	15965.43227	17978.20896	
9.14_129.9364m/z	129.9363708	9.14175	neg	1795.17616	1602.877352	1454.693286	970.7965514	896.5089175	913.5153296	1465.985703	1206.755187	1257.70359	
9.14_277.0329m/z	277.0329191	9.14175	neg	1771.530011	1651.291977	1762.005273	1674.099491	1933.764732	1694.660603	1922.286013	1837.624612	2164.682906	
9.16_481.2056m/z	481.2056431	9.155683333	neg	2315.759399	2284.480578	2800.092431	913.9432795	1448.26452	982.4524912	1986.93648	1927.387819	1948.757314	
9.17_344.9429m/z	344.9429305	9.167966667	neg	4546.127323	4341.24062	4289.509004	4654.259182	5229.466716	4700.700328	5534.950774	4585.512672	4915.339538	
9.17_704.8156m/z	704.8155713	9.167966667	neg	3801.37714	2798.916592	4414.606649	3820.183948	4717.002801	2860.664226	4400.603741	4007.69698	4676.060391	
9.17_918.8061m/z	918.8060904	9.167966667	neg	2954.015733	2983.603257	4070.871871	3507.081912	4397.754761	2893.225654	3728.25664	4107.610494	5147.190223	
9.18_360.9745m/z	360.9744624	9.176816667	neg	2121.707144	2374.805699	2820.956224	2314.070361	2804.769218	1951.711523	2508.035667	2291.426483	2545.465229	
9.19_358.2602m/z	358.2602136	9.191983333	neg	6896.164932	6220.706635	5912.206862	6055.235983	7558.190561	6506.411166	7301.395856	6810.911136	6073.16522	
9.19_401.1640m/z	401.1639775	9.191983333	neg	666.9366122	691.5580716	750.9393193	0.001403199	77.35028245	0.001403199	160.850476	281.0849049	281.9938624	
9.20_182.9215m/z	182.9214908	9.202566667	neg	639.7512664	677.9306956	776.5973483	736.3098938	957.103747	595.8489463	750.3264871	667.7718768	897.5677853	
9.22_524.8342m/z	524.834227	9.2201	neg	1843.187637	2323.470309	1636.249566	1468.32595	1980.283701	1782.629273	1776.287794	1206.012606	1317.153879	
9.23_918.8060m/z	918.8060031	9.228916667	neg	3480.635538	3541.629736	4166.261862	3542.109299	3617.570812	3774.899696	3690.428193	3745.731098	3618.744437	
9.25_414.9461m/z	414.9461341	9.248216667	neg	3033.299792	2624.307029	2918.596669	3082.768063	3644.432507	3259.125768	3473.9884	3008.362765	2432.903624	
9.25_590.8237m/z	590.823711	9.248216667	neg	6900.772156	6055.721475	6342.831164	6305.267659	6498.899053	6301.311205	7331.510038	7688.704218	5852.618507	
9.26_222.9783m/z	222.9782994	9.258733333	neg	598.5798102	734.0345206	527.8962954	631.4244714	612.5490235	755.842308	714.2545638	687.7407123	509.2225276	
9.26_658.8115m/z	658.8115029	9.258733333	neg	5382.855544	4912.347052	4274.103138	3519.33652	4679.772309	5002.885554	5201.241995	5325.554041	4374.884268	
9.28_156.8949m/z	156.8948642	9.278033333	neg	743.1839573	731.6043169	498.9349653	586.9710041	686.9950056	706.2855816	734.5297128	702.2255646	622.3651541	
9.28_187.9420m/z	187.9419641	9.278033333	neg	2802.872215	2294.127411	1955.938212	1600.562878	2080.787368	1868.26605	2317.837437	1961.878306	1703.365724	
9.29_377.1584m/z	377.1584278	9.288466667	neg	843.0199533	1078.3099	1071.550337	1226.195218	1157.422276	992.0837494	1167.796665	1360.551318	1157.541881	
9.29_445.1459m/z	445.1459316	9.288466667	neg	421.0455348	317.4634626	149.8272101	468.8153319	388.9111091	220.3287019	334.4878664	362.265723	327.8580067	
9.32_497.1385m/z	497.1385493	9.321783333	neg	7217.256648	7581.161505	5137.641102	7597.43217	9614.19014	7620.78027	6176.569275	6070.268782	7944.239467	
9.32_565.1259m/z	565.1259055	9.321783333	neg	5119.238702	4093.316895	2939.776681	4703.596002	6055.104524	4780.632789	3970.884356	3744.244964	4925.791211	
9.33_311.2463n	292.2284621	9.332316667	neg	7150.789264	6510.475407	6189.887689	5702.144365	6783.810811	6779.221293	7358.448463	6740.586666	6778.892558	
9.33_353.1317m/z	353.1316633	9.332316667	neg	439.6455167	367.2902885	184.7859529	507.7308962	545.9800742	506.8891628	380.7667187	366.166363	408.6475985	
9.33_390.2499m/z	390.2499309	9.332316667	neg	3904.107156	3189.552798	3519.449011	3096.232636	3514.692975	3465.774271	4179.618206	3734.002876	3666.05283	
9.33_633.1134m/z	633.1133652	9.332316667	neg	3335.101168	2874.235896	1602.407788	3421.215649	4546.530831	2846.019944	1952.765499	2440.928894	4024.499477	
9.34_704.8152m/z	704.8152484	9.342833333	neg	4358.005278	4123.993989	3861.140074	4125.687327	5304.61839	4718.028101	5029.292978	5031.422264	4716.579883	
9.35_549.8569m/z	549.8568535	9.353316667	neg	3162.371057	2980.917872	1887.36612	2630.056898	2775.173738	2523.489833	2324.808561	3612.434137	3798.761768	
9.36_360.9744m/z	360.9744326	9.36055	neg	2276.144308	1863.944746	2146.394236	1384.931009	1912.580966	1592.226477	2014.87577	2029.146334	2095.059156	
9.36_361.2234m/z	361.223446	9.36055	neg	233.7437255	395.9108456	412.738186	130.9451704	339.6256913	320.0394713	123.9509587	165.7609177	134.9510585	
9.38_164.9273m/z	164.9272875	9.37835	neg	501.977043	438.8161774	593.8899656	469.4753654	460.3503132	412.2719363	566.5361133	420.8665725	434.3390901	
9.39_197.9024m/z	197.9023734	9.387716667	neg	399.8937412	311.3005891	354.9062909	274.5731287	354.6203766	261.6173033	283.8002759	409.5872331	436.8243888	
9.39_482.9334m/z	482.9333761	9.387716667	neg	3028.076549	2863.694657	3441.769439	2238.584735	2386.363352	2235.17401	2793.241866	2828.608335	3033.962739	
9.40_103.9202m/z	103.9202359	9.396466667	neg	133.4609025	155.851303	143.0017225	126.260799	142.1305559	120.7539641	159.7371378	113.8065419	138.4794617	
9.40_347.8893m/z	347.8892826	9.396466667	neg	1161.766807	1210.413707	1113.421035	828.279417	762.325494	697.079938	1045.983388	1190.591412	1027.225575	
9.41_339.9117m/z	339.9116851	9.4114	neg	7479.780316	6164.578007	5580.790524	5378.843905	4750.820363	4820.566963	6135.848334	5725.780571	5091.112864	
9.41_571.0861m/z	571.0861003	9.40525	neg	821.2614953	770.7924621	714.0504145	507.9383481	837.777888	430.1613099	878.006374	596.5617718	1183.756577	
9.41_809.8509m/z	809.8508754	9.40525	neg	3316.066117	3149.140302	4419.422136	1283.656208	2516.901683	2472.760953	3455.631809	2701.113113	2088.496696	
9.42_156.8948m/z	156.8947738	9.4245	neg	538.1861918	582.605876	716.6011908	644.7239143	457.2616817	449.6015944	720.1894357	427.5582312	438.7523575	
9.42_277.0330m/z	277.0329651	9.4245	neg	780.4204729	858.0365403	1053.331888	965.2470197	592.3724846	511.1620505	930.4111176	624.0323868	693.5513409	
9.46_367.9067m/z	367.906716	9.455966667	neg	5323.00379	4197.207079	4559.77676	4023.208568	3384.228108	3371.523204	4846.801573	3315.276847	3172.951842	
9.47_344.9428m/z	344.9428114	9.473733333	neg	1707.909477	1929.80787	2617.748623	2356.623136	1796.734746	1776.640453	2344.362368	1874.416818	1843.086483	
9.47_477.8661m/z	477.8661251	9.466483333	neg	1350.813534	1249.19139	1945.786465	2056.93038	1149.612979	1180.096962	789.6828267	1006.063598	1545.102652	
9.48_395.8103m/z	395.8103026	9.482033333	neg	1066.794773	1290.444823	1357.652028	1346.121137	1558.851569	1599.960848	1527.271156	1250.895419	1710.971984	
9.50_362.8755m/z	362.8755065	9.5047	neg	24635.04516	21475.26988	20828.09457	18853.73201	21929.8953	21261.86311	23385.43571	20999.01487	22157.1212	
9.50_809.8507m/z	809.8507331	9.5047	neg	2792.258188	3343.35848	3492.694986	2189.33807	4700.727431	4555.675721	5556.914672	3528.490275	4807.502337	
9.53_242.8746m/z	242.8746458	9.52575	neg	370.2708224	403.6920832	308.2585269	224.6484782	453.0297687	407.9652008	602.0810654	439.2205223	628.4419146	
9.54_288.9918m/z	288.9917554	9.5362	neg	1407.571402	1343.19556	1029.346545	1200.628016	1533.727242	1606.189838	1534.265302	1512.203385	1458.861747	
9.54_360.9744m/z	360.9744322	9.5362	neg	805.9244194	692.9227812	640.8228873	596.0551605	864.9534779	971.3612826	881.2791331	751.5212744	885.8175459	
9.54_685.8329m/z	685.832945	9.543566667	neg	1803.528113	1513.52543	1070.786006	787.7946627	2126.823353	1748.873176	1350.952745	1184.714572	1894.791273	
9.55_297.9036m/z	297.9035927	9.554083333	neg	2262.775956	2577.351224	2037.396931	1987.059444	1987.982429	2487.251342	2126.452116	1686.327656	2172.087259	
9.57_187.9419m/z	187.9419459	9.565266667	neg	1453.25144	1255.654338	962.8965514	790.1832667	1103.634736	1247.92969	989.4684057	1145.049286	1113.618155	
9.57_445.1459m/z	445.1459273	9.565266667	neg	927.4530836	1041.863978	1141.444851	1207.212149	923.086181	1157.258954	931.7342048	987.698589	1206.548017	
9.58_347.8893m/z	347.889271	9.575683333	neg	1397.948881	1145.436929	1297.823458	1312.160429	1267.644166	1356.750115	1234.610255	1426.353589	939.2328592	
9.58_513.1334m/z	513.1333701	9.575683333	neg	310.3070749	576.2937621	591.4105174	451.8224962	383.505966	268.0825918	218.061692	539.5954819	333.6478992	
9.58_726.8001m/z	726.8001198	9.575683333	neg	7825.09895	7071.47698	6084.42388	6369.002755	7325.751778	7107.235583	6748.512141	7088.041252	6802.264369	
9.61_475.8863m/z	475.8862676	9.607216667	neg	3124.171917	3008.195008	2085.690943	2213.849895	1626.969505	1934.651298	2520.738943	1997.563171	1813.039717	
9.62_414.9460m/z	414.9460397	9.611966667	neg	2651.526063	2880.790774	2500.469677	2669.208975	3222.847055	2305.4666	2742.288604	2718.211517	3256.03039	
9.62_524.8344m/z	524.8343899	9.611966667	neg	2380.303849	2805.740434	2339.718917	2433.442226	2058.873793	2452.90972	1750.357433	3259.685774	2453.982036	
9.65_1022.7465m/z	1022.746452	9.645683333	neg	7337.066951	8138.456305	6677.276616	7575.326053	8059.771264	7206.94724	8412.936443	7222.907072	7271.762151	
9.65_311.2463n	292.2284143	9.654433333	neg	9421.362836	9086.522295	8304.622794	8502.390704	9477.601509	9313.250393	9179.780227	9318.75716	9466.293637	
9.65_944.7300m/z	944.7299877	9.645683333	neg	2137.025721	2707.022343	1878.166163	2337.852561	2461.875614	1729.541365	1405.92403	1647.054304	2191.223585	

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Supplementary file Table S3. Raw positive data obtained from sequencing

ID	m/z	Retention time (min)	Ion mode	Metabolites	Compound ID	Super Class	Class	Sub Class	level	kegg	Score	Fragmentation Score	Adducts	Formula	Mass Error (ppm)	CK1	CK2	CK3	HN1	HN2	HN3	LN1	LN2	LN3
1.35_268.1036m/z	268.1036166	1.350266667	pos	Adenosine	86	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	**	C00212	58.1	95.1	M+H	C10H13N5O4	-1.548936074	45345.65261	45100.88042	46434.00605	52635.59657	51670.32612	51460.9282	40829.94021	47018.81117	46316.63561
3.47_311.1225n	312.1297735	3.468983333	pos	N2,N2-Dimethylguanosine	HMDB0004824	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	***		58.1	96.7	M+H, M+K, M+Na	C12H17N5O5	-1.515682806	246031.3311	200852.9021	243346.9032	297155.8702	287921.3528	245362.9554	177728.8654	181281.2609	234480.8662
1.87_297.1069n	320.0960524	1.872316667	pos	Nelarabine	85183	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified			57.9	95.6	M+H, M+Na, M+K	C11H15N5O5	-1.427955585	124099.0628	123968.0426	123777.3675	128914.4563	118159.9135	121381.4719	110133.7922	122139.4109	115856.1866
0.68_156.0765m/z	156.0765014	0.6788	pos	L-Histidine	21	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00135	57.6	96.9	M+H	C6H9N3O2	-1.622267271	295624.5235	307770.107	306088.4932	411186.638	442487.3254	442250.2741	426917.6578	420123.4759	433411.1192
5.66_176.0704m/z	176.0704019	5.656316667	pos	Indoleacetic acid	HMDB0000197	Organoheterocyclic compounds	Indoles and derivatives	Indolyl carboxylic acids and derivatives	*	C00954	57.6	90.9	M+H	C10H9NO2	-1.159842257	14516.62073	14129.62032	14154.97558	22399.33413	22642.91444	23257.16439	12929.76938	12580.23761	14278.45446
0.78_104.0708m/z	104.0708183	0.778966667	pos	L-2-Aminobutyric acid	35945	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C02356	57.2	91.1	M+H	C4H9NO2	2.069824307	10446.42517	10211.76108	10577.65691	16201.59073	15184.46274	15058.32528	11767.17934	12770.46682	14048.54846
3.33_384.1144m/z	384.1143569	3.330366667	pos	Succinyladenosine	HMDB0000912	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	***		56.7	90.5	M+H	C14H17N5O8	-1.649751778	63501.838	74032.72386	69362.06645	84872.38138	77795.67214	80080.34313	67708.50691	74038.39641	69578.3707
0.80_198.0871m/z	198.0871077	0.796983333	pos	N-Acetyl-L-Histidine	44784	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C02997	56.3	87.1	M+H	C8H11N3O3	-1.065413086	14296.73222	13837.27925	14642.60044	16628.7343	16093.46724	15479.64774	13758.97461	14962.72484	14812.44944
4.70_188.1279m/z	188.127905	4.701116667	pos	(E)-2-Butenyl-4-methyl-threonine	69263	Unclassified	Unclassified	Unclassified			56.1	83.8	M+H	C9H17NO3	-1.148109789	47954.18088	45374.98941	44318.9369	43891.73406	44614.6913	45096.07212	48344.79923	44560.99189	45410.31911
5.13_205.0737m	206.0810051	5.125733333	pos	Indolelactic acid	71	Organoheterocyclic compounds	Indoles and derivatives	Indolyl carboxylic acids and derivatives	*	C02043	55.9	82.9	M+H+H2O, M+H	C11H11NO3	-0.922918285	11783.13432	11917.35645	11332.55613	19551.88371	18382.06272	18322.22576	20131.92666	19022.90758	17996.42088
9.01_426.3206m/z	426.3206054	9.012583333	pos	Cholic acid	HMDB0000619	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	***	C00695	55.9	86.3	M+NH4	C24H40O5	-1.946050553	34694.61364	49791.97745	51489.05568	5293.01299	4265.794588	4634.553048	17300.95422	19633.19941	18540.61483
3.91_298.0966m/z	298.0965629	3.911966667	pos	5'-Deoxy-5'-<WBR>(methylthio)adenosine	3425	Unclassified	Unclassified	Unclassified			55.8	85.4	M+H	C11H15N5O3S	-0.921931563	15806.43992	16323.88201	16813.76936	17129.18297	16897.58646	16740.58216	11420.00624	12336.72299	12030.04024
11.75_282.2788m/z	282.2787651	11.7471	pos	Oleamide	4115	Lipids and lipid-like molecules	Fatty Acyls	Fatty amides	*	C19670	55.7	83.4	M+H	C18H35NO	-1.337110009	3535810.765	3439530.468	3424650.496	3454229.059	3599104.795	3633102.14	3727488.096	3509656.049	3615399.969
1.16_166.0721m/z	166.0721048	1.157483333	pos	7-Methylguanine	58012	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	*	C02242	55.6	86.3	M+H	C6H7N5O	-1.402524015	188023.4654	188949.0781	182758.4986	201815.9711	190214.5677	194956.3014	182802.7789	194388.6349	176750.7393
7.20_373.2731m/z	373.2731628	7.20385	pos	3α-Hydroxy-5β-chola-7,9(11)-dien-24-oic Acid	42909	Unclassified	Unclassified	Unclassified			55.6	84	M+H	C24H36O3	-1.585052794	87362.60358	106200.8867	101911.8987	39036.20602	37951.8536	34870.43807	46994.89032	58789.13053	56158.37553
4.29_195.0875m/z	195.087453	4.294383333	pos	Caffeine	1455	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	**	C07481	55.5	87.7	M+H	C8H10N4O2	-1.025191358	304036.3057	317749.7272	341119.3753	215053.6261	192605.6304	204992.429	233468.2503	264376.1433	256179.0735
1.59_220.0845n	221.0917737	1.589283333	pos	5-Hydroxy-L-tryptophan	364	Organoheterocyclic compounds	Indoles and derivatives	Tryptamines and derivatives	**	C00643	55.3	79.6	M+H-H2O, M+H	C11H12N2O3	-1.455859479	53013.29544	57108.36161	57942.41801	70852.85244	67445.69081	68499.03664	51516.45456	59132.50717	56510.8189
8.52_318.2998m/z	318.299758	8.517983333	pos	17-hydroxy stearic acid	LMFA02000135	Lipids and lipid-like molecules	Fatty Acyls	Octadecanoids			55.3	82.5	M+NH4	C18H36O3	-1.706964671	5957.208823	6138.129632	5854.391747	6347.441371	6490.379207	11784.55826	6898.350203	4292.710978	7586.271157
4.20_246.1697m/z	246.1696959	4.204866667	pos	2-Methylbutyroylcarnitine	HMDB0000378	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	***		55	78.6	M+H	C12H23NO4	-1.177633319	62663.14528	64739.04045	68070.37333	125914.0588	115419.5898	119509.1482	86336.42328	95494.87778	90197.99496
8.72_272.2580m/z	272.257971	8.719016667	pos	C16 Sphingosine	53900	Lipids and lipid-like molecules	Sphingolipids	Sphingoid bases			55	79.9	M+H	C16H33NO2	-1.602811843	7883.647928	8507.569401	7043.027161	8262.844035	8590.169147	11268.94916	6857.196088	7446.97753	8869.356277
4.93_447.0914m/z	447.0914371	4.927016667	pos	Baicalin	49507	Phenylpropanoids and polyketides	Macrolides and analogues	Unclassified		C10025	54.9	79.3	M+H	C21H18O11	-1.682941586	191.0070616	131.8666824	468.4027014	15168.89748	13521.33207	12829.73551	0.001403199	0.001403199	0.001403199
4.47_373.2732m/z	373.2731628	4.466083333	pos	3β-Hydroxychola-5,7-dien-24-oic Acid	43006	Unclassified	Unclassified	Unclassified			54.9	80.2	M+H	C24H36O3	-1.500778944	11922.79654	12984.04125	9931.06716	4239.644648	4284.849138	4893.174633	10604.55777	11431.8421	8341.990067
0.88_281.1119n	282.1191326	0.8802	pos	N6-Methyladenosine	HMDB0004044	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	***		54.8	79.3	M+H, M+Na	C11H15N5O4	-1.948715702	141695.2946	169209.7666	165316.8581	149852.9593	162345.5875	158182.5662	158688.5407	153673.6587	164732.0307
8.48_301.2844m/z	301.2844114	8.4786	pos	Prosafirinine	LMSP01080051	Lipids and lipid-like molecules	Sphingolipids	Sphingoid bases			54.8	80.6	M+NH4	C17H33NO2	-1.918458448	6404.594515	610.9015031	831.8534826	1257.151645	2846.138576	716.7466903	1196.177384	9655.866319	655.8982374
0.76_162.1122m/z	162.1121691	0.758666667	pos	L-Carnitine	34532	Organic nitrogen compounds	Organonitrogen compounds	Quaternary ammonium salts	**	C00318	54.7	77.6	M+H	C7H15NO3	-1.866632448	170586.5003	158612.0086	166652.2869	278300.7563	273208.564	281661.8173	169546.913	172023.4067	161388.8414
5.40_349.2368m/z	349.236839	5.396716667	pos	Protomycinolide IV	71020	Unclassified	Unclassified	Unclassified			54.7	78.7	M+H	C21H32O4	-1.427099768	7700.567244	9429.348984	8966.346525	8305.027405	8929.873033	8543.172045	6893.952073	8777.543176	7822.887399
0.66_188.1754m/z	188.1754261	0.657416667	pos	N1-Acetylspermidine	3323	Organic acids and derivatives	Carboximidic acids and derivatives	Carboximidic acids	*	C00612	54.6	85.6	M+H	C9H21N3O	-1.670125412	66165.51226	72803.03049	81533.65862	74818.24573	70439.34063	70279.25778	67090.91089	74466.28077	75446.08541
2.05_189.0998n	212.0890299	2.048666667	pos	Alexine	68133	Unclassified	Unclassified	Unclassified			54.6	77.2	M+H+H2O, M+Na, M+H	C8H15NO4	-1.499182088	198237.7588	210785.9443	224658.109	143991.2663	131760.2428	131425.9119	174817.9644	200364.1191	188199.72
6.72_262.0626m/z	262.0625624	6.7199	pos	Desmethylflumazenil acid (Ro 15-6877)	2729	Unclassified	Unclassified	Unclassified			54.6	76.5	M+H	C12H8FN3O3	1.212915041	0.001403199	0.001403199	0.001403199	46425.04663	44041.35487	47956.18552	0.001403199	0.001403199	0.001403199
6.50_219.1741m/z	219.1740571	6.4952	pos	Zerumbone	91709	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		54.5	76.7	M+H	C15H22O	-1.304663971	6215.455308	6831.12681	5834.822627	3539.912936	3525.797254	3965.841297	5620.887497	5653.437294	5487.961761
1.33_120.0575n	121.0648021	1.327966667	pos	p-Tolualdehyde	66526	Benzenoids	Benzene and substituted derivatives	Benzoyl derivatives	**	C06758	54.4	74.1	M+H, M+NH4	C8H8O	0.090238002	8377.916969	8374.43682	8486.618993	9367.271531	9210.898522	9040.56547	8407.817532	9263.939992	9045.642109
6.28_376.0820m/z	376.082017	6.276683333	pos	4-[(4'-O-Acetyl-alpha-L-rhamnosyloxy)benzyl]isothiocyanate	HMDB0032802	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			54.4	81.4	M+Na	C16H19NO6S	-1.4501167	10568.2128	9700.979261	11272.53764	16700.12873	17542.02783	16388.566	16540.07034	19535.69198	18640.09682
0.94_373.2731m/z	373.2731214	0.9443	pos	3β-Hydroxychola-5,16-dien-24-oic Acid	43009	Unclassified	Unclassified	Unclassified			54.4	78.4	M+H	C24H36O3	-1.612002624	10136.44207	10790.86216	11079.31802	4403.07181	4235.09636	3729.11286	5761.019163	8052.877154	
14.93_282.2786m/z	282.2786333	14.927	pos	12-amino-octadecanoic acid	LMFA01100008	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			54.3	76.5	M+H-H2O	C18H37NO2	-1.696993087	2787014.67	2593228.248	2591329.544	2678954.495	2891773.003	2883888.358	2788877.345	2651034.62	2797575.005
3.04_219.1104n	220.1176861	3.043116667	pos	Pantothenic Acid	241	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols	**	C00864	54.3	75.1	M+H, M+Na	C9H17NO5	-1.200185703	55855.82337	64890.36145	74783.17289	143834.0664	133589.2489	129408.0353	96070.01877	96984.12634	102741.2763
0.68_308.1578n	309.1650422	0.6788	pos	1-[(5-Amino-5-carboxypentyl)amino]-1-deoxyfructose	HMDB0034879	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			54.2	77.9	M+H, M+Na	C12H24N2O7	-1.899607489	28675.3736	28026.05212	28116.58374	36459.22764	37771.28783	42078.74914	26056.38015	26775.47218	28458.53839
0.78_146.0809m/z	146.0809355	0.776966667	pos	L-trans-5-Hydroxy-2-piperidinecarboxylic acid	HMDB0029426	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		54.2	75.7	M+H	C6H11NO3	-1.614302259	77592.13749	80479.40477	81912.16616	31529.68222	30414.85105	31374.28489	28494.08773	29993.89975	29452.99227
3.78_246.1212m/z	247.1284581	3.781933333	pos	L-beta-aspartyl-L-leucine	62015	Organic acids and derivatives	Peptidomimetics	Hybrid peptides	*		54.1	75.8	M+H, M+Na	C10H18N2O5	-1.584586662	1570.912536	1967.225096	1454.120406	18541.08408	18625.3543	12961.33145	1504.35956	1427.454127	
0.80_310.1128m/z	310.1128049	0.796983333	pos	N-Acetylneuraminic Acid	24101	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C19910	54	77.5	M+H	C11H19NO9	-1.464659673	18653.41169	19885.42057	20404.10893	22280.65357	22543.51375	22025.225	16874.19037	19101.78779	17792.34309
6.31_399.2009m/z	399.2008745	6.308766667	pos	Cinncassiol E	71845	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		54	76	M+H	C20H30O8	-1.179956247	11225.53192	14769.99134	13935.13276	14825.41281	14467.54777	13782.85785	14469.40217	12809.41164	14514.55396
3.76_146.0598m/z	146.0598308	3.759483333	pos	4-formyl Indole	96392	Unclassified	Unclassified	Unclassified			53.9	73.4	M+H	C9H7NO	-1.444009853	9209.253314	10111.82055	10425.13301	13092.87059	11817.08039	11948.49136	10056.87684	12174.92511	11356.15273
5.28_550.1680n	573.1572038	5.284233333	pos	Neoliquiritin 2''-apioside	HMDB0040544	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides			53.9	73.4	M+H, M+Na	C26H30O13	-1.178776411	45555.76411	48319.60225	53329.99784	852.078437	1042.73746	971.6246298	6480.710363	7989.696279	7790.389725
15.08_338.3410m/z	338.341016	15.08395	pos	13Z-Docosenamide	64926	Unclassified	Unclassified	Unclassified			53.8	75.1	M+H	C22H43NO	-2.150622777	392181.4958	330533.5592	363673.9952	376208.9132	361858.2564	381607.2075	416104.1703	362561.2521	445328.4211
0.74_240.0231n	241.0304236	0.73955	pos	L-Cystine	17	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00491	53.7	80.8	M+H, M+Na	C6H12N2O4S2	-2.923429181	52164.28075	46629.42055	49403.6884	87555.90348	96276.8895	91405.66366	73006.7118	61749.38764	76737.36835
4.99_173.1170m/z	173.1170164	4.991816667	pos	9-hydroxy-5Z-nonenoic acid	74606	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			53.7	72	M+H	C9H16O3	-1.187503461	28695.7671	27158.23058	27029.16316	26876.57297	27335.41113	26075.23935	30227.29683	27377.10171	28109.64023
0.88_188.1158n	189.1230861	0.8802	pos	Nε-Acetyl-L-lysine	63103	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C02727	53.6	72.9	M+H, M+Na	C8H16N2O3	-1.502813612	59279.25641	67290.92297	66221.74223	82835.71411	80758.63581	80884.248	69044.28926	74270.2206	71587.71184
4.23_192.0653m/z	192.0653423	4.2272	pos	5-Hydroxyindoleacetic acid	HMDB0000763	Organoheterocyclic compounds	Indoles and derivatives	Indolyl carboxylic acids and derivatives	***	C05635	53.6	71.3	M+H	C10H9NO3	-0.92798515	12432.03167	12745.95762	13053.75055	12983.10886	11958.60368	11928.69428	12230.17766	13147.26684	13145.92225
6.90_313.2247n	314.2320238	6.8951	pos	9-Decenoylcarnitine	LMFA07070048	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		53.5	73.3	M+H, M+Na	C17H31NO4	-1.791262172	360744.4674	369706.5314	393647.4335	575192.8047	545015.1901	508945.1621	335236.1433	383437.3353	408514.4314
1.16_123.0440m/z	123.0440312	1.199716667	pos	4-Hydroxybenzaldehyde	62451	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C00633	53.4	69.7	M+H	C7H6O2	-0.202157175	13593.26753	15061.64	15450.70457	18616.81672	17409.84337	16215.42434	16727.83204	16995.70169	17408.2093
1.16_282.1192m/z	282.1191808	1.157483333	pos	1-Methyladenosine	6888	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	*	C02494	53.3	72.4	M+H	C11H15N5O4	-1.777339821	190287.2721	159325.6385	170413.8028	192409.362	142256.2883	140729.4574	161705.3064	188941.6898	157888.9181
0.78_118.0863m/z	118.0862667	0.776966667	pos	L-Valine	35	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00183	53.2	71.8	M+H	C5H11NO2	0.099931793	494266.4894	537149.8383	532336.5423	803052.3064	746456.9305	779660.8755	639476.2928	614616.5102	616217.6434
4.61_243.1468n	244.1540878	4.610866667	pos	2-Ethylacrylylcarnitine	6417	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters			53.2	71.8	M+H, M+Na	C12H21NO4	-1.015103534	17729.12011	18814.36195	19337.8684	12450.68629	13061.73095	10666.38959	14497.35911	14071.95774	16155.24858
8.07_389.2679m/z	389.2679074	8.074933333	pos	1α-hydroxy-25,26,27-trinorvitamin D3 24-carboxylic acid	41963	Unclassified	Unclassified	Unclassified			53.2	72.8	M+H	C24H36O4	-1.876816964	71648.84935	90011.26761	104788.7975	19885.25547	18022.09134	17488.59449	47661.75625	53796.44122	55554.79964
4.02_180.0533n	181.0605855	4.024633333	pos	Nicotinuric acid	1499	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C05380	53.1	75.5	M+H+H2O, M+Na, M+H	C8H8N2O3	-0.966678851	42046.7517	44073.71906	45499.37088	72057.62822	65508.87717	66705.05993	47849.73959	52790.73491	52193.86054
8.07_370.2504n	353.2470788	8.074933333	pos	Antibiotic SB 202742	HMDB0041206	Benzenoids	Benzene and substituted derivatives	Unclassified			53.1	71	M+H+H2O, M+H	C24H34O3	-1.155779999	964113.4687	1228893.327	1407344.153	28394.71626	29457.75908	29109.46639	65864.60196	76042.10748	
0.80_190.1184m/z	190.1183554	0.796983333	pos	N6-Carbamoyl-DL-Lysine	85017	Unclassified	Unclassified	Unclassified			53	71	M+H	C7H15N3O3	-1.387326499	9770.283291	7401.846462	8627.080132	9745.044468	8540.202582	7947.633113	7735.325521	8581.771215	7849.254594
0.88_241.0075n	242.0147434	0.8802	pos	3-Mercaptolactate-cysteine disulfide	HMDB0006512	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		52.9	69.1	M+H, M+Na	C6H11NO5S2	-1.649288094	85441.19541	86457.36925	90768.50835	95605.06593	88434.121	86263.19673	73221.92808	85080.95919	78861.8112
3.98_190.0497m/z	190.0496848	3.979183333	pos	4-(2-Aminophenyl)-2,4-dioxobutanoic acid	HMDB0000978	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C01252	52.9	67.4	M+H-H2O	C10H9NO4	-0.892152762	44131.65657	48096.73932	47982.74648	64854.8819	60064.6366	61700.38827	51256.45889	57316.86823	52620.45423
9.93_460.2685m/z	460.2685409	9.9276	pos	3-O-Acetylepisamarcandin	HMDB0031958	Phenylpropanoids and polyketides	Coumarins and derivatives	Unclassified	*		52.8	67.4	M+NH4	C26H34O6	-1.862095067	292847.0337	232952.247	303083.3286	326969.9341	209497.3983	226804.3133	213400.2163	190608.7662	287781.8803
12.77_279.1798m/z	279.1794683	11.18926667	pos	Rudbeckin A	67850	Unclassified	Unclassified	Unclassified			52.7	68.4	M+H	C17H26O3	-1.277366382	1298.54671	7660.208553	5486.131921	7536.424103	7480.296742	7305.137989	6627.255383	7051.100433	
5.72_364.2245n	347.2212442	5.720466667	pos	Tetrahydrocortisone	HMDB0000903	Lipids and lipid-like molecules	Steroids and steroid derivatives	Hydroxysteroids	*		52.7	68.4	M+H-H2O, M+H	C21H32O5	-1.218791568	32188.99115	32587.50607	34649.50138	39983.27519	40753.1364	37461.58165	33835.69182	29983.33943	29508.87501
0.72_170.0921m/z	170.0920694	0.717716667	pos	3-Methyl-L-histidine	3293	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C01152	52.5	72.9	M+H	C7H11N3O2	-1.973455579	87350.4463	87872.49281	93950.98629	113997.1564	118201.5388	118220.1132	97186.40688	93929.26978	95565.27951
12.88_264.2449n	282.2787279	12.87801667	pos	9,12,15-Octadecatrien-1-ol	LMFA05000216	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols			52.5	67	M+H, M+NH4	C18H32O	-1.510772465	773648.3715	638870.9398	618172.3574	607935.3934	619123.4578	660993.7061	704359.0225	669756.8481	646641.4321
3.78_482.1055n	505.0944231	3.781933333	pos	(-)-Epigallocatechin 7-gallate	96003	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	*		52.5	68.6	M+H, M+Na	C22H20O13	-1.078563357	17410.21273	18223.5556	19627.36188	9865.251547	9765.441202	10342.16131	14979.18949	14975.81358	12998.39329
1.19_263.1105n	263.1109958	1.193366667	pos	Arsenobetaine	HMDB0000194	Organic acids and derivatives	Peptidomimetics	Hybrid peptides	**	C01262	52.5	68.4	M+Na	C10H18AsNO3	2.226830724	45.56256144	2153.198798	137.0770655	47.52261144	18556.63263	1105.65363	97.75809	46.22497739	
0.68_133.0970m/z	133.0969791	0.6788	pos	D-Ornithine	6910	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00515	52.4	66.6	M+H	C5H12N2O2	-1.324350564	1246.720548	1603.897098	1326.551238	3770.678671	3993.000161	4955.308456	1892.041739	1615.33049	1780.034237
0.82_258.0848n	259.0920971	0.818116667	pos	Ribothymidine	85160	Nucleosides, nucleotides, and analogues	Pyrimidine nucleosides	Unclassified	*		52.4	68	M+H, M+Na	C10H14N2O6	-1.416348937	34872.97349	35763.9094	34871.79878	38531.31422	38589.20045	38096.42252	32761.18164	35531.01996	35267.1051
3.26_231.1468n	232.1540327	3.258783333	pos	Butyryl-L-carnitine	964	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*	C02862	52.4	65.1	M+H, M+Na	C11H21NO4	-1.306224871	214630.7452	228531.369	234938.5044	533577.1436	557185.3378	522525.3875	324986.0522	331207.5649	321585.5773
3.74_254.1018m/z	254.1018393	3.73775	pos	Austdiol	HMDB0030858	Organoheterocyclic compounds	Azaphilones	Unclassified	*		52.4	67.4	M+NH4	C12H12O5	-1.947561163	4983.32237	5209.681769	5660.62947	6749.885125	7232.9817	6161.5575	4536.627072	5140.047879	5073.34356
10.63_297.2664n	280.2631082	10.63171667	pos	4E,14Z-Sphingadiene	LMSP01080002	Lipids and lipid-like molecules	Sphingolipids	Sphingoid bases			52.3	75.2	M+H-H2O, M+K	C18H35NO2	-1.288015901	90682.66249	74152.63432	72734.44273	77771.07334	90036.38252	98648.73304	80751.89505	68265.73262	71518.9655
9.75_315.2769n	338.2659494	9.7507	pos	(4OH,8Z,t18:1) sphingosine	53909	Unclassified	Unclassified	Unclassified			52.3	70.5	M+H, M+NH4	C18H35NO3	-1.383846992	12609.1443	13385.7424	14427.04857	12537616178	167885.4126	134778.3672	158917.4399	134856.0149	141614.1064
10.19_460.2686m/z	460.2686318	10.1851	pos	Cinobufagin	LMST01130032	Unclassified	Unclassified	Unclassified			52.1	64.4	M+NH4	C26H34O6	-1.656442268	17906.43334	18066.83834	12587.50255	16413.86623	18466.48447	17740.0383	14774.40874	14777.40339	15176.2183
9.01_372.2638n	373.2731335	9.012583333	pos	3alpha-Hydroxy-5beta-chola-7,9(11)-dien-24-oic Acid	LMST04010330	Unclassified	Unclassified	Unclassified			52.1	66.4	M+H-H2O, M+H	C24H36O3	-1.610736918	260663.4875	364818.6928	372956.6833	36720.65622	34767.53938	35474.74493	127239.5112	145603.2442	132033.4604
0.76_190.0586n	191.0659111	0.758666667	pos	L-β-aspartyl-L-glycine	62014	Organic acids and derivatives	Peptidomimetics	Hybrid peptides	*		52	65.2	M+H, M+Na	C6H10N2O5	-1.771694552	39689.61024	41710.25278	38959.47977	63240.94029	60223.33296	60103.15054	37774.27547	36537.74906	38900.43191
0.78_129.0657m/z	129.0657079	0.776966667	pos	2-amino-4-cyano-butanoic acid	35948	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates		C05717	52	64.2	M+H	C5H8N2O2	-1.140209781	30134.48713	31082.10834	30828.06272	50220.11847	48117.5693	47089.53619	40790.62739	42443.10511	43754.50941
1.20_164.0471n	182.0809796	1.199716667	pos	4-hydroxycinnamic acid	306	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	**	C01772	52	69.1	M+H, M+NH4, M+H-H2O	C9H8O3	-1.233004652	241242.6653	277424.1039	280265.3835	347530.5023	329496.5831	338682.2377	290192.4036	343640.3388	318422.7501
1.12_139.0399n	139.0499079	1.115783333	pos	Undecanedioic acid	65716	Unclassified	Unclassified	Unclassified			51.9	64.1	M+H	C11H20O4	-1.492035672	11.25.53205	1287.552291	1282.82697	1228.42697	1356.668841	1157.010298	9616.498637	11105.04513	10263.03176
7.52_251.1274m/z	251.1274117	7.5231	pos	3-carboxy-4-methyl-5-pentyl-2-furanpropanoic acid	LMFA01150047	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		51.9	64.6	M+H-H2O	C14H20O5	-1.393976228	9503.783905	9674.109036	10136.17925	15927.50873	14694.78643	14845.65352	11017.81763	12389.79178	12330.9928
0.82_228.1108n	229.118057	0.818116667	pos	Prolylhydroxyproline	HMDB0006695	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***		51.8	64.4	M+H, M+Na	C10H16N2O4	-0.992860516	74322.36009	78893.768	80558.18131	119197.6697	116046.8024	114580.4032	66011.36644	74442.36634	70523.74122
4.43_105.0337m/z	105.0336989	4.42815	pos	Tropolone	HMDB0259299	Unclassified	Unclassified	Unclassified			51.8	62.1	M+H-H2O	C7H6O2	1.702081237	10363.77622	11527.8642	11931.0144	4732.529518	4310.287107	4493.05096	7998.219089	9268.082257	8550.590932
4.75_107.0857m/z	107.0857078	4.7

10.46_277.1795m/z	277.1794764	10.45796667	pos	Panaquinquecol 2	HMDB0038938	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		51.3	61.3	M+H	C17H24O3	-1.248097884	16259.33747	10096.22137	12462.82121	10945.73578	12497.07746	12605.80907	13023.88502	13368.26314	14599.90123
5.58_506.2510n	507.2583567	5.581883333	pos	11-Hydroxyprogesterone 11-glucuronide	HMDB0010364	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	*		51.3	61.1	M+H-H2O, M+H	C27H38O9	-1.092129406	28542.75571	28060.84803	35585.39244	39586.7741	37794.10074	41952.38164	27957.70443	27898.91706	27237.16873
10.33_278.2475m/z	278.247466	10.32878333	pos	Crucigasterin 277	LMSP01080036	Lipids and lipid-like molecules	Sphingolipids	Sphingoid bases			51.2	61.6	M+H	C18H31NO	-1.352952698	26884.07757	26131.63055	26772.98568	26225.43682	27072.31503	28402.50282	28094.28574	28462.72635	28627.41518
2.00_366.1422n	367.149428	2.004416667	pos	Tryptophan 2-C-mannoside	HMDB0240296	Organoheterocyclic compounds	Indoles and derivatives	Indolyl carboxylic acids and derivatives			51.2	62	M+H, M+Na	C17H22N2O7	-1.500869794	149106.6559	153768.7377	157816.5623	165584.3458	156773.5856	158520.093	139492.7493	160204.1159	145012.5843
4.20_217.0970m/z	217.096972	4.204866667	pos	5-Methoxytryptophan	HMDB0002339	Organoheterocyclic compounds	Indoles and derivatives	Tryptamines and derivatives	*		51.2	57.5	M+H-H2O	C12H14N2O3	-0.77759544	12409.08722	12705.99855	13494.54372	8078.077885	7701.180695	7639.810807	10871.89	11884.79475	11221.0223
0.76_126.0218m/z	126.0218441	0.758666667	pos	Taurine	HMDB0000251	Organic acids and derivatives	Organic sulfonic acids and derivatives	Organosulfonic acids and derivatives	**	C00245	51.1	64.2	M+H	C2H7NO3S	-0.770957281	11543.54013	9518.773234	10411.59784	30419.12169	28852.39299	30426.37097	11811.95101	11286.32177	10687.51387
1.50_233.1128m/z	233.1128448	1.500483333	pos	N6-Acetyl-LL-2,6-diaminoheptanedioate	63453	Unclassified	Unclassified	Unclassified			51.1	60.3	M+H	C9H16N2O5	-1.522000584	9805.693827	9771.322623	10129.88457	16990.27236	15492.06716	15704.22616	9650.122373	10539.99214	10051.80397
4.81_191.1065m/z	191.1064932	4.814066667	pos	C12:5n-1,3,5,7,9	73918	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			51.1	59.9	M+H	C12H14O2	-0.857286201	4130.952732	4478.563701	5057.931001	6163.491354	5481.075302	6095.860176	4556.995524	4722.741627	4974.609533
1.14_204.1228m/z	204.1227904	1.137683333	pos	L-Acetylcarnitine	HMDB0000201	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	***	C02571	51	58.2	M+H	C9H17NO4	-1.201781096	50273.91959	44185.10661	46519.29616	130995.9616	84377.20433	88483.68808	65039.27748	74496.12494	63874.25392
15.52_156.0762m/z	156.0762154	15.51933333	pos	L-2-Amino-3-(1-pyrazolyl)propanoic acid	HMDB0034267	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			51	62	M+H	C6H9N3O2	-3.466969139	6522.69233	1393.899251	1095.61431	2989.122527	10583.29221	13481.63044	9987.147397	0.723626582	0.245451348
2.18_297.1069n	298.1141691	2.178633333	pos	1-Methylguanosine	6324	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	*	C04545	50.9	61.1	M+H, M+Na	C11H15N5O5	-1.433697371	28180.19046	29354.8318	31939.93261	31183.07652	28866.40613	29832.62545	25767.77922	30285.26467	27879.02313
6.44_301.2249n	301.2321613	6.45815	pos	Nonanoylcarnitine	HMDB0013288	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		50.9	59.3	M+H, M+Na	C16H31NO4	-1.4062422	214648.1769	220857.2177	172814.3565	186124.4148	178107.6187	185899.8855	258873.1746	259997.0818	207303.8947
6.61_569.1258m/z	569.1257994	6.613233333	pos	6''-O-Malonylwistin	HMDB0039083	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavonoid O-glycosides			50.9	63.2	M+Na	C26H26O13	-1.395490135	30616.9595	28660.48715	31311.54253	22268.28326	18632.33286	18402.40477	620.1170554	655.9787331	276.0556722
8.13_406.2713n	407.2785465	8.13135	pos	3-Oxocholic acid	57908	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	*		50.8	60.2	M+H, M+Na	C24H38O5	-1.61025226	75602.20447	77190.70604	82132.68853	43650.93897	40789.77132	40014.99548	58978.84904	74300.13471	62971.11965
3.91_209.0806m/z	209.0806259	3.911966667	pos	5-(3',4'-dihydroxyphenyl)-gamma-valerolactone	86073	Benzenoids	Phenols	Benzenediols	*		50.8	59.4	M+H	C11H12O4	-1.006552887	1438.623911	1336.173654	1206.213222	996.8347375	902.5305149	952.1069001	4588.529938	5261.022882	4971.317188
5.06_267.1467n	268.153986	5.058233333	pos	Codonopsine	68144	Unclassified	Unclassified	Unclassified			50.8	61.3	M+H, M+Na	C14H21NO4	-1.304917526	21650.96616	23314.73115	22884.5252	13209.28834	13907.40237	13527.85542	15146.81072	17337.65668	15470.73683
5.35_135.1167m/z	135.1166834	5.351683333	pos	(S)-(-)-Perillyl alcohol	41074	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids		C02452	50.8	56.9	M+H-H2O	C10H16O	-0.943336987	5887.863034	5979.861242	5983.700179	3502.396264	3453.59933	3276.424455	4951.542747	5158.696917	5182.06036
5.33_205.0858m/z	205.0858219	5.329033333	pos	D-Hydroxykynurenine	HMDB0031668	Organoheterocyclic compounds	Azaphilones	Unclassified	*		50.7	58.6	M+H-H2O	C12H14O4	-0.444585761	10617.39468	11153.62169	11423.53172	2295.692627	2300.239378	2463.184671	2868.538511	2603.242319	2579.765763
4.66_304.0894n	305.0966356	4.656183333	pos	N-Acetylaspartylglutamic acid	44358	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C12270	50.6	61.6	M+H, M+Na	C11H16N2O8	-4.295716526	4409.114099	4285.228534	5016.044236	9421.553906	10683.44848	9227.665505	6013.543015	5190.171031	6291.864633
7.43_584.3188n	607.307916	7.432366667	pos	Cholic acid glucuronide	HMDB0002577	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	*		50.6	56.6	M+H-H2O, M+Na, M+H	C30H48O11	-1.475754588	302219.0805	300574.0888	347273.7858	58032.72473	57391.0346	53109.35076	126247.9868	154520.3388	146322.0844
0.90_102.1280m/z	102.1279558	0.898483333	pos	Triethylamine	70265	Organic nitrogen compounds	Organonitrogen compounds	Amines	*	C14691	50.5	55.5	M+H	C6H15N	2.273355767	5507.602471	5453.380973	5352.197572	6225.980996	6598.736093	5959.98639	7273.943792	6704.078725	7019.790189
8.60_490.2772n	513.2663812	8.602816667	pos	12-Hydroxy-13-O-D-glucuronoside-octadec-9Z-enoate	HMDB0060118	Lipids and lipid-like molecules	Saccharolipids	Unclassified	*		50.5	56.7	M+H-H2O, M+NH4, M+Na, M+H	C24H42O10	-1.270893929	98191.29045	104300.8129	121108.1259	134867.4449	131424.1377	144862.8908	109744.3909	126963.3874	126405.274
0.76_342.1156n	343.1047942	0.758666667	pos	Lactulose	916	Organic oxygen compounds	Carbohydrates and carbohydrate conjugates	Carbohydrates and carbohydrate conjugates		C07064	50.4	57.6	M+H, M+K	C12H22O11	-1.864728917	275384.4625	279704.8661	282383.994	162536.1824	144722.1752	160351.9434	240335.6835	202516.7737	216144.169
2.68_356.0963n	357.1035517	2.677116667	pos	2-O-beta-D-Glucopyranuronosyl-D-mannose	HMDB0039722	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			50.4	59	M+H, M+Na	C12H20O12	2.244245991	14349.47781	13995.67015	15108.38561	21207.69629	20457.13572	20784.7181	14237.68493	15512.0643	16975.16247
3.83_260.1368n	261.1440413	3.825583333	pos	gamma-Glutamylleucine	HMDB0011171	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***		50.4	57.3	M+H, M+Na	C11H20N2O5	-1.756446904	68437.46619	71863.51432	76342.1693	98003.29278	90259.30099	88443.84085	82456.23561	91381.56856	91202.80416
4.27_189.1002n	190.1071337	4.272416667	pos	(2S)-2-{[1-(R)-Carboxyethyl]amino}pentanoate	66366	Unclassified	Unclassified	Unclassified			50.4	62.4	M+H-H2O, M+K, M+H	C8H15NO4	0.532151122	5064.290001	4880.310441	5391.416638	4973.276016	4736.680409	4396.950292	4985.050956	5047.608528	5147.196311
4.75_166.0992m/z	167.106471	4.7456	pos	2E,6E,8E-decatrienoic acid	34881	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			50.4	55.1	M+H-H2O, M+H	C10H14O2	-0.930704782	66692.05021	67166.35939	71560.51276	60946.84497	57318.43185	56640.52261	59858.69771	64202.7006	61722.04468
5.22_230.1515n	231.1588094	5.21995	pos	Dodecanedioic acid	5596	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*	C02678	50.4	56.5	M+H, M+Na, M+H-H2O	C12H22O4	-1.200239213	21558.13789	22883.80025	23731.10369	23280.39052	22084.87286	21661.70403	22029.03219	23998.75952	23529.20736
1.33_329.0520n	330.0593207	1.327966667	pos	cAMP	92	Nucleosides, nucleotides, and analogues	Purine nucleotides	Cyclic purine nucleotides	**	C00575	50.3	57.5	M+H, Na	C10H12N5O6P	-1.444991112	20203.14533	20619.03597	21831.18421	21466.04279	20409.4472	20122.7265	17691.7834	19319.36641	19861.28006
7.18_357.2509n	358.2581953	7.182883333	pos	(9Z)-3-hydroxydodecenoylcarnitine	LMFA07070024	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters			50.3	57.6	M+H, M+Na	C19H35NO5	-1.691657254	364761.3375	364180.1408	379345.4439	479168.8621	432021.7243	424303.2983	280363.7877	307812.6603	330116.4905
5.40_285.1936n	286.20089	5.396716667	pos	2-Octenoylcarnitine	HMDB0013324	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		50.2	55.5	M+H, M+Na	C15H27NO4	-1.384146005	240255.2024	252863.5766	268858.5418	612226.1862	554684.9915	576252.1935	294908.605	335297.6987	325833.4928
6.00_364.2246n	347.2212797	5.995733333	pos	Allotetrahydrocortisone	HMDB0248161	Unclassified	Unclassified	Unclassified			50.2	55.5	M+H-H2O, M+H	C21H32O5	-1.115070769	30501.19712	33935.34172	30919.13823	29949.23051	30093.96983	31982.52217	30713.48928	32443.72265	32722.40058
0.68_486.2051n	487.2124045	0.6788	pos	Glucosylgalactosyl hydroxylysine	HMDB0000585	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		50.1	60.3	M+H, Na	C18H34N2O13	-1.976608286	22163.91014	24810.70632	24193.05187	21016.41137	21656.03274	27063.95013	19625.81296	21814.46189	23359.81946
1.44_306.0816n	309.0815703	4.4062	pos	D-Erythroascorbic acid 1'-a-D-glucoside	89427	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			50.1	54.3	M+H	C11H16O10	-0.171425345	8301.888289	8758.02724	8944.31424	7634.18048	7067.70578	7625.85372	9338.50501	9677.865342	9328.50428
1.57_146.0810m/z	146.0809571	1.56695	pos	4-acetamidobutanoate	44719	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C02946	50	53.9	M+H	C6H11NO3	-1.464852019	21790.94138	22891.46837	24394.47455	22915.88252	21158.82686	20728.41865	22240.48707	23607.2036	22969.73765
4.11_294.1213n	295.1285294	4.114783333	pos	Tyrosylhydroxyproline	HMDB0029106	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		50	54.8	M+H, M+Na	C14H18N2O5	-1.083547902	35628.7815	36716.94996	39676.68325	45836.5201	41209.26067	42904.93767	44038.00993	49724.7683	48872.23488
6.05_309.1936n	310.2008757	6.0535	pos	(2E,5Z,7E)-decatrienoylcarnitine	LMFA07070016	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters			50	54.6	M+H, M+Na	C17H27NO4	-1.322987749	271105.3421	285334.1339	272045.5573	494341.4215	496032.8328	488187.5345	335359.2489	390943.7878	351659.4816
1.37_227.0771m/z	227.0771236	1.372566667	pos	Azacitidine	HMDB0015660	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		C11262	49.9	54.1	M+H-H2O	C8H12N4O5	-1.465413125	26908.53788	26475.45959	29243.1977	40377.22529	38332.88663	37199.20826	36125.64805	41279.50032	39211.25287
3.82_127.0399m/z	127.0399234	3.889633333	pos	4-PYRIDINIC ACID	44509	Organoheterocyclic compounds	Pyridines and derivatives	Pyranones and derivatives	***	C11918	49.9	53.8	M+H	C6H5O2	-0.326008927	14498.64079	12274.40396	13136.26018	11305.24491	12397.73752	11498.2042	11827.00377	12340.09749	12340.09749
4.75_118.0652m/z	118.0651764	4.7456	pos	Indole	HMDB0000738	Organoheterocyclic compounds	Indoles and derivatives	Indoles	***	C00463	49.9	52	M+H	C8H7N	0.433741748	11567.90615	11573.64671	11984.69868	11005.81569	10644.1369	10323.21608	11311.32295	10893.22538	11328.16694
4.79_197.0807m/z	197.0806529	4.7912	pos	3-(4-Hydroxy-3-methoxyphenyl)propionic acid	3803	Phenylpropanoids and polyketides	Phenylpropanoic acids	Unclassified			49.9	53.7	M+H	C10H12O4	-0.930353779	5020.595546	5448.030033	5558.840599	1932.66885	1721.625696	1730.768146	4088.663492	4630.037196	4599.08079
8.68_591.3131m/z	591.3130523	8.6834	pos	(3a,5b,7a)-23-Carboxy-7-hydroxy-24-norcholan-3-yl-b-D-Glucopy	HMDB0002430	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	*		49.9	54.1	M+Na	C30H48O10	-1.611904515	71073.54716	79299.25087	79709.30061	9916.108786	9989.044162	9505.410484	31793.19593	40402.04189	40441.81499
5.96_315.2770n	338.2659828	9.56185	pos	6-hydroxysphingosine	53903	Lipids and lipid-like molecules	Sphingolipids	Sphingoid bases			49.8	54.3	M+H-H2O, M+Na, M+H	C18H37NO3	-1.174552219	127975.095	117294.7827	104811.4772	125208.8261	127364.8493	128034.5862	129130.8121	118341.3199	108009.6211
0.76_129.0425n	147.0761505	0.758666667	pos	Pyroglutamic acid	HMDB0000267	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C01879	49.7	51.2	M+H, M+NH4	C5H7NO3	-0.957765458	123515.1117	118653.781	102219.9015	198758.23	192999.6208	190215.4628	146839.6884	124782.7144	132096.3866
8.41_278.2356n	274.2735595	8.405166667	pos	Cytidine triphosphate	41556	Lipids and lipid-like molecules	Sphingolipids	Sphingoid bases	*		49.7	54.1	M+H, M+Na	C18H35NO2	-1.816652216	374557.9648	348099.9573	386579.6381	331603.1466	298808.4363	279269.9092	439785.8779	439785.8779	439785.8978
1.42_218.0479m/z	218.0478587	1.415933333	pos	Tyramine-O-sulfate	58408	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		49.6	58.4	M+H	C8H11NO4S	-1.366422337	990.0228432	1239.190884	998.1228196	2580.280856	2317.122833	2469.745735	845.8797836	933.8420031	873.9667034
3.96_188.0683n	211.0574742	3.956866667	pos	Tetrahydro-2,5-furan-diacetic acid	HMDB0059767	Organic acids and derivatives	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives			49.6	50.5	M+H, M+Na, M+H-H2O	C8H12O5	-0.758291924	32616.77925	33831.7484	34480.93526	59320.45486	58311.14573	59664.69758	36148.14123	40159.67598	36594.25667
3.98_496.1212n	519.1104526	3.979183333	pos	4'-Methyl-(-)-epigallocatechin 3'-glucuronide	HMDB0041675	Phenylpropanoids and polyketides	Isoflavonoids	O-methylated isoflavonoids	*		49.6	55.1	M+H, Na	C22H24O13	-0.963441929	16734.67895	15771.05124	17958.51429	12035.7128	11447.3455	11526.7701	13355.20698	15905.49238	16542.09988
4.11_262.0951n	263.102261	4.114783333	pos	L-cis-Cyclo(aspartylphenylalanyl)	87613	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		49.6	51.2	M+H-H2O, M+H	C13H14N2O4	-0.830845757	7080.467191	6916.615077	7768.136581	8083.592867	7713.991549	7738.196877	6467.675081	7367.536728	6595.655073
8.57_303.1215n	304.1287357	8.561516667	pos	Indoxyl glucuronide	HMDB0013240	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		49.6	53.2	M+H-H2O, M+H	C15H17N3O4	-1.474022561	11943.14284	13051.42539	13491.84401	21289.18301	19405.018	19837.01418	10346.41333	11489.79352	11542.38951
5.84_240.1722n	223.1689355	5.843716667	pos	7-oxo-11E-Tetradecenoic acid	45868	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			49.6	52.5	M+H-H2O, M+H	C14H24O3	-1.336180161	28337.50734	28109.06337	29816.35642	25805.87035	25728.70439	26227.87809	29600.47758	31987.02448	32932.02253
0.80_132.0766m/z	132.0766282	0.796983333	pos	Creatine	7	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00300	49.5	50.2	M+H	C4H9N3O2	-0.951640491	14440.79147	14729.98156	15345.98066	19837.2739	19554.77633	20481.45859	13864.75299	15635.49196	15003.37529
1.16_149.0508n	150.0580582	1.157483333	pos	L-Methionine	26	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00073	49.5	56.6	M+H, M+Na	C5H11NO2S	-1.796970993	34009.74362	33360.68744	30973.47193	31509.22037	28158.24966	28455.502	28849.93123	29531.33357	26614.58586
2.42_99.0687n	122.0576695	2.421616667	pos	δ-Valerolactam	62467	Organoheterocyclic compounds	Piperidines	Piperidinones	*		49.5	51.5	M+H, Na	C5H9NO	2.742391279	17430.51396	19128.32257	19841.99231	3334.795026	3572.345704	3663.606222	13721.80191	18164.75517	15508.81633
3.85_229.1178m/z	229.1178167	3.845583333	pos	(S)-ATPA	69667	Unclassified	Unclassified	Unclassified	*		49.5	54.8	M+H	C10H16N2O4	-2.045979218	6668.003579	7040.432242	8365.760422	8332.915419	7953.01335	7542.623332	6462.012801	6607.464212	6896.468395
5.26_491.2634m/z	491.2633813	5.26135	pos	3,17-Androstanediol glucuronide	HMDB0010321	Lipids and lipid-like molecules	Benzenoids	Benzenes and substituted derivatives	*		49.5	54.9	M+Na	C25H40O8	3.934461226	6701.240178	7933.340984	7714.755332	3843.124663	3936.256486	4150.18391	6263.926436	6967.140161	7054.286517
5.35_208.1097n	209.1169842	5.351683333	pos	12-oxo-5E,8E,10Z-dodecatrienoic acid	74733	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			49.5	53.3	M+H-H2O, M+H	C12H16O3	-1.114031987	7944.008092	8540.843536	9044.15576	7452.971033	7637.874601	8029.777688	6144.728521	6451.173416	6494.430808
7.20_355.2626m/z	355.2625669	7.20385	pos	delta2-THA	74388	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			49.5	53.2	M+H	C24H34O2	-1.665128689	59091.22496	71895.89465	69526.58102	30865.06483	29225.75552	26648.61539	33697.1961	41909.99326	39374.89376
0.78_263.1113n	264.1185449	0.776966667	pos	Creatine riboside	HMDB0240254	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			49.4	53.4	M+H, M+Na	C9H17N3O6	-1.774091359	52637.53207	53194.4238	53555.46257	150332.8938	140332.5499	132355.9818	81080.52463	80905.12204	81391.74929
2.18_191.0580n	209.0917859	2.178633333	pos	Desmethyldeschlorobenzoyl Indomethacin	828	Unclassified	Unclassified	Unclassified			49.4	50.5	M+H, M+NH4	C10H9NO3	-1.346650625	17945.04335	18202.14157	19550.3395	25612.33368	24142.9026	24041.44132	22051.37733	25661.55388	23378.98724
6.61_155.0569n	156.0585445	5.4428	pos	4-Methylcoumarin	88418	Phenylpropanoids and polyketides	Coumarins and derivatives	Coumarins and derivatives	*		49.4	50.5	M+H	C10H8O2	-1.008355977	6915.596561	7125.150905	6916.396961	2540.449639	2653.167733	2617.204048	4378.752502	4778.198266	4436.403561
6.16_300.2166m/z	300.2166248	6.162416667	pos	3-hydroxynonanoyl carnitine	HMDB0061635	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		49.4	51.8	M+H-H2O	C16H31NO5	-0.977295601	96010.02485	103202.7721	108275.2603	149862.9709	153937.3513	147109.9906	99261.88119	134379.1805	117161.1563
8.28_490.2773n	513.2664596	8.280116667	pos	10-Hydroxy-octadec-12Z-enoate-9-beta-D-glucuronide	HMDB0060120	Lipids and lipid-like molecules	Saccharolipids	Unclassified	*		49.4	51.3	M+H-H2O, M+NH4, M+Na	C24H42O10	-1.101023301	107884.4883	122866.9902	126233.994	111379.4744	95921.02783	100982.7183	94507.03337	108737.5033	116890.8705
0.82_527.1573m/z	527.1572627	0.818116667	pos	1-Kestose	44694	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C03661	49.3	56.6	M+Na	C18H32O16	-1.969399707	62248.36081	59595.73285	57841.61382	41407.72213	36007.97218	36430.17093	27536.88133	25550.82914	26243.613
0.84_237.0303n	238.0375862	0.8386	pos	S-Cysteinosuccinic acid	86255	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		49.3	55.5	M+H, Na	C7H11NO6S	-1.680282805	27613.39841	27545.82795	28341.07372	31931.66079	31853.06004	29658.70772	22762.98675	25950.55126	24691.70047
1.14_198.0750m/z	198.0749951	1.137683333	pos	5-Acetylamino-6-amino-3-methyluracil	58239	Organic nitrogen compounds	Organonitrogen compounds	Arylamides	**	C16366	49.3	55.3	M+H-H2O, M+Na, M+H	C7H11N3O3	-1.529209717	13712.57292	14032.26176	15829.8242	13825.34332	11077.1908	10999.8249	11709.35519	9827.853076	10233.2958
1.29_270.1556m/z	270.1556467	1.285033333	pos	Arginylhydroxyproline	HMDB0028710	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		49.3	53	M+H-H2O	C11H21N5O4	-1.459836552	5548.10441	5863.546021	6115.881072	10316.04228	9910.740293	10006.17842	7032.988473	7804.150479	8020.554355
11.46_205.0857m/z	205.0857135	11.45555	pos	Monoisobutyl phthalic acid	HMDB0002056	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*		49.3	50.3	M+H-H2O	C12H14O4	-0.932739025	38753.93869	32677.71592	36447.04975	39458.16717	40068.18197	43464.41551	39689.77146	37468.16579	40635.41649
5.15_208.1098n	209.1171328	5.148116667	pos	(Z)-3-Oxo-2-(2-pentenyl)-1-cyclopenteneacetic acid	86789	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		49.3	52.5	M+H-H2O, M+H	C12H16O3	-0.765390577	3707.091149	3628.521097	3807.604073	5288.708466	5082.558927	5150.366993	4014.947855	4107.551755	3737.22333
1.22_238.0931m/z	238.0931434	1.22075	pos	Biopterin	247	Organoheterocyclic compounds	Pteridines and derivatives	Pterins and derivatives	*	C06313	49.2	57.9	M+H	C9H11N5O3	-1.359319631	2769.855114	3416.014082	3292.949885	3608.178964	3805.785781	4137.021544	2384.062526	3538.054881	3425.253408
14.86_143.0813m/z	143.0813079	14.86423333	pos	Piracetam	HMDB0256585	Unclassified	Unclassified	Unclassified			49.2	50.6	M+H	C6H10N2O2	-1.380174124	128018.7932	123383.9569	124225.0145	124738.1375	131793.3523	128156.8269	135761.4365	125161.6329	129119.3307
5.24_409.1460m/z	409.1459803	5.238862333	pos	8NAL-N-glucuronide	HMDB0060498	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		49.2	52.1	M+Na	C16H24N2O8+	1.087217857	20874.26826	30681.10754	21334.59178	22661.08216	29894.6137	30587.46019	22880.30625	22508.72947	
4.79_176.0704m/z	176.0704131	4.7912	pos	Betamiporon	HMDB0034250	Benzenoids	Benzene and substituted derivatives	Unclassified	*		49.1	48.5	M+H-H2O	C10H11NO3	-0.993950439	11133.05066	11103.1904	11716.85666	18065.6987	16268.15399	16047.18888	8649.382138	9971.567987	9571.555572
0.74_132.0534n	133.0606471	0.73955	pos	D-Asparagine	65674	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C01905	49	49.9	M+H, M+Na, M+H-H2O	C4H8N2O3	-0.919387325	16342.39581	13130.02027	13389.24879	23985.39584	23148.04971	21699.18998	18659.73485	17891.90688	18748.74584
2.34_237.0866m/z	237.0866195	2.342433333	pos	L-Formylkynurenine	HMDB0060485	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C02700	49	58.3	M+H	C11H12N2O4	-1.541168316	4795.567527	4996.2087	4457.792729	5905.600773	6748.700278	7141.916207	5734.173208	5951.721875	5525.233176
3.91_325.0300n	326.0372751	3.911966667	pos	Urothion	HMDB0002377	Organoheterocyclic compounds	Pteridines and derivatives	Pterins and derivatives	*		49	53.5	M+H, Na	C11H11N5O3S2	-1.023062547	11460.46109	12030.50737	13109.97411	16013.00262	16086.65208	13801.37363	11776.6578	13399.41741	13507.12503
5.26_320.1828n	320.1828402	5.26135	pos	Dinor-10-NO2-CLA	LMFA11120008	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			49	50.2	M+H	C18H27NO4	-1.308216051	5483.773621	5623.291676	54927.13792	30371.31577	29408.02311	29697.11557	40058.4073	42433.61981	43030.35512
0.70_175.1438m/z	175.1437963	0.698133333	pos	Tranexamic Acid	HMDB0014447	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		C12535	48.9	55.8	M+NH4	C8H15NO2	-1.960103825	67779.24971	71188.36112	73392.38245	78452.36483	83333.97938	81319.01935	72678.42085	72938.32417	73941.43186
0.74_137.0707m/z	137.0707365	0.73955	pos	Trigonellinamide	274	Organoheterocyclic compounds	Pyridines and derivatives	Pyridinecarboxylic acids and derivatives	**	C02918	48.9	54	M+H	C7H8N2O	-1.490767203	32260.56

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6.48_202.1435m/z	202.1434812	6.476883333	pos	(E)-10-Oxo-8-decenoic acid	LMFA01030949	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*	45.9	37.4	M+NH4	C10H16O3	-1.568145296	11128.19174	11460.34436	8824.330993	13522.93828	14150.68845	15718.45041	13033.37118	13582.98512	10734.14324
2.09_181.0493m/z	181.0492842	2.0913	pos	Monomethyl phthalate	58100	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives		45.8	32.2	M+H	C9H8O4	-1.3941975	6711.790346	7378.751699	7363.826586	6741.226891	6287.590692	6384.927878	5966.139615	6670.15621	6364.680221
2.50_221.0917m/z	221.0917411	2.499733333	pos	gamma-Glutaminyl-4-hydroxybenzene	HMDB0029451	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	45.8	36.4	M+H-H2O	C11H14N2O4	-1.375924002	26894.04452	27348.4063	28018.61823	21216.05861	21311.40128	22220.98807	27276.72121	31984.84749	30180.86478
5.98_213.1484m/z	213.1483751	5.97975	pos	10-Hydroxy-3,7-dimethyl-2E,6E-decadienoic acid	45792	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates		45.8	33.6	M+H	C12H20O3	-0.687398077	6551.7781	6270.810689	6688.209109	5388.713253	5845.406315	5809.596679	5665.43005	5866.164488	5576.992491
7.16_237.1482m/z	237.1481685	7.16055	pos	12,13-Dimethyl-5,14-dioxabicyclo[9.2.1]-tetradeca-1(13),11-dien-	LMFA07040039	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters		45.8	41.5	M+H	C14H20O3	-1.492612044	11998.55335	12017.37872	12378.03982	11953.02564	10820.53398	10408.58281	9696.583397	10579.68276	11238.37976
4.68_232.1904m/z	232.1904429	4.678916667	pos	12-hydroxy-10-dodecenoic acid	LMFA01050168	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates		45.7	36.3	M+NH4	C12H22O3	-1.294395516	3499.957166	3902.853805	4118.040794	3789.696873	3616.516676	4175.996188	3569.758175	3986.309923	3597.467112
15.06_447.0989m/z	447.0987776	15.05856667	pos	Paederoside	67939	Unclassified	Unclassified	Unclassified		45.6	56.2	M+H	C18H22O11S	7.215373555	24132.4102	62623.36605	29542.0522	144589.19	92029.46457	31829.93256	16914.28033	7053.94446	24422.94922
2.58_250.0931m/z	250.0931085	2.578	pos	Zidovudine	HMDB0014638	Nucleosides, nucleotides, and analogues	Pyrimidine nucleosides	Pyrimidine 2',3'-dideoxyribonucleosides	**	C07210	45.6	33.4	M+H-H2O	C10H13N5O4	-1.337399369	19729.92365	19934.20934	21014.34471	20465.94368	17386.38065	20049.37664	17148.71217	21479.84431	20553.31699
3.65_145.1333m/z	145.1332795	3.648783333	pos	N-Acetylcadaverine	6592	Organic acids and derivatives	Carboxylic acids and derivatives	Carboxylic acid derivatives	*	45.6	33.9	M+H	C7H16N2O	-1.804319325	276.9586018	288.3143063	331.0192119	531.7210302	395.5393209	403.2893362	1086.934038	1240.681659	1171.362904
5.50_328.2115m/z	328.2114579	5.49815	pos	O-sebacoylcarnitine	LMFA07070100	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters		45.6	32.1	M+H-H2O	C17H31NO6	-1.134305546	12876.6571	14929.64016	14599.21752	18877.0506	17452.49535	17918.69054	15787.22293	14940.63892	16085.00381
5.59_374.2532m/z	374.2531793	5.590966667	pos	O-(11-carboxyundecanoyl)carnitine	LMFA07070083	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters		45.6	34.5	M+H	C19H35NO6	-1.433198711	17349.00984	18819.56859	19250.76253	18794.78024	18743.98467	22302.99477	13606.70661	15797.73974	15136.21473
1.26_190.0475m/z	213.0369453	1.264483333	pos	2,4-dihydroxy-2-heptenedioic acid	36007	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates	**	C06201	45.5	33.2	M+H, M+Na, M+H-H2O	C7H10O6	-1.397172686	7501.540789	7922.567421	7922.03478	11754.18291	11308.4132	10976.87667	7237.53222	8385.832164	7759.501472
15.07_296.2579m/z	296.2579047	15.06696667	pos	10,12,14-octadecatrienoic acid	LMFA01030154	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates		45.5	32.5	M+NH4	C18H30O2	-1.800948032	189217.0018	194187.4336	184109.4235	201027.1778	215247.2304	208110.135	222286.6162	191751.5492	209406.4637
3.85_195.0762m/z	195.0762315	3.845583333	pos	2-Pyridylacetylglycine	1311	Unclassified	Unclassified	Unclassified		45.5	33.1	M+H	C9H10N2O3	-0.964383375	20754.17287	20526.02437	22634.08271	23371.68337	22466.66701	20844.73926	21089.46698	22915.75786	22646.11926
3.98_316.1752m/z	316.1751892	3.979183333	pos	3,7,8,15-Scirpenetetrol	HMDB0037560	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*	45.5	32.8	M+NH4	C15H22O6	-0.921678212	13251.05847	13980.33229	13892.67286	26472.08822	24297.81626	24595.89729	14322.96186	16554.01171	15802.16528
4.25_365.0838m/z	365.0838164	4.249833333	pos	6-[4-(2-carboxyethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxylic	HMDB0125169	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	45.5	35.1	M+Na	C15H18O9	-1.421799581	5913.295968	5651.530173	6438.269938	1311.043989	906.0160656	1111.609941	2703.677676	2689.673433	2692.63728
4.90_262.1212n	305.110293	4.904516667	pos	Tyrosyl-Threonine	86007	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	45.5	43.6	M+H, M+Na	C13H18N2O5	-1.377521262	30225.02256	33437.74054	31635.52686	38240.28378	36876.39701	37247.85038	29143.90001	34235.6237	32900.20174
0.58_191.1428m/z	191.1427572	0.576333333	pos	2,2,6,7-Tetramethylbicyclo[4.3.0]nona-1(9),4-dien-8-one	91722	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*	45.4	31.3	M+H	C13H18O	-1.495699866	409202.9858	332920.6479	272275.4884	182273.7664	176037.3917	159053.6723	276926.07007	224594.792	209502.0188
1.20_244.1540m/z	244.1540481	1.199716667	pos	1-((4-amino-2-propylpyrimidin-5-yl)methyl)-2-methylpyridinium	34498	Unclassified	Unclassified	Unclassified		45.4	40.4	M+H	C13H17N5	-6.678596613	2554.03182	3412.96315	3597.889909	4524.811754	3699.555875	4021.770324	3099.408999	4153.036564	4110.736307
10.16_191.1791m/z	191.1791443	10.16326667	pos	3,5,7-Trimethyl-2E,4E,6E,8E-undecatetraene	97470	Lipids and lipid-like molecules	Fatty Acyls	Hydrocarbons		45.4	32	M+H	C14H22	-1.487319861	4875.495295	3590.657627	10377.04936	4794.993113	1493.845248	3547.438367	10708.65201	5426.34303	2537.188943
4.20_268.1524m/z	268.152421	4.204866667	pos	Isovalerylcarnitine	LMFA07070076	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*	45.4	32.3	M+Na	C12H23NO4	2.007412303	11298.12475	10990.7668	11819.81626	12080.44212	10791.11114	11370.11861	11043.44608	12542.94357	12557.99917
4.43_118.0652m/z	118.0651714	4.42815	pos	2-Acetyl-4-methylpyridine	HMDB0037071	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds		45.4	36.4	M+H-H2O	C8H9NO	0.33848024	19885.80315	21531.84308	22072.28238	10065.97197	8813.203146	9003.151424	15253.3602	17387.65188	16418.9116
4.91_372.1052m/z	395.0944373	4.814066667	pos	Dihydroxyellagic acid 4-O-glucuronide	HMDB0041723	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	45.4	33.8	M+H, M+Na	C16H20O10	-1.208233006	17167.22995	20390.11351	4824.287233	4432.205656	4251.969986	14538.9077	16262.56813	15368.39404
5.22_460.1023n	461.1095981	5.21595	pos	Glycitein 7-O-glucuronide	96099	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavonoid O-glycosides	*	45.4	44	M+H, M+Na	C22H20O11	3.825658381	10591.88927	10778.24232	10553.61462	10213.27502	9392.789528	9136.546176	11724.30679	12696.71038	12967.19955
5.78_591.3169m/z	591.31693	5.778566667	pos	Urobilinogen	HMDB0004158	Organoheterocyclic compounds	Tetrapyrroles and derivatives	Bilirubins	**	C05791	45.4	30.2	M+H	-1.323849726	103559.8142	93026.36452	115069.7627	87073.99629	81295.03074	79773.74069	110705.966	120013.9814	111259.7797
6.91_387.2135m/z	387.2135191	6.909216667	pos	Sativic acid	HMDB0302836	Lipids and lipid-like molecules	Fatty Acyls	Octadecanoids		45.4	34.7	M+K	C18H36O6	-2.377131873	197700.1636	46676.00268	651267.2338	59921.78478	49959.18113	52389.68092	54593.34981	56721.86521	122841.1683
4.70_124.0887n	142.1224905	4.701116667	pos	2E,6E-Octadienal	46424	Lipids and lipid-like molecules	Fatty Acyls	Fatty aldehydes		45.3	29.4	M+NH4, M+Na, M+H	C8H12O	-1.208921058	20783.53609	19479.31509	19407.71221	19712.26997	20106.76045	19668.30314	21132.71	19376.51435	19829.9027
5.04_342.2270m/z	342.2269954	5.035783333	pos	Dinor-PGE2	LMFA03010210	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids		45.3	32.5	M+NH4	C18H28O5	-1.554907714	12038.48493	12532.00957	13502.77761	11071.818	10165.37179	9753.604358	10690.21311	11278.50546	10904.88801
5.24_308.1522m/z	308.1522478	5.238683333	pos	5-Amino-2,3-dihydro-6-(3-hydroxy-4-methoxy-1-oxobutyl)-2,2-dim	93249	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans		45.2	42.2	M+H	C16H21NO5	9.762783056	11186.01427	12592.11979	12832.50946	17116.22573	16587.27452	15846.04999	11631.84414	13162.23137	12987.27987
5.37_411.1621m/z	411.1621418	5.374266667	pos	beta-D-Glucopyranosyl-11-hydroxyjasmonic acid	HMDB0039964	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*	45.3	31.9	M+Na	C18H28O9	-1.059732199	29516.08728	31628.37745	33865.99411	39080.05377	39066.70696	39795.34102	28203.58401	28555.09696	29422.09545
5.93_180.1147n	198.1486514	5.933983333	pos	Jasmolone	HMDB0030039	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols	*	45.3	33.2	M+H, M+NH4	C11H16O2	-1.623606757	7117.285092	6988.778027	6543.63943	5625.116328	7284.615134	6898.125485	8095.771054	6260.712916	7439.808042
6.55_314.2321m/z	314.2320674	6.5509	pos	10-Deoxymethynolide	LMPK04000034	Lipids and lipid-like molecules	Polyketides	Macrolides and lactone polyketides	**	C11993	45.3	32.1	M+NH4	C17H28O4	-1.747299395	24171.97108	27429.19832	26306.91285	26116.24632	24764.54221	23350.22628	21583.1216	22942.27834	24269.08822
0.84_144.1017m/z	144.1017035	0.8386	pos	4-heptynoic acid	HMDB0103489	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates		45.2	35.3	M+NH4	C7H10O2	-1.598993884	214022.1863	216719.119	222076.7615	526218.2512	493773.0015	485020.6807	186660.1692	215927.7092	203141.3662
7.01_265.1848m/z	265.1848382	6.991666667	pos	gamma-Glutamyl-S-methylcysteine	88096	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	45.2	37.8	M+H	C9H16N2O5S	-1.631358034	24282.85161	2656.727584	2784.387764	2788.387764	2746.636504	2720.105067	2198.544554	2907.889033	
4.16_174.1486m/z	174.1486401	4.159533333	pos	3R-aminononanoic acid	35938	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates		45.2	42.9	M+H	C9H19NO2	-1.242869681	1398.592088	1176.083048	1464.41013	791.3982636	841.137446	905.1146634	1733.539526	1636.267641	1468.653514
5.10_306.1730m/z	306.173006	5.103066667	pos	Cetraxate	65612	Unclassified	Unclassified	Unclassified		45.2	39.6	M+H	C17H23NO4	9.90062322	1483.489807	1557.317565	1685.816627	2340.939087	2352.20138	2580.528079	2166.826051	1450.483178	1606.592882
5.54_141.1272m/z	141.1272015	5.543066667	pos	1-Nonen-4-one	91121	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds		45.2	34.1	M+H	C9H16O	-1.356651581	1541.896774	1692.417445	1621.049055	1441.015459	1291.819595	1285.373006	1552.859851	1471.337288	1480.149686
5.72_308.1852m/z	308.1852302	5.720466667	pos	Laurenobiolide	HMDB0036771	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*	C09492	45.2	31.5	M+NH4	C17H22O4	-1.394049847	8733.839836	8893.345776	8644.238421	7434.385154	7420.827306	7041.80051	10943.77323	9559.403213	9507.037116
7.48_469.1207m/z	469.1208353	7.480483333	pos	3,6,7-Trihydroxy-4'-methoxyflavone 7-rhamnoside	LMPK12111586	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides		45.2	29.2	M+H-H2O, M+H, M+Na	C22H22O10	-1.383521834	11796.4864	11879.44851	10477.38877	102892.9738	102399.1357	105580.8939	113026.4209	110656.4209	
8.10_203.1792m/z	203.1791811	8.104816667	pos	Preisocalamendiol	HMDB0035391	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		45.2	29.3	M+H-H2O	C15H24O	-1.117568936	4731.601826	4836.029457	5511.660414	2996.259829	3272.557507	3030.897417	4858.81628	5321.895218	4886.658826
0.88_203.1388m/z	203.1388011	0.8802	pos	N-Acetylisoputreanine	HMDB0094713	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		45.1	29.2	M+H	C9H18N2O3	-1.077283013	225849.1468	261568.8964	256116.6107	244011.9798	230421.3637	230046.138	210797.6002	226453.6485	218520.7442
14.70_388.1039n	371.1005737	14.70206667	pos	Eszopiclone	HMDB0014546	Organoheterocyclic compounds	Pyrrolopyrazines	Cyclopyrrolones		45.1	47.3	M+H-H2O, M+H	C17H17ClN6O3	-3.102803926	478431.3276	12459.91315	36048.66809	15906.55604	10569.41983	11490.33295	11973.72223	16898.87351	17655.27144
0.60_126.0913m/z	126.0912874	3.604716667	pos	2-Methyl-5-propyloxazole	92666	Organoheterocyclic compounds	Azoles	Oxazoles		45.1	27.6	M+H	C7H11NO	-0.423792801	8913.681491	9547.606513	10296.51457	12270.39173	10133.17066	10127.16475	9026.644643	11174.55063	9773.572156
4.05_135.0552m/z	135.0551748	4.046633333	pos	N1-Methyl-4-pyridone-3-carboxamide	HMDB0004194	Organoheterocyclic compounds	Pyridines and derivatives	Pyridinecarboxylic acids and derivatives	**	C05843	45.1	28.7	M+H-H2O	C7H8N2O2	-1.752506565	2746.657447	2895.686702	2982.525856	4538.413468	4233.314885	4391.151437	3017.831524	3430.169402	3429.702259
5.89_463.1837m/z	464.1909653	5.759966667	pos	Dihydromorphine-3-glucuronide	HMDB0060821	Alkaloids and derivatives	Morphinans	Unclassified	*		45.1	30.2	M+H, M+Na	C23H29NO9	-1.171627858	18345.65167	18979.56843	22341.92403	56899.06923	51657.80978	45584.82723	30696.59853		
6.61_312.2164m/z	312.216433	6.613233333	pos	2-trans,4-cis-Decadienoylcarnitine	HMDB0013325	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*	45.1	31	M+H	C17H29NO4	-1.612548764	52614.94657	51103.41133	58827.85938	97952.03142	88137.73656	79326.54458	45211.55082	52743.78803	52122.09013
10.16_135.1166m/z	135.1166296	10.16326667	pos	1-Isopropyl-2-methylbenzene	92028	Benzenoids	Benzene and substituted derivatives	Cumenes		45	32.6	M+H	C10H14	-1.471109764	1553.290561	1191.123231	2918.922889	1413.638763	756.123721	1135.115277	2889.019682	1421.740109	870.617258
2.70_100.0760m/z	100.0759541	2.699483333	pos	2,5-Dihydro-2,4-dimethyloxazole	95009	Organoheterocyclic compounds	Azolines	Oxazolines		45	28.6	M+H	C5H9NO	2.662657681	2049.649812	2696.98036	2449.621215	2146.583657	2566.733073	2260.920622	2969.557365	2806.076528	2865.548416
5.06_477.1724m/z	477.1724219	5.058233333	pos	1-(2-Hydroxyphenylamino)-1-deoxy-beta-D-gentiobioside 1,2-carl	HMDB0037551	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		45	32	M+NH4	C19H25NO12	2.006215424	2322.780596	2003.521179	2176.295347	8791.00472	7032.253996	7752.276324	2121.641352	2432.976353	2303.213768
5.79_413.1779m/z	413.1778699	5.790033333	pos	(+)-11-Epoxyol-9,10-dihydrojasmonic acid 11-beta-D-glucoside	LMFA09020206	Lipids and lipid-like molecules	Fatty Acyls	Octadecanoids		45	31.1	M+Na	C18H30O9	-0.854277677	10347.05751	12004.72308	18723.16251	15944.51652	14723.75785	8229.114809	9003.918803	9256.828612	
7.18_229.1255m/z	229.1254564	7.182883333	pos	(S)-Menthone 8-thioacetate	92305	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*	45	30.2	M+H	C12H20O2S	-0.968412751	2374.562011	2484.162195	2499.030445	3534.604226	3170.379797	3214.301097	1666.723262	1774.7741	2181.487991
3.24_322.1232m/z	322.1232472	3.238016667	pos	Saxitoxin	HMDB0029368	Phenylpropanoids and polyketides	Saxitoxins, gonyautoxins, and derivatives	Unclassified	*	C13757	44.9	28	M+Na	C10H17N7O4	-0.586736211	13354.14823	13523.06211	13144.45472	23058.89025	23697.09679	22942.39209	17751.78239	16632.75228	16952.95755
4.02_339.0951n	362.0841167	4.024633333	pos	5-Hydroxy-6-methoxyindole glucuronide	HMDB0010163	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C03033	44.9	30.1	M+H, M+NH4, M+Na	C15H17NO8	-0.805370258	13664.09027	14831.61366	15734.00524	16362.76096	14660.11488	15063.71071	12898.2802	13826.70194	14359.8577
4.59_162.0548m/z	162.0548055	4.58805	pos	Indole-3-carboxylic acid	HMDB0003320	Organoheterocyclic compounds	Indoles and derivatives	Indolecarboxylic acids and derivatives	***	C19837	44.9	28.5	M+H	C9H7NO2	-0.927645752	3233.306784	3470.189607	3440.007284	3816.714912	3896.82797	3584.015429	3129.401137	3236.611141	3273.079699
7.56_257.2259m/z	257.2259314	7.553266667	pos	5α-Androst-16-en-3α-ol	41837	Unclassified	Unclassified	Unclassified		44.9	29.5	M+H-H2O	C19H30O	-1.625946065	7078.742009	6629.392507	6197.403051	8817.083544	9042.540175	9031.616127	5968.841648	6564.300988	5729.782304
3.80_298.1621m/z	298.162123	3.80375	pos	Hydroxyhomocarnitine	LMFA07070072	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*	44.8	32.3	M+Na	C13H25NO5	-1.346770103	1515.974909	1667.950987	2035.191781	3416.453417	2950.218234	2991.785491	1691.137712	2165.629944	1993.180398
4.45_342.1697m/z	342.1696767	4.451133333	pos	1-(2,5-dihydro-6,8-dihydroxy-3-methyl-1-benzoxepin-7-yl)-3-pheny	LMPK12120501	Unclassified	Unclassified	Unclassified		44.8	28.4	M+NH4	C20H20O4	-0.950128486	280.966502	2607.805011	2347.627511	1693.450972	3236.583055	808.8867825	3022.933593	3135.87746	1932.0747
4.90_204.0785n	205.0856994	4.904516667	pos	3-Butylidene-7-hydroxyphthalide	68011	Organoheterocyclic compounds	Isocoumarans	Isobenzofuranones	*	44.8	36.4	M+H-H2O, M+H	C12H12O3	-0.808674791	5124.26453	5063.181727	5753.445035	1463.155691	1274.879659	1521.070723	1700.549388	1653.966844	1736.227625
4.99_154.0991n	172.1329179	4.993181667	pos	4-oxo-2-Nonenal	45397	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds		44.8	34.5	M+H, M+NH4, M+H-H2O	C9H14O2	-1.72599608	415174.7066	398884.1732	396757.4793	396008.9017	415784.1037	401460.0218	450106.7564	401660.7343	422683.4388
5.28_269.1624n	270.1696273	5.284233333	pos	Tetranor-8-NO2-CLA	LMFA01120009	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates		44.8	28.8	M+H, M+Na, M+H-H2O	C14H23NO4	-1.327460501	73697.28059	76795.03505	81831.4099	43107.10522	37463.96053	38217.25616	42790.43493	47922.54445	47890.773
4.40_221.1534m/z	221.1533547	5.396716667	pos	Tetradec-11-ynedioic acid	LMFA01031094	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates		44.8	29.9	M+H	C14H22O4	-1.142734162	4243.525893	5021.045275	5358.654857	4088.473464	4471.348504	4482.243664	4323.983249	4492.543329	4622.502033
6.84_338.2320m/z	338.2319732	6.8409	pos	Oryzalide A	HMDB0037591	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*		44.8	30	M+NH4	C19H28O4	-1.910523778	39579.12635	38546.30216	41714.78027	73839.75825	74933.64043	65878.63072	38008.68186	38748.17834	40926.42771
8.48_230.2475m/z	230.2474936	8.4786	pos	Xestoaminol C	53933	Lipids and lipid-like molecules	Sphingolipids	Sphingoid bases		44.8	28.8	M+H	C14H31NO	-1.515669295	16749.81561	16005.25067	18934.9479	17702.78186	17103.57837	26442.00907	19717.1518	12218.08344	22009.31949
8.48_342.2633m/z	342.2633336	8.4786	pos	2-Hydroxylauroylcarnitine	LMFA07070032	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*	44.8	30	M+H-H2O	C19H37NO5	-1.534786642	44848.47782	48929.53552	59721.27662	41437.02425	38194.0844	40896.34132	38086.25829	36895.82883	39182.71355
10.88_295.2508n	318.2399399	10.8797	pos	(4E,8E,10E-d18:3)sphingosine	LMSP01080013	Lipids and lipid-like molecules	Sphingolipids	Sphingoid bases		44.7	28.7	M+H, M+Na, M+K	C18H33NO2	-1.113092994	433425.0745	409307.2653	400522.4065	429273.0816	444408.6786	441836.3843	447744.3782	427333.6207	430621.5706
13.11_270.2787m/z	270.2786618	13.10638333	pos	2-E-Heptadecenal	HMDB0000228	Lipids and lipid-like molecules	Fatty Acyls	Fatty aldehydes		44.7	28.4	M+H	C17H32O	-1.900565075	2774.525893	5021.045275	5358.654857	4088.473464	4471.348504	4482.243664	4323.983249	4492.543329	4622.502033
2.48_290.1594m/z	290.1594097	2.484216667	pos	3-Methylglutarylcarnitine	HMDB0000552	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*	44.7	28	M+H	C13H23NO6	-1.397998048	14927.36998	17851.85578	16553.47822	33283.43662	32033.27789	34264.60543	18148.77532	20044.16477	20569.6375
4.45_181.0970m/z	181.096977	4.451133333	pos	L-2-Amino-3-(4-aminophenyl)propanoic acid	86943	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	44.7	28.8	M+H	C9H12N2O2	-0.983192211	5067.120682	6435.028696	6745.962541	638.7008741	722.8911179	673.2110683	1178.778289	1299.029058	1193.823756
5.58_312.2086n	313.2157439	5.581883333	pos	Ethisterone	HMDB0060580	Lipids and lipid-like molecules	Steroids and steroid derivatives	Androstane steroids	*	C14487	44.7	28.3	M+H-H2O, M+H	C21H28O2	-0.911707295	7479.696819	6905.590278	8682.301028	10367.01277	9706.153013	10784.99521	7392.206001	7348.45888	7263.473832
5.01_462.0792n	485.0683695	5.013433333	pos	5,6,7,2'-Tetrahydroxyflavone 7-glucuronide	LMPK12111077	Unclassified	Unclassified	Unclassified		44.6	29	M+H, M+Na	C21H18O12	-1.273703667	4375.640898	3957.858207	4592.032346	24342.76982	22684.94594	21624.54994	7085.646418	8202.432767	7480.172801
7.51_318.2093m/z	318.2092823	7.50885	pos	Glycopyrrolate	3132	Benzenoids	Benzene and substituted derivatives	Unclassified		44.6	37.5	M+H	C19H27NO3	9.180705082	38667.15959	38247.49035	44511.15034	33275.14536	34547.15315	33911.2938	21293.80161	25301.41093	24023.1439
11.41_322.1062m/z	322.1062304	1.807733333	pos	gamma-L-Glutamyl-L-cysteinyl-beta-alanine	66204	Unclassified	Unclassified	Unclassified		44.5	32.7	M+H	C11H19N3O6S	-1.564550725	4496.544068	4774.101276	4800.007135	12377.32759	11726.91623	9911.485966	5882.747596	6451.001913	5635.621637
4.75_138.1045n	121.1011946	4.7456	pos	(2E,6E)-2,6-Nonadienal	HMDB0031261	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*	44.5	26.7	M+H-H2O, M+H	C9H14O	0.128502248	5227.134082	5113.698296	5643.665942	4622.101157	3977.469264	4264.061265	5002.419222	5015.420318	4949.683319
5.70_218.1668n	219.1740967	5.69755	pos	6,8,10,12-pentadecatetraenal	75363	Lipids and lipid-like molecules	Fatty Acyls	Fatty aldehydes		44.5	26.7	M+H-H2O, M+H	C15H22O	-1.316187858	6074.641682	5403.975104	4781.91543	4195.201333	4358.703696	3925.418986	6350.768377	5749.907962	5655.750086
7.33_210.1253n	211.1325679	7.332033333	pos	(-)-Jasmonic acid	3345	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C08491	44.5	26.9	M+H, M+Na	C12H18O3	-1.441903547	105473.2534	99983.39129	87238.98094	104526.1771	118181.9724	112077.1515	116765.5264	108423.3012	114430.2527
9.93_119.0856m/z	119.0856355	9.9276	pos	alpha-Methylstyrene	70026	Benzenoids	Benzene and substituted derivatives	Phenylpropenes		C14395	44.5	27	M+H	C9H10	0.920870983	3550.065139	2756.517277	3752.091635	4315.431151	2317.262593	2797.977989	2687.875245	2341.47518	3502.200099
13.37_174.1275m/z	174.1274784	13.37201667	pos	Pestalotiollide A	HMDB0256280	Unclassified	Unclassified	Unclassified		44.4	26.2	M+H	C12H17NO	-1.295063322	107955.6143	137334.9302	127776.4812	140707.2375	149603.6314	154155.6168	151694.6434	141590.8338	145995.588
15.06_264.0897m/z	264.0896504	15.05856667	pos	Cyprodinil	HMDB0034853	Benzenoids	Benzene and substituted derivatives	Aniline and substituted anilines		C10914	44.4	36.3	M+K	C14H15N3	-0.467172217	665.1880719	11612.24535	1698.355409	1787.406924	1074.692086	810.9968961	609.0041629	614.0982187	475.2702151	
3.67_197.0667m/z	197.0666892	3.671416667	pos	1,9-Dimethyluric acid	58078	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	*		44.4	31.6	M+H	C7H8N4O3	-1.159508162	70238.20118	71630.5742	75686.56983	103526.9311	87291.85511	80021.29121	69383.47865	74881.38069	78134.18046
3.85_120.0444m/z	120.0443893	3.845583333	pos	2-Aminobenzoic acid

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7.14_391.1354m/z	391.1354116	7.13965	pos	b-D-Glucopyranosiduronic acid, 6-(3-oxobutyl)-2-naphthalenyl	1377	Unclassified	Unclassified	Unclassified			40.8	20	M+H	C20H22O8	-8.542003539	12290.82239	14849.20223	14439.58428	23437.84549	22689.75812	22763.43287	15337.0055	16398.52561	15541.6534
0.90_157.0737n	175.1074828	0.898483333	pos	Ethadione	HMDB0031876	Unclassified	Unclassified	Unclassified			40.7	7.8	M+H, M+NH4	C7H11NO3	-1.190473162	56616.58465	58958.73331	60716.87573	33548.07028	31090.68807	29593.38664	38446.18169	41126.30339	39530.78504
14.87_231.1238m/z	231.1237713	14.87405	pos	Prenyl glucoside	HMDB0031876	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*	C09808	40.7	11.2	M+H-H2O	C11H20O6	4.317255213	141210.0473	139047.926	136663.5175	145158.9756	151748.2457	147361.2663	154706.5586	143398.504	151298.1676
4.07_214.1546m/z	214.1546371	4.069116667	pos	Fasoracetam	HMDB0252174	Unclassified	Unclassified	Unclassified			40.7	20.9	M+NH4	C10H16N2O2	-1.8673683	430.2137286	544.188855	423.5294178	496.3107679	1971.834306	689.965744	310.9677001	310.5825908	711.0244227
4.45_207.1378m/z	207.1378205	4.451133333	pos	3-Acetoxy-3-methyl-1-phenylbutane	90021	Benzenoids	Benzene and substituted derivatives	Unclassified			40.7	12	M+H	C13H18O2	-0.658434291	5216.079345	4813.492032	4793.302626	4039.84965	3640.625008	3193.967074	4210.146483	3746.456167	3693.770348
5.08_182.1901m/z	182.1901263	5.081	pos	Dicyclohexylamine	70260	Unclassified	Unclassified	Unclassified			40.7	7.54	M+H	C12H23N	-1.103159883	8454.122125	6898.580526	5769.619411	7072.250229	4385.419947	4444.441229	6525.962792	6310.755087	5643.491285
5.26_261.1726n	262.179848	5.26135	pos	Bufuralol	HMDB0249434	Unclassified	Unclassified	Unclassified			40.7	7.97	M+H+H2O, M+H	C16H23NO2	-1.13322494	18782.84891	20770.3287	20986.87024	12287.26029	11855.08869	11733.10059	15267.20906	16961.71499	16179.52176
6.15_416.1547m/z	416.1546581	6.149866667	pos	6'-Apiosyllotaustralin	HMDB0034207	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			40.7	11.7	M+Na	C16H27NO10	4.937769356	11614.58642	13636.66015	13670.074	8374.165749	8925.794616	8210.92483	7942.00756	10617.46984	9158.502045
0.72_265.1112m/z	265.1112061	0.717716667	pos	Thiamine	229	Organoheterocyclic compounds	Diazines	Pyrimidines and pyrimidine derivatives	**	C00378	40.6	15.3	M+H	C12H16N4OS	-2.092085632	2538.594472	1837.78513	2828.655079	6430.01294	5498.929822	4544.886143	1566.230851	2033.040592	2009.445676
1.16_152.0332n	153.0404607	1.157483333	pos	Oxypurinol	866	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	*	C07599	40.6	8.04	M+H, M+NH4	C5H4N4O2	-1.585730302	25585.04108	28652.83443	29106.48069	32306.22755	32006.69539	32382.11181	22337.9238	25547.8776	24728.92523
1.52_455.1296m/z	455.1295914	1.52285	pos	Pinostrobin 5-O-glucoside	LMPK12140143	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides			40.6	22.7	M+Na	C22H24O9	-3.845036318	7052.926554	7356.771885	7923.132322	5597.541932	6111.537123	5396.344318	5761.319577	7899.898037	6861.171298
1.61_247.1662m/z	247.1661827	1.611133333	pos	R-cucujolide III	LMFA07040047	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters			40.6	21.1	M+Na	C14H24O2	-2.97991879	1420119.3392	135687.8943	132340.8328	129827.0323	142569.042	139320.0916	136717.0413	131931.5894	137949.8759
1.74_180.1017m/z	180.1017477	1.741883333	pos	2,3-Dihydro-5-(3-hydroxypropanoyl)-1H-pyrrolizine	94562	Organoheterocyclic compounds	Pyrrolizines	Unclassified			40.6	7.96	M+H	C10H13NO2	-0.879012458	5644.872169	5693.458519	6438.316711	2014.481322	1883.593619	1902.358103	980.2268149	1107.138782	933.6316742
12.91_226.9511m/z	226.9511312	12.90603333	pos	3-Chloro-2-methylidenelactone	HMDB0060368	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*	C18309	40.6	33.1	M+K	C7H5ClO4	1.791708206	780009.9342	779833.6351	800671.7568	827392.1935	865290.3965	858523.2457	819043.6141	865354.4337	
14.90_123.0916m/z	123.0915867	14.89778333	pos	2-Ethyl-5-methylpyrazine, 9Cl, 8Cl	HMDB0041568	Organoheterocyclic compounds	Diazines	Pyrazines			40.6	11.7	M+H	C7H10N2	-0.721405049	1111.945128	1031.356246	1335.706844	1433.969717	894.8008858	1141.111768	1812.803795	1202.192673	1156.723252
2.07_151.0612m/z	151.0612391	2.069333333	pos	7-Methylhypoxanthine	HMDB0003162	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives			40.6	6.74	M+H	C6H6N4O	-1.32030489	25123.27562	25231.82156	27495.32015	28596.99798	27132.00461	26175.5162	23917.93865	27329.45404	25281.96067
2.16_240.0854n	241.0927115	2.157266667	pos	D-glycero-L-galacto-Octulose	HMDB0029954	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			40.6	9.27	M+H, M+Na	C8H16O8	3.821968265	19016.5407	20027.31967	21475.04195	26902.18886	25341.06354	24240.75577	20554.64212	23910.6333	22068.92649
4.43_343.1382m/z	343.1382316	4.42815	pos	Veratrostin A	95141	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*		40.6	9.55	M+H	C16H22O8	-1.497927087	4687.001998	5642.31011	5706.359604	6930.226428	5785.619624	5675.359102	5653.510175	6832.269082	5737.019517
5.82_226.1435m/z	226.1434625	5.821	pos	Jasmine ketolactone	LMFA08030150	Organoheterocyclic compounds	Oxocins	Unclassified	*		40.6	7.82	M+NH4	C12H16O3	-1.477162394	6393.475903	6377.946879	8091.52756	2752.045462	2847.026583	2662.782437	3963.492816	5104.285821	5300.169564
6.34_400.2688m/z	400.2688448	6.339133333	pos	(5Z)-13-carboxytridec-5-enoylcarnitine	LMFA07070018	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters			40.6	9.47	M+H	C21H37NO6	-1.301171578	27298.8861	32565.6705	34311.47823	33166.18965	33143.57808	30631.34395	19527.82242	24926.69925	23777.51088
1.35_173.1163n	174.1235334	1.350266667	pos	apo-[3-methylcrotonoyl-CoA:carbon-dioxide liqase (ADP-forming	HMDB0059607	Organic acids and derivatives	Carboximidic acids and derivatives	Carboximidic acids			40.5	7.75	M+H, M+Na	C7H15N3O2	-0.98047835	33244.51235	45454.20371	40636.86187	45520.20862	46821.27982	88213.84281	23129.106	25745.08231	28509.13764
14.79_136.0214m/z	136.0213578	14.79195	pos	Benzothiazole	HMDB0032930	Organoheterocyclic compounds	Benzothiazoles	Unclassified			40.5	6.6	M+H	C7H5NS	-1.398008907	339945.954	314808.6257	314641.252	326449.8742	348655.756	348345.6043	341098.6856	324708.2764	333542.1
2.70_270.0531m/z	270.0531189	2.004416667	pos	4-Hydroxydiflamethoxazole	HMDB0060529	Benzenoids	Benzene and substituted derivatives	Benzenesulfonamides	*		40.5	14.5	M+H	C10H11N3O4S	-4.402253367	5882.159785	5780.763145	6316.602888	2819.469841	2499.694042	2468.402452	2904.070426	3479.519645	2952.40672
4.09_282.1675n	305.1566805	4.091916667	pos	Hexaethylene glycol	HMDB0061822	Organic oxygen compounds	Organooxygen compounds	Ethers			40.5	7.47	M+H, M+Na, M+NH4	C12H26O7	-1.219706711	37706.61765	39603.22724	35105.26439	51757.62901	34846.75799	34170.65125	37443.76282	36893.79357	37933.30722
4.45_423.1619m/z	423.1618554	4.451133333	pos	Corchoionoside B	HMDB0030975	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		40.5	10	M+Na	C19H28O9	-1.743624575	9863.908117	9465.865012	10444.65191	5624.024483	4329.495852	4909.779222	7118.683011	7914.162072	7404.372688
4.70_289.1132m/z	289.1132	4.701116667	pos	11-dimethylaminoyl-undecanoic acid	HMDB0000037	Lipids and lipid-like molecules	Fatty Acyls	Other Fatty Acyls			40.5	11.9	M+H+H2O	C13H27AsO3	-3.684911939	4165.498008	4197.755344	4147.88401	8170.545839	8403.888359	8028.598852	3704.669082	4060.171858	4165.903681
5.06_372.2376m/z	372.237607	5.058233333	pos	5-hydroperoxy-7-[3,5-epidioxy-2-(2-octenyl)-cyclopentyl]-6-hepter	LMFA01040028	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			40.5	8.28	M+NH4	C19H30O6	-1.290937623	6087.383947	6101.223125	6899.408349	12510.56509	11441.8122	11442.49772	4665.3537	5485.300171	5491.115345
5.70_215.1519n	238.1409668	5.69755	pos	N-Nonanoylglycine	HMDB0013279	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		40.5	8.58	M+H+H2O, M+Na, M+H	C11H21NO3	-0.978753504	13318.46177	11589.3801	10989.16365	11286.98706	13375.00407	11301.69069	13795.99019	10884.75737	11890.48617
8.51_158.1537m/z	158.1537248	8.509533333	pos	(3Z,6Z)-3,6-Nonadien-1-ol	HMDB0030957	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		40.5	5.82	M+NH4	C9H16O	-1.540609948	15047.02263	13859.06115	13470.20813	15227.93378	16414.5241	15039.39412	16211.10783	14314.68232	15418.95813
1.24_119.0161m/z	119.0161317	1.243033333	pos	Dihydro-4-mercapto-3(2H)-furanone	94335	Organoheterocyclic compounds	Dihydrofurans	Furanones			40.4	8.48	M+H	C4H6O2S	0.041033978	1686.016796	1989.439079	2044.644048	993.8618261	960.2348463	962.8793258	1078.139258	1172.276454	1142.5645
1.44_183.0510m/z	183.0509947	1.438283333	pos	7-Methyluric acid	HMDB0011107	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	**	C16355	40.4	7.13	M+H	C6H6N4O3	-1.493059462	8214.153773	9321.793512	9344.867674	12092.84992	10417.29404	11431.64909	9638.918362	10881.44466	10441.76288
4.25_252.1203m/z	252.120289	4.249833333	pos	Butenylcarnitine	HMDB0013126	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		40.4	6.23	M+Na	C11H19NO4	-1.48292597	2574.825613	2795.038315	2735.38392	1663.486047	1623.622952	1495.480202	2292.913356	2470.105155	2418.548813
4.43_275.0108m/z	275.0108488	4.42815	pos	Cysteinyl-Aspartate	HMDB0028771	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		40.4	15.9	M+K	C7H12N2O5S	4.228973651	4868.488968	5314.08244	5519.991267	2353.170627	2274.414306	2346.767846	3580.388405	4116.645411	3669.455616
4.99_291.1971m/z	291.1907342	4.991816667	pos	1-nitro-1-undecene	HMDB0062669	Organic oxygen compounds	Alkyl-type 1,3-dipolar organic compounds	Alkyl-type 1,3-dipolar organic compounds			40.4	6.41	M+NH4	C11H21NO2	-1.607903789	9973.98486	18839.0434	18645.66675	18336.62976	19840.7495	18634.76386	19931.69224	20770.41681	19931.69224
0.64_159.1489m/z	159.1489118	0.63615	pos	(R)-Pelletierine	HMDB0030324	Organoheterocyclic compounds	Piperidines	Unclassified	*		40.3	6.03	M+NH4	C8H15NO	-1.968614659	20285.86092	25848.47255	27731.13387	22197.68568	19507.44762	21604.69398	18326.84889	26611.23054	25386.31125
1.14_146.0922m/z	146.0921577	1.137683333	pos	4-amino-4-cyano-butanoic acid	LMFA01100037	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates	**	C05715	40.3	9.72	M+NH4	C5H8N2O2	-1.91612674	63147.33854	51681.80912	61602.01079	66488.16435	52521.43687	47208.85691	57050.34438	65352.11904	64119.3835
1.14_178.0530m/z	178.0530019	1.137683333	pos	Cycloalliin	HMDB0029417	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	*		40.3	7.45	M+H	C6H11NO3S	-1.348389207	5819.91418	6265.279343	6345.773315	3385.507355	3334.81325	3630.342216	4955.017569	6199.921189	5738.320468
10.05_304.2995m/z	304.2994536	10.04765	pos	BENZALKONIUM	HMDB0061822	Unclassified	Unclassified	Unclassified			40.3	7.94	M+H	C21H37N	-1.3947253	10983.58993	2455.944338	1475.865091	1298.811104	3698.783073	1217.94913	1562.226027	1550.265813	1435.059891
3.54_175.1228m/z	175.1227693	3.55	pos	4-Methyltryptamine (AMT)	3310	Unclassified	Unclassified	Unclassified			40.3	14.6	M+H	C11H14N2	-1.180895125	3205.2	4178.579973	3728.422998	1766.488501	1811.798764	2105.207022	1966.256707	2165.811167	2165.811167
4.09_132.0443m/z	132.0442973	4.091916667	pos	NAPQI	HMDB0060946	Organic nitrogen compounds	Organonitrogen compounds	Imines	*		40.3	4.43	M+H-H2O	C8H7NO2	-0.623188882	3711.799603	3997.824164	4189.566543	236.5939214	262.4639479	263.1525158	3471.594111	3962.845434	3623.230382
4.72_135.0439m/z	135.0439172	4.723666667	pos	ortho-Hydroxyphenylacetic acid	HMDB0000669	Benzenoids	Benzene and substituted derivatives	Phenylacetic acids	**	C05852	40.3	11.3	M+H-H2O	C8H8O3	-0.91204185	40668.71061	42257.09052	43198.64015	19363.01094	18386.13233	18464.58047	33472.81779	37106.70147	35491.17013
4.93_288.0837m/z	288.0837144	4.927016667	pos	N-Phenylacetylglutamic acid	HMDB0059772	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			40.3	8.97	M+Na	C13H15NO5	-1.995064042	2547.691366	2491.890653	2462.311832	4049.427518	4184.551196	4597.287093	2795.229814	3013.246195	2877.356891
5.40_254.1384m/z	254.1384287	5.396716667	pos	8-Azaspiro[4.5]decane-8-butanoic acid, 7,9-dioxo(buspirone met	1452	Unclassified	Unclassified	Unclassified			40.3	7.87	M+H	C13H19NO4	-1.01045025	2938.337256	2908.660937	3282.286295	5683.249668	5171.495697	5520.906676	2719.323116	3107.857912	3226.809066
0.86_233.1241m/z	233.1240566	0.859583333	pos	L-Acetopine	HMDB0039111	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			40.2	6.05	M+H	C9H16N4O4	-1.615078508	16773.36671	18559.12665	18991.10372	8758.762162	10169.13041	10494.31934	13917.25818	13373.28843	12991.10093
0.92_250.0375m/z	250.0375401	0.898483333	pos	4-Hydroxyphenylacetic acid sulfate	HMDB0240441	Organic acids and derivatives	Carboxylic acids and derivatives	Arylsulfates			40.2	13.6	M+NH4	C8H9O6S	-1.915617269	3241.645491	3565.979223	3962.055896	6584.726859	5897.922078	5612.543596	4456.888691	5098.777132	4961.57079
1.42_152.9947m/z	152.9947146	1.415933333	pos	3-oxo-4-pentenoic acid	LMFA01060166	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			40.2	3.79	M+K	C5H6O3	-1.206256944	341240.5232	324366.1895	310767.3918	321009.5641	338307.1548	330268.2138	351021.197	319527.7559	330148.7549
1.50_301.1406m/z	301.1405638	1.500483333	pos	Glyceryl 5-hydroxydecanoate	HMDB0032297	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		40.2	6.85	M+K	C13H26O5	-2.357959909	227275.0935	209789.7318	199158.3839	205491.4566	217112.9587	211273.5693	237562.6149	209582.4457	215256.2474
3.85_253.1155m/z	253.1154585	3.845583333	pos	Valylhydroxyproline	HMDB0029128	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		40.2	9.43	M+Na	C10H18N2O4	-1.8219	1643.290021	2612.688013	2207.322057	2848.287015	1918.562916	2406.58368	2625.604995	2952.58071	3112.145585
3.91_257.0695n	258.0768063	3.911966667	pos	1,3,5-Trihydroxy-10-methylacridone	95860	Organoheterocyclic compounds	Quinolines and derivatives	Benzoquinolines			40.2	11.8	M+H, M+Na	C14H11NO4	2.808855857	5624.143672	6296.883974	6310.756082	19949.20614	18158.93886	17635.28136	20137.0042	22958.94775	22130.76907
4.41_572.1850n	572.1922664	4.4062	pos	Amorphigenin C-glucoside	48015	Lipids and lipid-like molecules	Prenol lipids	Flavonoids			40.2	15.4	M+NH4	C29H32O12	-7.613724114	74166.89894	85616.899	80851.25009	47611.97824	45672.74663	47092.56108	90982.18308	90008.0274	92899.36274
4.45_270.0762m/z	270.0761966	4.451133333	pos	9-(2-Phosphonomethoxypropyl)adenine	HMDB0247572	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives			40.2	7.03	M+H-H2O	C9H14N5O4P	3.986043291	555.1858598	1449.614075	1622.550535	2960.018461	2793.406858	2443.047276	4197.566949	5541.14457	4037.079006
4.79_273.1305m/z	273.1304656	4.7912	pos	7,8-Dihydroneopterin	HMDB0002275	Organoheterocyclic compounds	Pteridines and derivatives	Pterins and derivatives	**	C04874	40.2	8	M+NH4	C9H13N5O4	-0.446381401	9336.901165	8713.513249	8527.479349	9850.728021	3545.2737	4411.566009	5433.236124	6132.136093	5119.165443
1.16_170.1051n	193.0969059	1.157483333	pos	(3xi,6xi)-Cyclo(alanylvalyl)	HMDB0033926	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			40.1	4.73	M+H, M+Na	C8H14N2O2	-2.60263143	1000.435202	932.0028924	862.7724119	20291.27958	17068.13364	17482.47297	1916.4206	2006.410277	2015.802936
1.81_220.0635m/z	220.0635047	1.807733333	pos	3-ethylphenyl Sulfate	HMDB0062721	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		40.1	5.78	M+NH4	C8H10O4S	-1.488212577	35379.97305	37453.41709	38302.19341	26279.57901	23781.79261	23685.54324	37905.0045	44017.87579	39219.81039
13.12_104.1073m/z	104.107262	13.12308	pos	Neurine	87532	Unclassified	Unclassified	Unclassified			40.1	9.38	M+H	C5H13NO	2.634105976	71470.6223	57.68582722	28.48922258	34.0652706	18.40229428	27.05511869	475.1350792	8.300441669	33.66065631
13.67_271.2740m/z	271.2740187	13.67386667	pos	Palmitoleamide	LMFA08010010	Lipids and lipid-like molecules	Fatty Acyls	Fatty amides			40.1	5.34	M+NH4	C16H31NO	-1.466933298	13073.95584	12828.01243	13617.46999	13223.78686	13430.21534	12340.59332	14602.3768	13038.05265	12172.6826
3.76_177.0787n	195.1126586	3.759483333	pos	5-[2H-Pyrrol-4-(3H)-ylidenemethyl]-2-furanmethanol	HMDB0040045	Organoheterocyclic compounds	Heteroaromatic compounds	Unclassified			40.1	12	M+H-H2O, M+NH4	C10H11NO2	-1.290990992	7997.344077	9055.339707	8756.552607	6411.798398	6277.485743	5968.2818	7271.422156	7813.619484	7446.132043
4.09_371.0942m/z	371.0941753	4.091916667	pos	Isoferuloyl C1-glucuronide	96107	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	*		40.1	14.1	M+H	C16H18O10	-8.370660642	6188.754876	6647.288219	7434.207096	5875.232898	5322.723649	5060.32919	5108.827542	6167.000852	5856.564254
5.93_130.1226m/z	130.1225629	5.933983333	pos	2-Methylcyclohexanone	HMDB0031539	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		40.1	2.57	M+NH4	C7H12O	-0.692618264	2572.818276	2129.90367	2188.88158	2174.466264	2663.403539	2469.580745	2898.966554	2148.983295	2593.906404
0.92_248.1487m/z	248.1487128	0.91985	pos	3-hydroxybutyrylcarnitine	LMFA07070037	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		40	9.76	M+H	C11H21NO5	-2.170386253	1483.113861	1792.623725	2143.844938	4377.643887	4624.712903	5060.612175	2592.290741	2414.118625	2227.347102
10.31_184.9853m/z	184.985334	10.30981667	pos	Phosphoenolpyruvic acid	HMDB0001024	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C03232	40	6.62	M+NH4	C3H5O7P	4.176618526	80221.52705	81284.9644	79437.03187	83976.9002	84792.5036	85104.6573	86221.1652	85827.15563	85827.15563
2.14_166.0488n	167.0561139	2.1354	pos	9-Methylxanthine	96280	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives			40	8.14	M+H, M+Na	C6H6N4O2	-1.43320675	52394.88093	51313.74303	56257.72652	85659.25928	84129.38623	81685.13176	74290.69533	80485.56628	75481.83242
2.28_136.0392m/z	136.03918	2.28185	pos	3-Hydroxyanthranilic acid	HMDB0001476	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	**	C00632	40	6.04	M+H-H2O	C7H7NO3	-0.815432916	1245.774194	1068.699781	1047.504015	1671.570934	1674.978642	1684.968008	1474.687744	1635.970572	1577.81335
3.47_180.0877m/z	180.0877197	3.468983333	pos	7-Aminomethyl-7-carbaguanine	HMDB0011690	Organoheterocyclic compounds	Pyrrolopyrimidines	Pyrrolo[2,3-d]pyrimidines	**	C16675	40	7.27	M+H	C7H9N5O	-1.489121785	21028.26061	17695.33399	21312.08165	25213.82586	25565.69169	21020.7237	15758.08026	16132.81547	20983.75537
4.36_326.1706m/z	326.170572	4.3623	pos	2-Carboxy-1-[5-(2-carboxy-1-pyrrolidinyl)-2-hydroxy-2,4-pentadier	HMDB0035173	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			40	7.41	M+NH4	C15H20N2O5	-1.54256302	3720.93388	4767.61757	5068.36641	6031.428182	5188.542682	4833.316097	1249.937581	1920.13366	1115.770547
2.47_208.1463m/z	208.1462827	4.473983333	pos	N-Succinyl-L,L-2,6-diaminopimelate	HMDB0012267	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C04421	40	7.42	M+NH4	C11H18N2O7	3.640657625	2204.152165	3907.870987	2204.152165	1892.611933	1882.098554	3139.127648	1440.977726	3205.746548	
4.97_407.1296m/z	407.1296371	4.970833333	pos	Naproxen glucuronide	1467	Unclassified	Unclassified	Unclassified			40	19.1	M+H	C20H22O9	-9.90229424	20463.35397	21298.62508	23888.77682	29683.40427	27004.42112	28170.69192	22044.611	24849.66613	24716.69979
5.40_168.0785n	151.0751657	5.396716667	pos	4-Ipomeanol	HMDB0030472	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		40	4.99	M+H-H2O, M+H	C9H12O3	-1.132428479	3309.568071	3393.318597	3543.535619	3820.719612	3901.061094	3654.707842	2984.897851	2984.79805	3119.374426
5.52_358.1491m/z	358.1490886	5.5209	pos	Simmondsin	HMDB0030394	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		40	6.28	M+H-H2O	C16H25NO9	-1.478031839	10600.62872	11020.56371	11674.80066	3600.547097	3133.622394	3638.89871	9798.932048	9121.722612	9567.775944
7.45_255.2350m/z	485.2350218	7.553266667	pos	Neryl rhamnosyl-glucoside	HMDB0029349	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		40	6.27	M+Na	C22H38O10	-1.506242913	22462.77584	23242.88552	21490.38625	24930.36811	26382.47606	25923.58752	32862.08467	31182.37048	32128.59409
3.93_151.0388m/z	151.0388125	3.9343	pos	3-Acetyl-4-hydroxy-6-methyl-2H-pyran-2-one	HMDB0033129	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds			39.9	5.75	M+H-H2O	C8H8O4	-0.940248413	3335.734924	3600.799657	3876.992706	1094.424837	1041.246146	1012.683073	2495.825089	2688.242312	2492.193576
4.97_295.1649m/z	295.164943	4.969116667	pos	Tyroyl-L-eucine	HMDB0029109	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		39.9	4.04	M+H	C15H22N2O4	-0.988103365	2238.427645	2243.757445	2178.47199	3070.193123	3057.273893	2987.714529	2299.695209	2177.072227	2224.395166
4.29_130.1589m/z	130.1589381	4.294383333	pos	1-Octene	HMDB0032449	Hydrocarbons	Unsaturated hydrocarbons	Unsaturated aliphatic hydrocarbons	*		39.9	1.35	M+NH4	C8H16	-0.78407696	7063.880683	5793.455383	5788.317996	5855.272319	7705.682818	8573.460493	4554.665547	3996.244885	7285.860126
4.43_292.0152m/z	292.0152307	4.42815	pos	Lamivudine-monophosphate	HMDB0060641	Nucleosides, nucleotides, and analogues	Nucleoside and nucleotide analogues	Unclassified	*		39.9	7.28	M+H-H2O	C8H12N3O6PS	0.246447895	7619.799485	7291.746671	7559.060562	4564.736146	4024.916012	4176.870541	6144.702441	6470.581369	6157.168054
5.66_130.0650m/z	130.0650417	5.656316667	pos	Isoquinoline	44763	Organoheterocyclic compounds	Isoquinolines and derivatives	Isoquinolines	**	C06323	39.9	3.09	M+H	C9H7N	-0.650472504	9248.625545	7804.842039	6950.322776	9353.532672	9067.260383	9021.81966	7254.284216	6031.606547	6711.894664
6.08_365.1202m/z	365.1202222	6.084383333	pos	Coniferin	HMDB0013682	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C00761	39.9	4.86	M+Na	C16H22O8	-1.363185165	32681.14878	34689.72959	36311.34289	28517.21474	27554.8613	28749.24354	30257.02258	36157.08358	33049.38846
5.64_369.3509m/z	369.3508928	0.535	pos	Cholesterol	163	Lipids and lipid-like molecules	Steroids and steroid derivatives	Cholestane steroids	**	C00187	39.8	7.06	M+H-H2O	C27H46O	-1.773177345	19872.139	19872.139	23969.10138	18142.13525	3068.434998	3588.225284	6232.084006	25780.73655	15086.39308
2.05_154.0861m/z	154.0860719	2.048466667	pos	3-(5-Methyl-2-furyl)prop-2-enal	HMDB0032400	Organic oxygen compounds	Heteroaromatic compounds	Unclassified	*		39.8	3.03	M+NH4	C8H8O2	-1.345922554	11884.76064	12257.35897	13269.41466	8390.91626	7553.369424	7910.36545	10522.95865	11820.92522	10983.99475
2.42_169.0969m/z	169.0969347	2.421616667	pos	Cyclo(deltaAla-L-Val)	69241	Unclassified	Unclassified	Unclassified			39.8	10.6	M+H	C8H12N2O2	-1.305290662	9563.483105	10352.54061	10199.61094	9680.271874	10522.28754	10491.66242	8381.259924	11036.0878	9469.224236
3.03_235.0798m/z	235.0798397	3.027516667	pos	Histidylglycine	HMDB0028885	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides

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0.88_126.0661m/z	126.0660939	0.8802	pos	2-O-Methylcytosine	58237	Organoheterocyclic compounds	Diazines	Pyrimidines and pyrimidine derivatives	*		38.9	0	M+H	C5H7N3O	-0.754660992	2618.756167	3488.492729	3545.524711	2328.189531	2276.959415	2350.826889	2675.820672	3182.740229	3301.995271
0.88_155.0449m/z	155.0448572	0.8802	pos	3-Imidazole-2-oxopropanoate	66039	Unclassified	Unclassified	Unclassified			38.9	0	M+H	C6H6N2O3	-1.696419921	8985.206553	8713.355075	8259.522856	9243.680534	7940.870712	8511.410005	8529.278221	8687.713002	8111.703924
1.14_188.0795n	211.0686219	1.137683333	pos	Glycylhydroxyproline	HMDB0011173	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.9	0	M+H, M+Na	C7H12N2O4	-1.156110707	11145.42466	12590.98777	14058.10782	11879.64473	10711.72901	11450.16988	10929.72159	16887.72775	13339.47356
1.16_213.1231m/z	213.1230931	1.157483333	pos	Prolylproline	HMDB0011180	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.9	0	M+H	C10H16N2O3	-1.299984288	16278.12103	16767.30611	18104.76573	20452.06925	18629.37763	19269.92158	15677.74781	18467.25027	17418.17801
1.16_230.1859m/z	230.1858828	1.157483333	pos	N1,N8-Diacetylspermidine	HMDB0041947	Organic acids and derivatives	Carboxylic acids and derivatives	Carboxylic acid derivatives	*		38.9	0	M+H	C11H23N3O2	-1.835433941	7740.659715	8853.031038	7328.74701	7671.204972	7837.156036	7956.68861	6659.158043	7521.560047	6509.347363
1.20_300.1550m/z	300.1549774	1.199716667	pos	Threonyltyrosine	HMDB0029073	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.9	1.55	M+NH4	C13H18N2O5	-1.488109736	4529.995152	5829.497207	5873.70225	128.9404374	0.001403199	0.001403199	3061.515551	3578.361318	3680.098691
1.22_225.0161m/z	225.016067	1.220725	pos	beta-L-fucose 1-phosphate	HMDB0304542	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C02985	38.9	0	M+H-H2O	C6H11O8P-2	0.831800028	2134.559626	2605.486156	2097.281557	2570.491305	2361.178366	2498.097021	2523.812324	2647.885443	2430.189941
1.22_268.0012m/z	268.0011815	1.22075	pos	RESAZURIN	HMDB0257158	Unclassified	Unclassified	Unclassified			38.9	2.23	M+K	C12H7NO4	2.251603033	8644.585596	9480.973327	9766.079353	16933.77908	16332.59528	16508.85498	11663.92696	12959.22893	12131.68668
1.31_271.0920m/z	271.0919841	1.30655	pos	N-Salicyloylaspartic acid	HMDB0039506	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			38.9	0.794	M+NH4	C11H11NO6	-1.890691768	4562.044443	4797.600696	5283.925504	6559.717339	5526.834142	5816.015643	4030.852942	5219.620394	5261.360068
1.33_163.0388m/z	163.0388164	1.327966667	pos	2-Hydroxy-3-(4-hydroxyphenyl)propenoic acid	HMDB0006915	Benzenoids	Benzene and substituted derivatives	Phenylpyruvic acid derivatives	**	C05350	38.9	0	M+H-H2O	C9H8O4	-0.855825178	2322.595772	2357.410482	1898.555229	1761.849546	1816.79717	1772.488744	1955.191539	1738.784058	1837.315776
1.42_115.0503m/z	115.0502569	1.415933333	pos	MALEIMIDE	HMDB0254312	Unclassified	Unclassified	Unclassified			38.9	0	M+NH4	C4H3NO2	0.547047943	211.4919913	194.1116978	189.3498816	215.5362104	229.7339057	238.6307822	220.3045414	218.0074735	270.3911781
1.46_144.0653m/z	144.0653271	1.458683333	pos	1,3,5-Trihydroxybenzene	HMDB0013675	Benzenoids	Phenols	Benzenediols and derivatives	*	C02183	38.9	0	M+NH4	C6H6O3	-1.527429428	3053.676707	3068.874686	3086.369435	3115.508254	2916.363639	3126.213355	2963.781011	2782.669816	2872.794507
1.46_321.0812m/z	321.0811937	1.458683333	pos	L-Ascorbic acid-2-glucoside	72159	Unclassified	Unclassified	Unclassified			38.9	0	M+H-H2O	C12H18O11	-1.270282516	12326.81759	15055.47298	15568.58461	4715.455748	4114.023237	5001.674258	3885.987729	4943.531407	5032.77349
10.06_181.1584m/z	181.1583923	10.06391667	pos	Methyl 10-undecenoate	HMDB0029585	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.9	0	M+H-H2O	C12H22O2	-1.510850375	1034.73953	938.9779671	791.9392761	846.5741732	1291.022465	1107.262887	952.461293	869.5780495	983.0394564
10.09_403.2321m/z	403.23207	10.08803333	pos	5S-HETE di-endoperoxide	74966	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids			38.9	0	M+H	C20H34O8	-1.428189574	5691.481597	5709.181144	6185.984789	6042.007815	7487.616739	5505.369695	7362.838566	5923.334278	6081.043691
10.31_205.1584m/z	205.1584413	10.30981667	pos	3-NOR-3-OXOPANASINSAN-6-OL	44489	Unclassified	Unclassified	Unclassified			38.9	0	M+H-H2O	C14H22O2	-1.126895949	2474.905204	2247.405183	2095.157767	2778.569793	2387.240637	2505.991515	2889.861405	2631.990263	2907.247335
10.86_496.3393m/z	496.3392749	10.85551667	pos	LysoPC(0:0/16:0)	HMDB0240262	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	***		38.9	0	M+H	C24H50NO7P	-0.991567886	7012.953952	4682.274178	5485.934517	4433.978934	4901.238726	5053.572054	5562.010647	4686.527455	6012.933479
10.91_332.2192m/z	332.2191951	10.91385	pos	N-cis-tetradec-9Z-enoyl-L-Homoserine lactone	64725	Unclassified	Unclassified	Unclassified			38.9	0	M+Na	C18H31NO3	-1.356502795	1817.704152	1685.177209	1664.735141	1691.680003	2302.676295	1820.847211	2485.329389	1451.613664	1081.746675
11.30_177.1636m/z	177.1635772	11.29856667	pos	Geranylacetone	HMDB0031846	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*	C13297	38.9	0	M+H-H2O	C13H22O	-1.029331721	1971.590674	1758.102144	2030.165428	1291.932515	2136.246234	2090.082574	1870.668388	1779.69864	2044.691609
12.80_154.1224m/z	154.1224253	12.80346667	pos	4-Methyl-2-pentyloxazole	HMDB0037857	Organoheterocyclic compounds	Azoles	Oxazoles			38.9	0	M+H	C9H15NO	-1.405478802	631.8636776	537.4810831	619.1848784	382.723392	474.8819479	637.0299675	530.306625	461.9902794	590.4938111
13.15_271.1660m/z	271.1660035	13.15121667	pos	4-(2-hydroxy-3-isopropyl-aminopropyl)benzoic scid	1354	Unclassified	Unclassified	Unclassified			38.9	0	M+NH4	C13H19NO4	3.041548265	1279.534715	1215.531883	1223.519258	1513.104101	1139.824774	1507.152667	1398.373258	1183.75472	1374.302495
13.21_371.1620m/z	371.1619771	13.2099	pos	11b-Hydroxyprogesterone	HMDB0304821	Lipids and lipid-like molecules	Steroids and steroid derivatives	Pregnane steroids	**	C05498	38.9	0	M+K	C20H28O4	0.179496078	4620.78848	3014.173009	3820.752712	3661.146776	3284.830452	4186.996646	3914.370873	7141.611641	4179.500349
13.33_228.1955m/z	228.1955144	13.33273333	pos	alpha-Tyrosol propanoate	88148	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		38.9	0	M+NH4	C13H22O2	-1.384766557	2661.660104	2014.585189	1813.376201	2136.567304	1733.977393	2117.146232	1857.332858	1862.616964	1862.616964
13.70_206.0665m/z	206.0665054	13.69921667	pos	cis-2-Methylaconitate	HMDB0006357	Organic acids and derivatives	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives	**	C04225	38.9	0	M+NH4	C7H8O6	3.147593956	775.7677695	650.7203185	643.4291213	914.757241	831.5653508	1003.289886	1076.019279	817.918767	708.2403162
13.73_101.0712m/z	101.0712229	13.73403333	pos	L-2,4-diaminobutyric acid	HMDB0006284	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C03283	38.9	0	M+H-H2O	C4H10N2O2	2.401458291	310.2334003	439.4064928	354.4469509	253.191143	321.7782667	223.8506208	326.3693016	263.5435179	299.8264479
13.90_213.1132m/z	213.113206	13.89973333	pos	gamma-Butyrobetaine Ethyl Ester Chloride	73569	Unclassified	Unclassified	Unclassified			38.9	0	M+K	C9H20NO2+	3.698455839	12946.31288	13224.98383	12580.27145	13876.52077	13869.20678	14429.16228	14307.55727	13215.35839	14110.01368
13.95_172.1118m/z	172.1117765	13.9479	pos	Biphenyl	HMDB0034437	Benzenoids	Benzene and substituted derivatives	Biphenyls and derivatives	**	C06588	38.9	0	M+NH4	C12H10	-1.942634049	535.0036355	883.7919373	533.0215991	656.7456831	549.6322384	697.2261417	703.3291461	568.1126117	470.732434
14.11_226.1586m/z	226.1586001	14.10851667	pos	2,4-Diphenyl-1-butene	HMDB0032563	Phenylpropanoids and polyketides	Linear 1,3-diarylpropanoids	Unclassified	*	C14562	38.9	0	M+NH4	C16H16	-2.046474304	227.476411	338.0014034	293.45682	307.6442162	360.3676501	289.3155988	255.6272702	252.6329832	289.5863848
14.64_116.1070m/z	116.1070323	14.63885	pos	Cyclohexanone	HMDB0003315	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*	C00414	38.9	0	M+NH4	C6H10O	0.426521632	202.1511455	247.1569647	294.1092032	386.1202769	289.1951414	337.93188	431.7668373	312.2422588	361.2493208
14.85_228.2317m/z	228.2317468	14.84533333	pos	10E,12E-Tetradecadien-1-ol	LMFA05000178	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols			38.9	0	M+NH4	C14H26O	-2.113278511	16198.60786	13386.09507	14736.48621	15671.68888	16722.7814	16310.33418	16915.56479	15398.74256	15516.00223
14.86_278.2474m/z	278.247437	14.86423333	pos	4,5-(methanoxyethano)isolongifol-4-ene	LMPR0103500012	Lipids and lipid-like molecules	Prenol lipids	Isoprenoids			38.9	0	M+NH4	C18H28O	-1.552688479	16602.72945	15286.56804	15040.64554	16651.17374	16804.95674	17274.36912	17781.02678	16592.58187	18003.13503
14.94_284.2941m/z	284.2941025	14.93678333	pos	3Z,13Z-octadecadien-1-ol	LMFA05000047	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols			38.9	0	M+NH4	C18H34O	-2.586893758	5072.630258	2266.484306	3373.258083	3513.954224	3360.455065	3571.068487	4284.830543	3744.473502	3810.167192
15.05_248.0584m/z	248.0584399	15.0502	pos	Proflavine	68897	Organoheterocyclic compounds	Quinolines and derivatives	Benzoquinolines		C11181	38.9	0	M+K	C13H11N3	-0.074221244	1417.567148	10775.08874	2199.788466	2682.474789	1329.480409	1211.454346	838.7839692	779.0059258	627.2878078
15.36_263.2469m/z	263.2465566	15.34891667	pos	Farnesyl acetone	265036	Unclassified	Unclassified	Unclassified	***		38.9	0	M+NH4	C18H30O	-1.46971073	3499.301741	3899.691585	4145.841418	4018.830869	2480.627777	4581.627777	3965.319017	2103.356308	3496.210687	1917.811537
15.41_271.2415m/z	271.2415489	15.41201667	pos	Taxa-4(20),11(12)-dien-5alpha-ol	LMPR0104390003	Lipids and lipid-like molecules	Prenol lipids	Isoprenoids	**	C11895	38.9	0	M+H-H2O	C20H32O	-1.659967277	4992.392134	7104.064133	7104.018389	413.5719788	462.8951579	467.0220915	764.6799838	429.6766434	710.4955966
2.03_214.0158m/z	214.015784	2.026633333	pos	Benzeneacetamide-4-O-sulphate	HMDB0059994	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		38.9	14.2	M+H-H2O	C8H9NO5S	-4.636430548	3240.109694	3067.224115	3232.20924	674.791932	613.7591449	540.5742916	6176.064763	6854.698597	6546.912133
2.20_309.0576m/z	309.0575698	2.200433333	pos	D-erythro-L-galacto-Nonulose	HMDB0029955	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			38.9	0	M+K	C9H18O9	-2.482311134	685.017601	1025.640534	966.5630962	63.5132832	0.001403199	53.25681033	2845.285347	3272.033518	3188.958105
2.36_194.1034m/z	194.1033523	2.360916667	pos	N-Benzooxazol-2-yl-guanidine	96363	Unclassified	Unclassified	Unclassified			38.9	0	M+NH4	C8H8N4O	-1.613577854	3368.005801	3236.278091	3114.260296	3230.155272	3290.072227	3247.665462	3206.018987	3285.516767	2761.460031
2.45_139.1009m/z	139.1009413	2.450033333	pos	3-Acrylamidopropyl trimethylammonium	34500	Unclassified	Unclassified	Unclassified			38.9	0	M+H	C9H18N2O	-1.132129552	772.2509389	781.3746213	842.1591803	701.3746213	842.1591803	1016.044271	1097.99527	1113.586923	934.9891927	1069.187997
2.47_231.1336m/z	231.1335791	2.465483333	pos	Hydroxyprolyl-Valine	HMDB0028876	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.9	0	M+H	C10H18N2O4	-1.539846068	2443.405744	3022.598123	2723.62921	3861.195561	3887.831365	4192.561919	3072.272338	3650.325855	3667.287038
2.58_154.0498m/z	154.0497662	2.578	pos	4-Nitroanisole	HMDB0246530	Unclassified	Unclassified	Unclassified			38.9	0.353	M+H	C7H7NO3	-0.6749872	4003.729419	3978.246113	3965.920205	4804.156136	4303.80748	4873.712877	2887.913569	3107.096873	3075.724281
3.03_262.0032m/z	262.0031835	3.027516667	pos	Sodium citrate	HMDB0303752	Unclassified	Unclassified	Unclassified			38.9	0	M+H	C6H8Na3O7+3	-1.545367845	2586.823892	3068.150052	3261.484436	281.1938573	124.2795003	361.8485682	2599.984977	2611.405454	2789.753037
3.52_184.0577m/z	184.057748	3.520533333	pos	DL-2-Aminoadipic acid	324	Unclassified	Unclassified	Unclassified			38.9	0	M+Na	C6H11NO4	-1.741749457	5647.93353	5106.936544	4707.582124	4483.573206	5089.424907	4832.894227	5913.378042	4874.981816	5460.897058
3.69_302.1595m/z	302.1594712	3.6941	pos	karalicin	LMFA05000671	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols			38.9	0	M+NH4	C14H20O6	-1.206262269	1308.823749	1224.576757	1274.372336	4042.866085	3301.024788	3058.900108	1493.791016	1708.059071	1664.72624
3.72_212.0712m/z	212.0712631	3.716333333	pos	gamma-Fagarine	HMDB0030195	Organoheterocyclic compounds	Quinolines and derivatives	Furoquinolines	*	C10676	38.9	0	M+H-H2O	C13H11NO3	2.872979803	1155.635104	1088.333907	1313.780978	2011.274409	1928.677195	2013.343582	673.7488271	1170.936514	880.1588244
3.76_417.1178m/z	417.1177651	3.759483333	pos	Daidzin	HMDB0033991	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavonoid O-glycosides	***	C10216	38.9	0	M+H	C21H20O9	-0.585275813	1086.630489	731.7195725	925.3095548	877.4105184	882.9149389	796.8347819	574.4865189	1222.91101	1061.515184
3.87_179.0945n	180.1017724	3.866916667	pos	2(N)-Methyl-norsalsolinol	58029	Organoheterocyclic compounds	Tetrahydroisoquinolines	Unclassified	*		38.9	0	M+H, M+NH4	C10H13NO2	-0.741015888	1560.52053	1456.622259	1562.466151	1252.220658	1676.05318	1317.14958	1584.135362	1418.099391	
3.93_356.9900m/z	356.9900031	3.9343	pos	2-Methyl-1,4-naphthalenediol bis(dihydrogen phosphate)	88651	Benzenoids	Naphthalenes	Unclassified			38.9	0	M+Na	C11H12O8P2	0.125185866	1035.728575	343.3543715	1375.48501	0.001403199	0.001403199	9.862498306	669.89353	1073.732518	947.7737325	
3.96_177.0545m/z	177.0544625	3.956866667	pos	trans-Ferulic acid	HMDB0000954	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	***	C01494	38.9	0	M+H-H2O	C10H10O4	-0.814602438	956.7138981	1125.894519	1262.577193	679.9869685	532.6172979	454.5884863	777.9453502	955.9892844	900.6789223
3.98_179.0581m/z	179.0581155	3.979183333	pos	4-Oxo-4-(3-pyridyl)-butanoic acid	5924	Organic acids and derivatives	Keto acids and derivatives	Gamma-keto acids and derivatives	**	C19569	38.9	0	M+H-H2O, M+H	C9H9NO3	0.778567227	3567.778781	4007.228862	4306.737507	3470.046026	3577.738781	4007.228862	2284.31147	3818.123819	3743.992722
4.00_255.0836m/z	255.0835618	4.002016667	pos	Glycerol 1-propanoate diacetate	87831	Lipids and lipid-like molecules	Glycerolipids	Triradylglycerols	*		38.9	0	M+Na	C10H16O6	-1.495470203	1617.657376	1644.143596	1797.922192	1947.055656	1771.938068	1854.805804	1383.112946	1726.532161	1612.187958
4.09_200.1523n	201.1595428	4.091916667	pos	Hexamethylene bisacetamide	HMDB0041901	Organic acids and derivatives	Carboximidic acids and derivatives	Carboximidic acids			38.9	0	M+H, M+Na	C10H20N2O2	-1.056853539	2372.588767	3176.648188	2832.745415	605.0102808	558.1049194	604.2433652	3284.295684	3836.415621	3687.712916
4.34_147.0438m/z	147.0438315	4.33965	pos	Coumarin	HMDB0001218	Phenylpropanoids and polyketides	Coumarins and derivatives	Unclassified	***	C05851	38.9	0	M+H	C9H6O2	-1.536440306	1344.364234	1351.01298	1364.928935	738.6458207	602.8450588	651.5144575	942.7873827	1244.988006	1081.608404
4.43_169.0857m/z	169.0857345	4.42815	pos	1-Ipomeanol	87002	Organoheterocyclic compounds	Heteroaromatic compounds	Unclassified	*		38.9	0	M+H	C9H12O3	-1.107690817	2225.147097	2532.735947	2436.379743	2512.540078	2409.123727	2237.128753	2191.514926	2306.874711	2131.681009
4.57_219.1127m/z	219.1127246	4.565116667	pos	2'-Aminobiphenyl-2,3-diol	66795	Unclassified	Unclassified	Unclassified			38.9	0	M+NH4	C12H11NO2	-0.395541583	571.9391607	569.9083676	734.997334	278.3849622	246.7714049	333.0870894	236.7214736	257.6311684	230.1557758
4.57_328.1187m/z	328.1186506	4.565116667	pos	Tianilast	43562	Unclassified	Unclassified	Unclassified			38.9	0	M+NH4	C18H17N5O2	2.144592799	4961.090107	614.6923795	557.6885994	616.0982881	478.6647374	573.8202249	564.0518595	418.2616425	
4.61_324.1105m/z	324.1104974	4.610866667	pos	Cynometrine	68408	Unclassified	Unclassified	Unclassified			38.9	0	M+K	C16H19N3O2	-1.359180858	3229.572269	3503.374964	3529.523406	189.2029967	218.2907264	174.9816968	363.4563664	462.1226718	441.2886941
4.70_152.1068m/z	152.1068015	4.701116667	pos	N-Methyltyramine	HMDB0003633	Benzenoids	Benzene and substituted derivatives	Phenethylamines	**	C02442	38.9	0	M+H	C9H13NO	-1.250593036	1664.185417	1569.525128	1712.173768	1690.222371	1725.555845	1585.91884	1804.997208	1588.4526	1677.448913
4.70_331.1723m/z	331.1723277	4.701116667	pos	(R)-1-O-b-D-glucopyranosyl-1,3-octanediol	86223	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		38.9	0	M+Na	C14H28O7	-1.285754572	270.0999079	898.1717255	182.0589431	5038.111744	52.56672392	0.001403199	38.68848628	646.39744	0.001403199
4.72_334.0660n	357.0551991	4.723666667	pos	2-(beta-D-Glucosyl)-sn-glycerol 3-phosphate	68368	Unclassified	Unclassified	Unclassified			38.9	0	M+H, M+Na	C9H19O11P	-1.610903184	1044.887141	2267.349672	2246.787918	1031.219271	1493.835515	1572.702471	3100.528668	3256.807487	3129.789566
4.75_153.1272m/z	153.1272239	4.7917	pos	Methyl 4-oxo-3-nonenoate	HMDB0029859	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	**		38.9	0	M+H-H2O	C10H18O2	-0.99145162	2732.723691	1291.572684	1527.979268	835.0436654	758.5220685	1027.922884	1207.823198	1496.388049	1494.794505
4.79_207.0263m/z	207.026312	4.7912	pos	4-O-Methylgallic acid	HMDB0013198	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*		38.9	0	M+Na	C8H8O5	-0.4454922	967.940142	1103.281554	1165.624919	424.6858025	364.1512915	411.0233728	283.9051445	272.1342297	281.7030319
4.84_444.2335m/z	444.2334904	4.836966667	pos	3-Hydroxyldocaine glucuronide	998	Unclassified	Unclassified	Unclassified			38.9	0	M+NH4	C20H30N2O8	-1.292892499	8311.102014	10188.60042	10921.12114	4825.02829	5036.025825	4882.524942	5550.138433	6839.517159	6658.166944
4.86_158.1174m/z	158.1173614	4.8596	pos	Lentiginosine	68160	Unclassified	Unclassified	Unclassified			38.9	0	M+H	C8H15NO2	-1.232997282	2566.438842	2663.134543	2793.844725	2551.181678	2306.96272	2304.2344	2625.456502	2638.436655	2796.210059
4.86_181.1221m/z	181.1220633	4.8596	pos	formyl 2E,4E,6Z-decatrienoate	97203	Unclassified	Unclassified	Unclassified			38.9	0	M+H	C11H16O2	-1.34872036	3774.118519	3730.185598	4013.397226	3770.087142	3580.422425	3589.663843	3404.881843	3291.993238	3396.462325
4.95_320.1827m/z	320.1827446	4.949833333	pos	(4Z)-Octadodecenyl)homoserine lactone	69239	Unclassified	Unclassified	Unclassified			38.9	0	M+H	C18H29NO3	-1.629924129	3771.579184	4433.919521	3950180.5234	218325.538	148841.8098	203134.8854	257557.7495	264587.2417	260289.8578
4.97_221.1534m/z	221.1534365	4.970833333	pos	Oblongolide	67771	Unclassified	Unclassified	Unclassified			38.9	0	M+H	C14H20O2	-0.771410899	2663.951289	2616.594777	3022.078311	2955.873354	2633.666182	2708.966888	2902.863141	2723.929754	2876.18576
5.13_160.0755m/z	160.0755172	5.125733333	pos	N-Hydroxy-1-aminonaphthalene	HMDB0062503	Benzenoids	Naphthalenes	Unclassified	**	C14789	38.9	0	M+H	C10H9NO	-1.088485328	791.7675556	712.4249144	756.9243132	1229.889956	1082.823026	1038.135718	1228.566923	1112.428034	1098.454812
5.17_181.0858m/z	181.0857878	5.1709	pos	3-Methoxybenzenepropanoic acid	62469	Phenylpropanoids and polyketides	Phenylpropanoic acids	Unclassified	*		38.9	0	M+H-H2O	C10H12O3	-0.737838294	1747.24394	1682.265961	1736.70017	2981.971714	2727.426144	2742.777317	1882.168033	1827.150203	1817.040885
5.35_153.1272m/z	153.1271962	5.351683333	pos	(±)-6-Methyl-5-hepten-2-yl acetate	86674	Organic acids and derivatives	Carboxylic acids and derivatives	Carboxylic acid derivatives	*		38.9	0	M+H-H2O	C10H18O2	-1.148173451	2870.759533	3076.041367	3039.210595	1822.347944	1858.140602	1790.777506	2651.330098	2883.392515	2741.377135
5.35_163.1138m/z	163.111762	5.351683333	pos	(±)-2-Methyl-3-(4-methylphenyl)propanal	HMDB0031856	Benzenoids	Benzene and substituted derivatives	Phenylpropanes			38.9	0	M+H	C11H14O	0.126390124	859.3954507	524.9890661	708.714462	1438.225504	1393.807973	1491.897038	1012.642147	961.8837609	914.3103886
5.44_225.1361m/z	248.1253881	5.396716667	pos	Terbutaline	HMDB0015009	Benzenoids	Phenols	Benzenediols	*	C07129	38.9	0	M+H, M+Na	C12H19NO3	-1.564483628	24899.63127	23602.88142	23926.88591	25059.68584	24538.23727	28040.79161	26177.56457		
5.40_376.1697m/z	376.1696948	5.396716667	pos	Fortimicin AO	71968	Unclassified	Unclassified	Unclassified			38.9	0	M+Na	C13H27N3O8	1.866573238	1435.38781	1312.813438	1223.861126	2937.072162	3147.278795	3045.068864	2013.491322	1787.471954	2172.102623
5.68_358.2583m/z	358.2582695	5.675716667	pos	Idebenone Metabolite (1,4-Benzenediol, 2-(10-hydroxydecyl)-5,6-	763	Unclassified	Unclassified	Unclassified			38.9	0	M+NH4	C19H32O5	-1.55824776	4361.668988	4556.361829	4262.604729	5241.159702	6796.156403	5202.951766	3964.137584	3239.532757	3677.007442
5.72_435.1621m/z	435.1621217	5.720466667	pos	1-Hexanol arabinosylglucoside	HMDB0031689	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		38.9	0	M+K	C17H32O10	-1.472875431	7924.583756	7446.806944	7860.54392	9069.167042	9215.850945	7577.823227	5992.973601	4766.843343	5147.719199
5.78_171.0625m/z	171.0624591	5.778566667	pos	2,3-Dihydroxy-3-methylpentanoic acid	LMFA01050469	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C06007	38.9	0	M+H	C6H12O4	-2.164004814	662.3420219	441.4580473	527.2523617	615.3592591	556.8307955	487.39342	688.920502	457.6695387	509.7402039
5.87_281.2260m/z	5.8665	pos	3-Methyl-19-nor-17alpha-pregna-1,3,5(10)-trien-17-ol	70609	Unclassified	Unclassified	Unclassified				38.9	0	M+H-H2O	C21H30O	-1.171672506	348.5583603	298.1969955	275.6967458	517.27379	597.4262409	578.2675731	299.4892948	441.8793031	330.1096607	
5.96_221.1897m/z	221.1896989	5.956833333	pos	2-trans,6-trans-Farnesal	HMDB0060356	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	**	C03461	38.9	0	M+H	C15H24O	-1.330426679	1418.418955	1281.098972	1370.513594	514.9245184	734.8725612	522.226092	1445.399041	1240.234317	1412.094451
6.00_541.2638m/z	541.2637997	5.995733333	pos	17-α, 21-dihydroxy-11,20-dioxo-5-β-pregnan-3-α-yl-β-d-glucuroni	4094	Unclassified	Unclassified	Unclassified			38.9	0	M+H	C27H40O11	-0.997331226	18296.99087	20044.72554	18078.76836	17807.50721	18251.07167	19425.239	17400.83167	19282.55592	18607.0324
6.01_251.1615m/z	251.1614799	6.01315	pos	Menthone 1,3-glyceryl ketal	HMDB0040004	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		38.9	0	M+Na	C13H24O3	-1.250724006	2697.574377	2967.113668	1465.146498	1800.352467	1642.235246	3150.913635	3158.674093	2101.990782	3132.255312
6.05_135.1167m/z	135.1166706	6.0535	pos	Isocitral	HMDB0030893	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		38.9	0	M+H-H2O	C10H16O	-1.027039432	1021.311825	1154.132128	891.1172784	705.0929549	748.6152547	669.9155445	915.1057252	1044.785829	899.8512979
6.16_402.2846m/z	402.2846101	6.162416667	pos	Sphingofungin F	53966	Lipids and lipid-like molecules	Sphingolipids	Sphingoid bases			38.9	0	M+NH4	C21H39NO6	-1.007486195	5003.768845	4743.713654	5012.750513	4672.324505	5974.635765

0.51_172.1116m/z	172.1115915	0.51135	pos	Acenaphthene	HMDB0247899	Unclassified	Unclassified	Unclassified			38.8	0	M+NH4	C12H10	-3.143682391	669.106214	517.5312652	619.3973143	946.3677486	650.4821438	807.8647785	754.0958322	729.4707005	981.0849722
0.54_116.0819m/z	116.0819007	0.535	pos	Dimethylimidazole	2539	Unclassified	Unclassified	Fatty acids and conjugates			38.8	0	M+NH4	C4H6N2O	0.635422949	7.750319339	91.19495956	140.4476037	6.088286357	18.14409654	89.27799938	29.84452537	84.7351265	178.2901229
0.54_280.2398n	263.2364853	0.535	pos	Linoleic acid	HMDB0000673	Lipids and lipid-like molecules	Fatty Acyls	Linoleic acids and derivatives	***	C01595	38.8	0	M+H-H2O, M+H	C18H32O2	-1.629721335	2219.436909	4580.710191	4802.066687	2982.05007	400.5336154	3386.111546	691.6349488	3319.825327	4055.433687
0.54_307.2627m/z	307.2626785	0.535	pos	11,14,17-eicosatrienoic acid	LMFA01030159	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C16522	38.8	0	M+H	C20H34O2	-1.561710064	892.7483522	2167.136844	1077.276915	941.8008475	27.38597822	1054.959474	60.69076542	1193.335876	1078.679065
0.54_359.1661m/z	359.1660625	0.535	pos	S-Japonin	91032	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.8	0	M+Na	C19H28O3S	2.754755837	1856.631304	2001.931042	5689.716472	3515.139948	0.001403199	7524.29194	255.4091573	5394.050653	3253.031372
0.58_113.0233m/z	113.0233421	0.576333333	pos	3-Hydroxy-2H-pyran-2-one	HMDB0032994	Organoheterocyclic compounds	Pyrans	Pyranones and derivatives			38.8	0	M+H	C5H4O3	0.193428993	221.6042598	191.7401283	272.2009942	272.9277368	180.650387	175.4201416	188.1470529	224.2861357	307.5592004
0.62_182.9849m/z	182.9848721	0.616683333	pos	Octafluorocyclobutane	HMDB0031292	Organohalogen compounds	Organofluorides	Unclassified	*		38.8	0	M+H-H2O	C4F8	4.673142905	472002.4137	470457.7599	475703.0451	476879.7787	437913.0682	500272.2625	478222.6982	462816.7233	473152.0263
0.62_220.9806m/z	220.980577	0.616683333	pos	1,3-Glyceryl dinitrate	1579	Unclassified	Unclassified	Unclassified			38.8	0	M+K	C3H6N2O7	-0.448599629	0.001403199	0.001403199	486.5973838	503.4165178	747.9161363	269.1523157	0.001403199	347.4995575	305.0846187
0.74_335.1323n	336.1395342	0.73955	pos	N4-(b-N-Acetyl-D-glucosaminyl)-L-asparagine	6292	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C04540	38.8	0	M+H, M+Na	C12H21N3O8	-1.810838471	12697.56099	9886.532386	11559.01732	12803.44859	13535.9209	12930.98034	10551.35676	9377.818746	8796.626602
0.78_205.0680m/z	205.0679839	0.776666667	pos	Mannitol	HMDB0000765	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	***	C00392	38.8	0	M+Na	C6H14O6	-1.509823925	34281.07474	31353.61434	32551.12633	27890.51574	23572.48858	23502.05039	26855.91172	28815.61185	26687.68401
0.78_219.0472m/z	219.0471864	0.776666667	pos	Gulonic acid	HMDB0003290	Organic acids and derivatives	Hydroxy acids and derivatives	Medium-chain hydroxy acids and derivatives	**	C00800	38.8	0	M+Na	C6H12O7	-1.718730507	24906.76626	23392.98952	23376.10693	23223.20125	23275.07509	22630.84735	21239.76695	23154.10457	21102.61693
0.84_262.0797n	263.0869016	0.8386	pos	Aspartyl-Glutamate	HMDB0028752	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.8	0	M+H, M+Na	C9H14N2O7	-1.471242936	13501.56069	13645.62467	13588.29655	15285.04444	14509.76027	13852.01424	11328.9967	11868.62766	11854.38137
0.86_148.0926n	187.05742	0.859583333	pos	R-3-(Methylthio)-1-hexanol	HMDB0040153	Organosulfur compounds	Thioethers	Dialkylthioethers			38.8	6.44	M+H, M+K	C7H16OS	2.974355023	17206.15423	17016.16264	16870.7383	12355.46029	11488.30736	12018.60848	11991.68667	13589.6746	12697.89789
0.88_128.0705m/z	128.0705009	0.8802	pos	Catechol	HMDB0000957	Benzenoids	Phenols	Benzenediols	***	C15571	38.8	0	M+NH4	C6H6O2	-0.945896587	3017.673085	3100.464723	3153.269423	2932.513542	3003.72902	2734.952889	2707.341723	2717.95188	2589.026356
0.88_166.0862m/z	166.0862225	0.8802	pos	1-Phenyl-1,2-propanedione	HMDB0035243	Benzenoids	Benzene and substituted derivatives	Phenylpropanes	**	C17268	38.8	0	M+NH4	C9H8O2	-0.219706509	1872.526381	2074.101681	2037.281264	1734.644134	1707.922426	1898.645793	1660.038755	1881.253966	1552.064746
0.88_172.0845n	173.0918252	0.8802	pos	Prolylglycine	HMDB0011178	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.8	0	M+H, M+Na, M+H-H2O	C7H12N2O3	-1.414754282	11740.55451	13044.00662	13492.80509	18717.52922	18740.15349	18651.06478	12474.94533	12872.71342	12340.02533
0.88_278.1230m/z	278.1230412	0.8802	pos	3-Furanmethanol glucoside	88828	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			38.8	0	M+NH4	C11H16O7	-1.488620199	21011.77755	21040.61182	22072.51657	18697.68376	16873.39584	17713.79931	15908.45411	17568.57334	17192.59964
1.14_188.1027m/z	188.1026703	1.137683333	pos	2,3,4-Trihydroxybenzylhydrazide	1291	Unclassified	Unclassified	Unclassified			38.8	0	M+NH4	C7H10N2O3	-1.749080436	11193.46542	10354.64673	11541.65328	17325.70566	13232.99113	10750.5621	9521.394234	13329.75889	10834.3315
1.16_235.1184m/z	235.1184338	1.157483333	pos	Acetylhydrazinopthalazinone	3165	Unclassified	Unclassified	Unclassified			38.8	0	M+NH4	C11H11N3O2	-2.387666601	11697.73049	12602.1244	12155.70767	10887.72042	9855.984763	10213.33391	10616.54616	11107.93478	10030.09954
1.16_240.1087m/z	240.1086918	1.157483333	pos	4a-Hydroxytetrahydrobiopterin	64413	Organoheterocyclic compounds	Pteridines and derivatives	Pterins and derivatives	**	C15522	38.8	0	M+H-H2O	C9H15N5O4	-1.648818876	27863.39931	30487.10796	29875.79489	31814.4177	31213.76539	30354.12721	29037.50708	30995.41627	27263.01228
1.20_199.0002m/z	199.0002249	1.199716667	pos	Dihydroxyacetone Phosphate Acyl Ester	62468	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C03372	38.8	0	M+H	C4H7O7P	0.046963895	279.4530844	214.1686058	291.9905591	277.6618515	309.9605024	288.4028572	269.6985534	299.5824643	235.4857872
1.35_289.2522m/z	289.2521534	1.350266667	pos	Sciadonic acid	LMFA01030380	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.8	0	M+H-H2O	C20H34O2	-1.432371537	103680.568	64812.73288	44678.56776	21345.44418	20214.76785	17555.55298	41203.12454	30519.37102	26725.88519
1.37_244.1541m/z	244.1540839	1.372566667	pos	3-Hydroxyoleoylcarnitine	LMFA07070041	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.8	0	M+H-H2O	C12H23NO5	0.959912151	4703.338505	5161.288	961.0638856	271.5182388	399.0803848	493.3974027	376.1159356	485.4275453	512.2863464	450.7533793
1.42_196.0578m/z	196.0577504	1.415933333	pos	2,6-Piperidinedicarboxylic acid	334	Unclassified	Unclassified	Unclassified			38.8	0	M+Na	C7H11NO4	-1.606707449	2006.206051	2065.706027	2152.827804	2247.334387	2324.572247	1879.562054	1804.669047	1977.445926	2067.844084
1.46_416.0267m/z	416.0267489	1.458683333	pos	Gossypetin 3-O-sulfate	LMPK12113267	Lipids and lipid-like molecules	Polyketides	Flavonoids			38.8	6.94	M+NH4	C15H10O11S	-3.665207275	12593.01183	14530.48286	13757.58558	3337.819949	3724.045874	3677.612779	3443.414427	4013.949241	4242.184894
1.70_115.0503m/z	115.0502611	1.697866667	pos	Dihydrouracil	285	Organoheterocyclic compounds	Diazines	Pyrimidines and pyrimidine derivatives	**	C00429	38.8	0	M+H	C4H6N2O2	0.501715274	770.7244808	870.1800303	779.2206193	875.7218582	879.129251	867.3547265	906.9971291	888.7338232	861.6439409
11.09_269.2082m/z	269.2082074	11.08833333	pos	8,8-Diethoxy-2,6-dimethyl-2-octanol	HMDB0034557	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols	*		38.8	0	M+Na	C14H30O3	-2.063725931	2154.314953	1530.190046	1450.76503	1675.273215	2049.440278	2151.135845	1903.800545	1747.540888	1967.181704
11.17_262.1434m/z	262.1433619	11.18926667	pos	Batatasin III	HMDB0030636	Phenylpropanoids and polyketides	Stilbenes	Unclassified	*		38.8	0	M+NH4	C15H16O3	-1.671453393	2798.746222	2318.961844	1800.191478	2074.675041	2505.824357	2803.463902	2591.299455	2251.655391	2586.404594
11.33_323.1824m/z	323.1824122	11.32543333	pos	Tetranor-PGF1alpha	LMFA03010213	Unclassified	Unclassified	Unclassified			38.8	0.768	M+Na	C16H28O5	-1.607099377	8332.236244	3346.337589	13274.4898	907.1392647	5183.664909	3714.789609	19271.57548	4394.031704	2592.564776
11.47_105.0426m/z	105.0425707	11.47106667	pos	Fomepizole	66749	Organoheterocyclic compounds	Azoles	Pyrazoles		C07837	38.8	0	M+Na	C4H6N2	3.06885126	1869.883866	1919.029453	2000.118312	1898.306195	1878.255501	2132.557866	1864.825731	1971.879805	2274.366141
11.81_527.3046m/z	527.3045542	11.81006667	pos	N3'-Acetyltobramycin	65882	Unclassified	Unclassified	Unclassified			38.8	0	M+NH4	C20H39N5O10	2.034754441	14365.81234	19625.73195	19549.25281	18907.58878	17098.54371	16895.52621	19727.17016	17085.26924	20492.96412
12.72_369.3511m/z	369.351065	12.72343333	pos	Lathosterol	166	Lipids and lipid-like molecules	Steroids and steroid derivatives	Cholestane steroids	**	C01189	38.8	0	M+H-H2O	C27H46O	-1.327462784	51860.54531	58186.53006	79968.08929	43769.70438	40565.15349	132632.7379	80796.37094	69245.36603	61650.56648
12.72_378.3572m/z	378.3571563	12.72343333	pos	1-O-(2R-hydroxy-octadecyl)-sn-glycerol	LMGL01020064	Lipids and lipid-like molecules	Glycerolipids	Monoradylglycerols			38.8	0.411	M+NH4	C21H44O4	-1.745989223	31337.84848	25912.19375	29059.79588	27308.02182	26066.43371	25981.39499	29007.69281	26511.02824	28003.22422
12.97_435.8090m/z	435.8090014	12.97438333	pos	Iodoquinol	HMDB0253533	Unclassified	Unclassified	Unclassified			38.8	0	M+K	C9H5I2NO	-0.513768861	9594.963779	9162.998454	8094.375199	8097.247837	9162.998454	8645.868408	10248.81769	8399.394331	8309.394331
13.23_392.3728m/z	392.3727604	13.23251667	pos	1-O-(2R-hydroxy-nonadecyl)-sn-glycerol	LMGL01020065	Lipids and lipid-like molecules	Glycerolipids	Monoradylglycerols			38.8	0	M+NH4	C22H46O4	-1.803519204	38434.88633	37439.2739	34129.91524	31126.03928	31998.92343	33238.03663	39148.95359	36998.96283	38005.93986
13.56_395.2198m/z	395.219788	13.5607	pos	PA(15:1(9Z)/0:0)	82340	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphates			38.8	0	M+H	C18H35O7P	1.195879924	2057.900655	2740.553982	2219.380679	2568.707934	2325.61792	2600.994565	2875.532202	2678.797198	2434.460933
13.81_284.2942m/z	284.2942306	13.81325	pos	Octadecanamide	HMDB0034146	Organic acids and derivatives	Carboximidic acids and derivatives	Carboximidic acids	*	C13846	38.8	0	M+H	C18H37NO	-1.978954827	29623.59675	26675.32293	26050.20193	23461.99639	25149.76199	24119.49747	26806.04359	24710.92089	26016.82501
13.97_310.3098m/z	310.3098412	13.97213333	pos	Geranylcitronellol	HMDB0032147	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	*		38.8	0	M+NH4	C20H36O	-2.053349301	5105.170756	5112.329018	4480.586407	7146.934592	3666.778105	4497.749033	4822.017875	4500.872736	4819.902288
14.04_322.2770m/z	322.2770282	14.0456	pos	Methadone blue	1222	Unclassified	Unclassified	Unclassified			38.8	0	M+K	C19H21NO3S	-1.583894568	1688.220736	2239.053436	23.06996553	23.64467216	0.001403199	671.5562114	0.001403199	671.5562114	0.001403199
14.19_228.1955m/z	228.1954539	14.19346667	pos	Citral propylene glycol acetal	HMDB0037286	Organoheterocyclic compounds	Dioxolanes	1,3-dioxolanes	*		38.8	0	M+NH4	C13H22O2	-1.672728773	1097.448144	877.2604414	673.0113245	509.5898372	769.0093381	696.8260996	967.5167385	741.4483179	670.6307279
14.33_310.3099m/z	310.3098531	14.33463333	pos	3,7,11,15-Tetramethyl-6,10,14-hexadecatrien-1-ol	LMFA05000210	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols			38.8	0	M+NH4	C20H36O	-2.0126291	2448.362324	2770.080158	2572.081931	2006.298715	2057.455506	1789.658041	2629.5926	2072.479921	4536.906217
14.59_226.1587m/z	226.1586587	14.59043333	pos	cis-1,2-Diphenylcyclobutane	70084	Phenylpropanoids and polyketides	Stilbenes	Unclassified		C14467	38.8	0	M+NH4	C16H16	-1.765241324	888.0711273	1203.148755	1150.9139	1124.019992	1310.667291	1213.166127	1350.28545	1220.914215	1124.645956
14.83_284.2940m/z	284.2940316	14.82528333	pos	Safingol (L-threo-sphinganine)	53955	Lipids and lipid-like molecules	Sphingolipids	Sphingoid bases			38.8	0	M+H-H2O	C18H39NO2	-2.521397295	6716.944533	6036.56524	6231.365686	5525.334434	6594.692433	6605.053182	6850.674694	5869.180116	7037.986119
15.10_167.0551m/z	167.0550863	15.10426667	pos	Arabinonic acid	HMDB0000539	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C00878	38.8	0	M+H	C5H10O6	0.432766701	14.87295573	807.9884655	42.46785028	7.192842669	8.068156784	5.994316786	20.47305493	18.51515746	13.44538299
15.27_245.0992m/z	245.0992485	15.27166667	pos	Isopropyl beta-D-glucoside	HMDB0032705	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		38.8	0	M+NH4	C9H18O6	-1.398043155	2140.228973	2222.988101	2175.267167	1246.179836	1159.736939	1182.488243	1384.296006	1531.180257	1478.139095
2.11_130.0862m/z	130.0861627	2.113216667	pos	2-Pyrrolidineacetic acid	HMDB0029444	Organoheterocyclic compounds	Pyrrolidines	Unclassified	*		38.8	0	M+H	C6H11NO2	-0.715415378	1646.993791	1092.957397	1306.061969	1192.234398	952.6944678	1140.857691	1228.200608	1197.837445	1196.1399
2.18_211.0710m/z	211.0710309	2.178633333	pos	2'-Deoxyuridine	91	Nucleosides, nucleotides, and analogues	Pyrimidine nucleosides	Pyrimidine 2'-deoxyribonucleosides	**	C00526	38.8	0	M+H-H2O	C9H12N2O5	-1.325496444	1216.170635	1406.048204	1475.7287	2383.796392	2269.20424	2164.633285	1263.834621	1484.475565	1393.330875
2.36_326.1454m/z	326.1454004	2.360916667	pos	2-O-alpha-D-Galactopyranosyl-1-deoxynojirimycin	HMDB0041337	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			38.8	0	M+H	C12H23NO9	2.591647392	52137.358	51097.27136	48725.03585	50073.72613	49809.43711	52302.06857	49188.39881	50693.07029	47551.70813
2.80_371.1009m/z	371.100886	2.804116667	pos	Camptothecin	3491	Unclassified	Unclassified	Unclassified			38.8	0	M+H	C20H16N2O4	1.891079994	1472.447409	1327.636345	1119.877534	1521.10766	1350.983387	1699.05071	1832.452122	1490.790418	1556.024768
2.82_144.0654m/z	144.0653524	2.821016667	pos	Methyl 2-furoate	HMDB0029750	Organoheterocyclic compounds	Furans	Furoic acid and derivatives	*		38.8	0	M+H	C6H6O3	-1.326748215	1886.598777	1291.029748	1562.591455	1212.958198	1494.548939	1551.256705	1646.019413	1321.267929	
3.07_118.0500m/z	118.0499639	3.07445	pos	Succinic anhydride	24050	Organic acids and derivatives	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives	*	C19524	38.8	0	M+H	C4H4O3	0.94372678	29.8425838	57.42175465	52.19266199	61.80538636	75.81362075	53.42206683	80.71125183	25.07382167	47.60156406
3.14_233.1532m/z	233.1531868	3.139516667	pos	(3beta,6beta)-Furanoeremophilane-3,6-diol	HMDB0035117	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.8	0	M+H-H2O	C15H22O3	-1.676985698	522.6383843	434.5078404	329.527772	270.5019601	311.5994583	268.3839367	413.4881763	330.3678405	314.7590422
3.22_334.1129m/z	334.1128834	3.215533333	pos	N-acetyl-O-acetylneuraminate	HMDB0060492	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			38.8	0	M+H-H2O	C13H21NO10	-1.065902943	2306.680639	1848.584097	2598.26244	0.001403199	0.001403199	51.45408058	1180.25806	1829.282396	1184.123475
3.26_302.1593m/z	302.1593334	3.258783333	pos	Etamiphylline	HMDB0041889	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives			38.8	0.326	M+Na	C13H21N5O2	2.105523648	6757.099123	7215.281016	7593.596402	12096.60975	12552.84167	11748.04972	9613.135493	10259.38489	10035.33001
3.28_187.0938m/z	187.093784	3.280766667	pos	Psoralene	43312	Unclassified	Unclassified	Unclassified			38.8	0	M+Na	C7H6O4	-1.801896705	39960.30422	32880.07292	29337.31441	35550.93477	41372.64456	37086.67566	40070.42762	32447.59887	33449.83357
3.54_289.2522m/z	289.2522028	3.5398	pos	Nicaltaxol	64023	Unclassified	Unclassified	Unclassified			38.8	0	M+Na	C20H34O2	-1.351398202	9179.940997	8859.629481	8413.756856	2204.136132	2102.80798	1840.042677	4812.309222	2119.18097	2634.823325
3.57_255.0836m/z	255.0835546	3.568016667	pos	Ethyl pyruvate	87833	Organic acids and derivatives	Keto acids and derivatives	Alpha-keto acids and derivatives	*		38.8	0	M+Na	C10H16O6	-1.526740294	2985.704604	3109.185467	2246.392901	2761.974822	2518.873758	3291.474033	2693.370397	3088.928128	2828.446894
3.57_413.2656m/z	413.2656249	3.568016667	pos	Pregnan-20-one, 17-(acetyloxy)-3-hydroxy-6-methyl-, (3a,5b,6a)-	1090	Unclassified	Unclassified	Unclassified	***		38.8	0	M+Na	C24H38O4	-1.551318963	3977.599177	4768.249661	2688.960376	1941.289995	2031.318779	2611.54646	4162.585041	3460.860832	2736.220416
3.78_348.1760m/z	348.1759927	3.781933333	pos	2'-N-Acetylparomamine	71791	Unclassified	Unclassified	Unclassified			38.8	0	M+H-H2O	C14H27N3O8	-1.462080936	1831.35482	1891.465885	1990.147085	3160.657957	2393.336453	3058.889815	1771.28687	2678.080894	2359.780697
3.80_378.0790m/z	378.0789708	3.80375	pos	2,5-Diimino-6-(5-phospho-D-ribitylamino)pyrimidin-4(3H)-one	72671	Unclassified	Unclassified	Unclassified			38.8	0	M+Na	C9H18N5O8P	1.270030732	2443.620337	2998.473633	3011.657118	663.273748	697.8141835	761.2792553	2134.909432	2199.909103	2424.834264
3.91_155.1379m/z	155.1378647	3.911966667	pos	3-Hydroxy-carnuranan	88702	Organoheterocyclic compounds	Coumarans	Unclassified	*		38.8	0	M+NH4	C12H15NO4	-1.010004675	681.1773553	691.9477405	663.6618047	575.4166429	630.8045078	596.2449815	431.6157139	597.7482093	529.0641394
4.00_149.1072m/z	149.1072218	4.002016667	pos	3-Methylindole	HMDB0000466	Organoheterocyclic compounds	Indoles and derivatives	Indoles	**	C08313	38.8	0	M+NH4	C9H9N	-0.785994071	1511.035173	1205.662744	952.1284949	507.445532	515.0273612	489.1842394	892.1734326	679.4978527	748.2390781
4.02_337.0526m/z	337.052609	4.024633333	pos	Salicyl phenolic glucuronide	619	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		38.8	0	M+Na	C13H14O9	-1.253680467	5381.347674	5970.329	5806.081423	567.9024082	705.5016775	619.8393266	792.580054	1073.725794	990.2122274
4.09_289.2522m/z	289.2522196	4.091916667	pos	Taxa-4(20),11(12)-dien-5α-ol	41257	Unclassified	Unclassified	Unclassified			38.8	0	M+H	C20H32O	-1.292228536	6087.423446	3778.183921	2868.836308	1108.50936	1212.310298	1226.942224	2437.76007	1870.754698	1742.353745
4.18_167.0815m/z	167.0815093	4.182316667	pos	2-methyl-3-Pyrimidin-2-yl-Propionic Acid	45030	Unclassified	Unclassified	Unclassified			38.8	0	M+H	C8H10N2O2	0.032019998	1610.549122	1451.330343	1474.21974	529.5460559	517.9974356	711.6770355	690.2015708	749.7789347	796.5068322
4.22_294.0994m/z	294.0993871	4.317083333	pos	Suberylglycine	5899	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.8	0	M+Na	C10H17NO5	-2.190575532	1498.887506	1480.609151	1391.326772	1896.72667	1598.887506	1700.979102	1318.761798	1665.668568	1508.957263
4.43_330.1179m/z	330.1179486	4.42815	pos	isorhamnetin 3-rutinoside-7-glucoside	HMDB0304580	Lipids and lipid-like molecules	Polyketides	Flavonoids	*		38.8	0	M+NH4	C14H16O8	-1.263686818	2006.990055	1884.525956	2091.064633	2144.20053	2019.013574	1930.555137	1757.378856	2262.971092	2142.393196
4.45_421.1098m/z	421.1097827	4.451133333	pos	5-(3',4'-dihydroxyphenyl)-gamma-valerolactone-3'-O-glucuronide	HMDB0029190	Benzenoids	Phenol ethers	Unclassified	*		38.8	0	M+Na	C18H22O10	-1.845941096	1314.938108	2019.181943	1757.661676	1876.797596	1447.513108	1855.255515	3562.517431	4678.115041	3532.704508
4.50_220.1694m/z	220.1694265	4.496783333	pos	(±)-Anisoxide	HMDB0030572	Organoheterocyclic compounds	Coumarans	Unclassified	*		38.8	0	M+NH4	C14H18O	-0.812571245	1532.727526	1731.465545	1558.485809	854.0872976	765.4746654	819.3556278	1307.208374	1688.952974	1556.003492
4.52_141.0908m/z	141.0908211	4.51925	pos	trans-4-Hydroxycyclohexylacetic acid	HMDB0000909	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols	*		38.8	0	M+K	C8H14O3	-1.170159758	2424.601216	2302.516178	2301.012028	2735.228981	3014.426119	2516.439618	2877.641497	2638.58489	2744.419378
4.63_425.1769m/z	425.1769471	4.63335	pos	N,N'-diacetylchitobiose	HMDB0062702	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C01674	38.8	0	M+H	C16H28N2O11	0.850898197	1160.395403	1401.354709	1449.477135	887.1523779	1579.579605	927.1749328	1277.417256	1450.131373	1512.771523
4.66_561.1936m/z	561.1936579	4.656183333	pos	Citrusin A	HMDB0039230	Lignans, neolignans and related compounds	Lignan glycosides	Unclassified	*		38.8	0	M+Na	C28H34O12	-1.076313328	7731.665701	7560.481066	7624.835806	6572.021655	6633.396251	2710.837474	2457.022047	2322.707698	
4.68_196.0942m/z	196.094164	4.678916667	pos	N-Isovalerylglycine methyl ester	6385	Unclassified	Unclassified	Unclassified			38.8	0	M+Na	C8H15NO3	-1.444622914	3300.328541	2982.635175	3027.992581	3679.461895	4006.671617	3683.102347	4122.9321	3235.850306	3657.845731
4.79_396.0661m/z	396.0661394	4.7912	pos	N-Acetylmuramic acid 6-phosphate	63225	Unclassified	Unclassified	Unclassified			38.8	0	M+Na	C11H20NO11P	-1.282231727	12364.20716	13999.76562	13243.89145	22271.53678	20273.13903	20413.19735	11208.64503	12592.76405	11127.51438
4.86_399.1257m/z	399.1256762	4.8596	pos	N-Isovalerylglycine ethyl ester	6385	Unclassified	Unclassified	Unclassified			38.8	0	M+Na	C10H17NO3	-1.306481647	17033.26201	18110.85719	17768.05096	26637.46129	25494.54793	25879.81649	18207.51059	19907.37105	20125.53702
4.90_536.1524n	559.1413809	4.904516667	pos	Vaccinoside	HMDB0034733	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		38.8	0	M+H, M+Na	C25H28O13	-1.08675633	18358.45705	20287.73508	21167.28924	140.4875031	0.001403199	0.001403199	755.7067239	996.2512101	771.7925723
5.13_423.1256m/z	423.1255624	5.125733333	pos	2,3-Butanediol apiosylglucoside	88905	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		38.8	0	M+K	C15H28O11	-1.971446029	4938.118891	4438.537512	5284.948878	8892.47626	7298.880036	7665.275786	5448.019908	6236.235181	5547.369249
5.17_173.1324m/z	173.1323602	5.1709	pos	beta-Damascenone	HMDB0013804	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		38.8	0	M+H-H2O	C13H18O	-0.614214238	88.23140404	212.3064286	124.4834073	61.07899924	18.92227511	36.91406609	115.4156491	0.008134117	21.41010149
5.19_209.1534m/z	209.1534242	5.193566667	pos	3-Hydroxy-beta-ionone	91835	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.8	0	M+H	C13H20O2	-0.875070752	2690.074647	2505.420835	2430.908441	1856.327691	1845.55311	1807.80797	2516.097398	2049.866579	1971.077041
5.19_273.0753m/z	273.0753373	5.193566667	pos	Cyclo(his-pro)	HMDB0250630	Organic acids and derivatives	Carboximidic acids and derivatives	Amino acids, peptides, and analogues	*		38.8	0	M+K	C11H14N4O2	2.150875072	1691.502039	2042.394449	1633.207739	1282.788362	1237.84374	1215.915261	1768.163252	1866.747156	1772.251626
5.26_297.2209m/z	297.2209364	5.26135	pos	Etretinate metabolite	2649	Unclassified	Unclassified	Unclassified			38.8	0	M+H	C21H28O	-1.200295339	1988.459394	2383.249851	2323.174583	1343.019765	1464.35605	1243.994265	1811.19652	2131.042144	2033.611576
5.35_321.1440m/z	321.1439555	5.351683333	pos	Iso-Olomoucine	96580	Unclassified	Unclassified	Unclassified			38.8	0	M+Na	C15H18N6O	1.762899434	442.3194703	417.3836244	507.719298	688.9690614	562.6294905	680.9441984	501.1051993	651.9434706	685.6437354
5.48_267

6.93_281.1740m/z	281.1739639	6.928783333	pos	Tetranor-PGE1	74976	Unclassified	Unclassified	Unclassified			38.8	0	M+H-H2O	C16H26O5	-2.588290606	605.189156	690.1706089	646.155643	790.913961	548.8255972	557.8357904	508.0242386	610.1131524	629.5746603
7.02_233.1534m/z	233.1534314	7.01515	pos	(Z)-8-Decene-4,6-diyn-1-yl 3-methylbutanoate	LMFA07010705	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohol esters	*		38.8	0	M+H	C15H20O2	-0.753285793	802.4569339	634.8447232	658.4580181	601.6026431	722.988614	628.6899013	645.2963266	475.5385986	617.8803175
7.05_219.1377m/z	219.1377236	7.046666667	pos	(R)-Pterosin B	HMDB0030759	Benzenoids	Indanes	Indanones	*		38.8	0	M+H	C14H18O2	-1.066487184	555.5015464	607.3224022	562.5210601	616.03939	712.1396026	606.6846386	693.008688	556.9250929	447.8867638
7.26_193.1585m/z	193.1584646	7.25695	pos	2,5-Diisopropyl-4-methylphenol	HMDB0029821	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		38.8	0	M+H	C13H20O	-1.181744959	2075.182712	1763.918699	1782.307232	1929.426121	1564.614003	1362.162422	1394.732906	1583.235451	1538.342952
7.29_593.3287m/z	593.3286994	7.294266667	pos	Epoxomicin	45091	Unclassified	Unclassified	Unclassified			38.8	0	M+K	C28H50N4O7	-4.344914166	63805.33302	91350.91139	79126.55582	14768.29653	16737.87409	15001.21291	41907.75026	57320.3142	51278.54089
7.33_230.1514n	253.1405569	7.332033333	pos	Dipropyl hexanedioate	HMDB0041614	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.8	0	M+H+H2O, M+Na	C12H22O4	-1.896144464	13560.26128	13882.19455	11809.3838	15921.40937	15691.27608	16017.54323	11935.34828	13517.51423	12618.43851
7.37_837.3547m/z	837.3546573	7.36631667	pos	Kurilensoside H	LMST05050017	Lipids and lipid-like molecules	Sterol Lipids	Steroid conjugates			38.8	0	M+Na	C32H54O11	-1.914084025	24418.65594	25466.8611	25243.17448	23695.17104	24531.38663	25292.04692	21812.97076	28002.74216	25049.80064
7.45_195.1377m/z	195.1376844	7.448183333	pos	(±)-Myrtenyl acetate	HMDB0035126	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		38.8	0	M+H	C12H18O2	-1.400144788	2396.746015	2207.715342	2169.091294	2145.80742	2639.175107	2323.739661	2047.046725	2265.854045	1898.915765
7.45_549.3050m/z	549.3050156	7.448183333	pos	PERUVOSIDE	43469	Unclassified	Unclassified	Unclassified			38.8	0	M+H	C30H44O9	-1.447763251	5769.499114	5507.339794	7105.728842	1048.542777	833.9926705	919.194432	2655.187996	3000.092967	2805.129345
7.61_513.1358m/z	513.135815	7.606533333	pos	6-Feruloylglucose 2,3,4-trihydroxy-3-methylbutylglycoside	HMDB0036214	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		38.8	0	M+K	C21H30O12	-2.25535149	5759.311885	4812.049635	4721.728904	3586.26568	6326.761852	5666.48626	5958.020063	6194.648459	4693.141202
7.78_120.0808m/z	120.0807953	7.780633333	pos	(R)-(-)-2-Phenylglycinol	45040	Unclassified	Unclassified	Unclassified			38.8	0	M+H+H2O	C8H11NO	0.142728523	1737.958539	1491.93668	1170.331171	679.3861372	771.8824191	689.6239338	1217.671989	913.6425481	847.2731147
7.95_163.0388m/z	163.0387563	7.950883333	pos	4-Coumaryl alcohol	HMDB0003654	Phenylpropanoids and polyketides	Cinnamyl alcohols	Cinnamyl alcohols	***	C02646	38.8	0	M+H	C9H9O3	-1.321559469	960.1709826	570.0993255	585.6648402	1085.318462	562.0422076	662.1397137	899.1853255	752.3666531	589.2433891
7.95_358.2502n	359.2574371	7.950883333	pos	24,25,26,27-Tetranor-23-oxo-hydroxyvitamin D3	HMDB0060114	Lipids and lipid-like molecules	Steroids and steroid derivatives	Vitamin D and derivatives	*		38.8	0	M+H+H2O, M+H	C23H34O3	-1.53314805	18836.12844	16807.24097	18409.14251	12525.04365	11455.2098	10314.14238	12469.01443	13751.22171	11390.44554
8.98_437.2140m/z	437.2140036	8.982066667	pos	methyl 5-hydroperoxy-6,8,9,11-bisepidioxy-12,14-eicosadienoate	74484	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			38.8	0	M+Na	C21H34O8	-1.412486118	5967.588573	7955.15963	7736.499373	2558.549844	2771.390738	2424.429763	3473.604556	4122.449937	4025.483721
9.93_281.1379m/z	281.1379046	9.9276	pos	Nigellic acid	HMDB0036094	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.8	1.49	M+H	C15H20O5	-1.590689458	5703.19433	3888.201862	5982.911816	7767.590139	3622.647998	4125.635208	3536.383985	3091.479597	5911.034071
9.96_285.2031m/z	285.2031247	9.958533333	pos	Arginyl-Lysine	85629	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.8	0	M+H-H2O	C12H26N6O3	-0.747134878	4357.805502	5292.472496	2500.785956	5267.638345	1548.882761	1867.813343	2866.861405	3242.770268	2851.492593
0.51_138.1022m/z	138.1022066	0.51135	pos	Benzamidine	65652	Unclassified	Unclassified	Unclassified			38.7	0	M+NH4	C7H8N2	-3.058256208	289.9583646	1227.521625	156.2554525	580.8139312	215.6864611	1085.36181	1893.03899	456.1927181	1072.995071
0.54_145.0525n	184.0128992	0.535	pos	3-Methyleneoxindole	65836	Unclassified	Unclassified	Unclassified			38.7	0	M+NH4, M+K	C9H7NO	-2.007905159	591.5141659	934.0554749	1045.474448	876.1712273	182.6099487	1016.553626	550.8661147	822.3357945	1089.972214
0.54_494.2674m/z	494.2673645	0.535	pos	15-HETE-DA	75532	Lipids and lipid-like molecules	Fatty Acyls	Fatty amides			38.7	0	M+K	C28H41NO4	1.422400573	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	480.3808272	185.4477365	0.001403199	1553.692916
0.62_106.0377m/z	106.0377238	0.616683333	pos	5-Aminoimidazole	HMDB0003929	Organoheterocyclic compounds	Azoles	Imidazoles	**	C05239	38.7	0	M+Na	C3H5N3	1.877319369	165.5788051	184.3690217	201.4067748	326.3191927	397.810782	309.2021637	281.5177117	325.5074707	307.7831195
0.64_148.0272m/z	148.0271771	0.63615	pos	2-Aminomethylpyrimidine (hydrochloride)	44990	Unclassified	Unclassified	Unclassified			38.7	0	M+K	C5H7N3	0.199797429	489.566691	1008.908474	750.0509334	840.9509804	952.7073753	997.6596087	1249.284829	1184.150467	1039.616516
0.68_110.0714m/z	110.0713595	0.6788	pos	4-Pyrimidine Methanamine (hydrochloride)	45035	Unclassified	Unclassified	Unclassified			38.7	0	M+H	C5H7N3	0.786636952	15494.08719	16392.97132	17203.63247	21991.66968	23983.89816	24804.82361	23019.05513	22763.18779	22978.10677
0.68_162.1002m/z	162.1074388	0.6788	pos	2,6-Diamino-5-hydroxyhexanoic acid	HMDB0245508	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C16741	38.7	0	M+H-H2O, M+H	C6H14N2O3	-1.620195101	3139.691956	3587.444049	3578.083333	3911.66127	4075.166318	4796.136173	3381.790161	3660.630221	3620.531173
0.70_246.1808m/z	246.1808074	0.698133333	pos	Lysyl-Valine	85866	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.7	0	M+H	C11H23N3O3	-1.674728279	1656.09841	1915.091881	2477.60734	2329.528707	2339.342873	2941.936722	2346.96142	2139.993744	2407.881278
0.74_219.1338m/z	219.1337879	0.73955	pos	Isoleucyl-Serine	85821	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.7	0	M+H	C9H18N2O4	-0.667573819	2323.590369	3012.448897	2745.67186	2065.509967	3285.835988	2351.800669	1809.224704	1859.152741	1909.441917
0.76_115.0865m/z	115.0864537	0.758666667	pos	Ornithine	HMDB0000214	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***	C00077	38.7	0	M+H-H2O	C5H12N2O2	-1.026905468	4466.981405	4212.887013	3671.418514	8063.088786	8118.666163	8030.734487	4129.644323	3302.181441	3740.118573
0.76_130.0610m/z	130.0610201	0.758666667	pos	ALBIZZIINE	43854	Unclassified	Unclassified	Unclassified			38.7	0	M+H-H2O	C4H9N3O3	-0.563230781	1382.597442	1664.681696	1660.239729	2614.7121	2919.186112	2809.604716	1592.975171	1429.055351	1134.595873
0.80_233.0628m/z	233.0627598	0.799833333	pos	MANNOHEPTULOSE	HMDB0254327	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C08236	38.7	0	M+Na	C7H14O7	-1.797552191	17954.07132	20395.31615	21098.26725	16656.6839	17208.01868	18285.76856	18293.72752	20822.21158	18798.65704
0.84_130.0975m/z	130.0975034	0.8386	pos	4-Guanidinobutanal	63476	Unclassified	Unclassified	Unclassified			38.7	0	M+H	C5H11N3O	0.116421343	28.89384504	45.34095676	105.7257548	41.98894324	72.48192959	0.001403199	118.4289832	117.2524319	62.19968576
0.84_271.0897m/z	271.0897244	0.8386	pos	Threonylglutamic acid	HMDB0029060	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.7	0	M+Na	C9H16N2O6	-1.34026091	2554.204687	2086.185279	2099.401718	2897.964083	2767.840736	2604.572127	2674.93435	2683.666536	2691.625891
0.88_146.1172m/z	146.1172443	0.8802	pos	4-Trimethylammoniobutanoic acid	HMDB0001161	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C01181	38.7	0	M+H	C7H15NO2	-2.142068295	5437.211663	6714.404591	6190.964096	6247.394476	6148.239257	9570.371255	3914.306438	4312.821755	4394.0784
0.88_260.1964m/z	260.1963789	0.8802	pos	Isoleucyl-Lysine	85518	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.7	0	M+H	C12H25N3O3	-1.887565716	1326.048306	2523.614233	2656.34141	1958.270447	1709.666149	2063.41413	3626.454805	3903.910702	4064.184108
0.90_113.0234m/z	113.0233774	0.898483333	pos	Citraconic acid	LMFA01170099	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C02226	38.7	0	M+H-H2O	C5H6O4	0.438481414	459.5822891	299.8656569	379.7471498	197.2222162	360.558742	303.6843152	405.3713472	272.8433148	304.8091796
0.92_130.0651m/z	130.0610255	0.91985	pos	L-Alloisoleucine	66872	Unclassified	Unclassified	Unclassified			38.7	0	M+H-H2O	C4H9N3O3	-0.526696675	0.001403199	0.001403199	0.001403199	0.001403199	90.11422055	50.25852602	0.001403199	0.001403199	0.001403199
1.16_159.0529n	177.0867215	1.157483333	pos	N-Methyl-2-oxoglutaramate	66012	Unclassified	Unclassified	Unclassified			38.7	0	M+H, M+NH4	C6H9NO4	-1.670893616	5486.818344	4791.886744	4846.785143	5493.99658	4881.732725	4770.60946	4599.951338	4616.24867	3676.375846
1.16_364.1165m/z	364.1164577	1.157483333	pos	Monocrotaline	HMDB0034363	Organoheterocyclic compounds	Pyrrolizines	Unclassified	*	C10350	38.7	0	M+K	C16H23NO6	2.344122456	2349.798718	2636.950923	2987.948923	2797.15008	2761.533444	2374.136014	1907.406852	3133.23672	2096.324357
1.20_215.1025m/z	215.1025238	1.199716667	pos	L-Dopa	HMDB0000181	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***	C00355	38.7	0	M+NH4	C9H11NO4	-0.55575034	1456.180273	2359.837756	2147.789491	0.001403199	262.7855086	275.3924318	191.0570491	837.5358507	743.6484699
1.24_260.0560m/z	260.0560345	1.243033333	pos	2-Phthalimidoglutaric acid	2816	Unclassified	Unclassified	Unclassified			38.7	0	M+H	C13H11NO6	2.474934704	1458.465461	1755.107194	1974.695793	1622.123285	1686.812047	1819.703879	1565.616211	1501.529076	1505.79462
1.50_279.0946m/z	279.0946912	1.500483333	pos	4-beta-D-Ribofuranosyl)-1,4-dihydronicotinamide	HMDB0011648	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C15497	38.7	0	M+Na	C11H19NO5	-1.761462873	10417.12227	10975.05625	8910.453888	9102.629276	10465.40238	8979.507534	9824.5987	9843.461001
1.68_193.0970m/z	193.0969937	1.6764	pos	Gentianine	HMDB0303030	Unclassified	Unclassified	Unclassified			38.7	0	M+NH4	C10H9NO2	-0.916054159	0.001403199	143.8178807	38.96130549	1333.312395	1052.273429	1310.032078	27.9679116	163.6177149	31.44563071
10.09_270.2190n	293.2082418	10.0880333	pos	3-keto palmitic acid	LMFA01060051	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.7	0	M+H, M+Na	C16H30O3	-1.76123951	8337.977286	6389.681153	14069.58824	7765.3354	5785.153944	6818.41871	14991.02178	7628.851977	4939.000738
10.43_263.2366m/z	263.2366353	10.4331	pos	6,10,14-Trimethyl-5,9,13-pentadecatrien-2-one	89972	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	*		38.7	0	M+H	C18H30O	-1.169671784	4004.760461	2934.116077	2654.826555	2838.085842	3281.140135	2707.273034	2985.698408	3442.453394	3597.487789
10.60_263.2366m/z	263.236588	10.59638333	pos	Ricinenic acid	LMFA01030117	Lipids and lipid-like molecules	Fatty Acyls	Lineolic acids and derivatives	*		38.7	0	M+H-H2O	C18H32O2	-1.263365867	34390.26102	33073.12876	30692.89411	31687.47654	32129.7493	33287.82405	34027.615	32756.61558	30915.33125
10.65_179.1428m/z	179.1428332	10.64673333	pos	(Z)-4-Hydroxy-6-dodecenoic acid lactone	HMDB0032331	Organoheterocyclic compounds	Lactones	Gamma butyrolactones	*	C03107	38.7	0	M+H-H2O	C12H20O2	-1.062631738	2031.704754	1796.950044	1493.664015	1568.112287	1772.810175	1795.25717	1719.522153	1479.647827	1364.552336
10.68_235.1690m/z	235.1690313	10.67216667	pos	Curcumenol	71448	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*	C16942	38.7	0	M+H-H2O	C15H24O2	-0.961557789	2153.559061	1986.970527	1962.636897	2315.111362	1998.975527	1962.636897	2435.881004	2096.356365	2084.790845
10.82_605.5493m/z	605.5493075	10.82321667	pos	DG(O-16:0/18:6(0/0:0)	HMDB0111146	Lipids and lipid-like molecules	Glycerolipids	Diradylglycerols	*		38.7	0	M+Na	C37H74O4	2.361881525	10281.53014	9874.828188	8876.353251	6045.962838	7463.606299	5777.029031	8049.741679	8102.981268	8810.737514
10.96_219.1741m/z	219.1741021	10.9597	pos	2-Hydroxyacorenone	HMDB0030916	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		38.7	0	M+H-H2O	C15H24O2	-1.014944977	3021.742477	3359.102414	2554.347193	2960.898004	3119.139199	2950.937683	3028.947353	2998.358409	2733.292586
10.98_209.1533m/z	209.15334	10.97861667	pos	Acetal R	HMDB0036824	Benzenoids	Benzene and substituted derivatives	Unclassified	*		38.7	0	M+H	C13H20O2	-1.279288721	2804.268339	2685.704347	2147.559318	2080.605421	2186.32522	2375.184154	2253.784453	2492.840747	2284.812153
11.04_271.1688m/z	271.1688318	11.03985	pos	Cybutryne	68695	Unclassified	Unclassified	Unclassified			38.7	0	M+NH4	C11H19NS5	-4.386546207	6270.492354	5559.725644	5941.616781	6421.755785	7043.074942	6987.39953	6900.842196	6893.762231	6238.218566
12.16_259.2052m/z	259.2052802	12.07935	pos	Stearonic acid	LMFA01030357	Lipids and lipid-like molecules	Fatty Acyls	Linoleic acids and derivatives	**	C16300	38.7	0	M+H-H2O	C18H28O2	-1.309386072	2101.570911	2254.746251	2773.852947	2201.742273	3440.739441	2511.100649	2857.278061	2418.523538	2930.250719
12.22_199.1691m/z	199.1691049	12.21766667	pos	12-Hydroxydodecanoic acid	6465	Organic acids and derivatives	Hydroxy acids and derivatives	Medium-chain hydroxy acids and derivatives	*	C08317	38.7	0	M+H-H2O	C12H24O3	-0.700959934	1197.277759	1347.613429	953.2318008	1052.453076	1106.57726	1277.49338	1410.65309	970.405871	1128.572075
12.46_204.1382m/z	204.1381582	12.45588333	pos	(E)-2-Tridecene-4,6,8-triyn-1-ol	87296	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		38.7	0	M+NH4	C13H14O	-0.711391728	363.6220822	183.5716911	364.9951043	273.8157417	252.9032642	355.316955	363.2422718	351.5025311	403.7602913
13.09_369.3511m/z	369.3510982	13.08768333	pos	5α-cholest-8-en-3β-ol	41660	Lipids and lipid-like molecules	Steroids and steroid derivatives	Cholestane steroids	**	C03845	38.7	0	M+H-H2O	C27H46O	-1.241381334	2959.572281	3596.102965	4018.266307	2094.022941	1586.668615	4945.113778	4646.333912	3112.698602	2369.150743
13.16_425.2866m/z	425.2866221	13.16496667	pos	Sorbitan palmitate	86566	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.7	0	M+Na	C22H42O6	-1.833517673	13645.44047	13312.30031	13296.73108	14287.31894	11942.53335	13266.90541	13653.98143	12042.08332	14508.97397
13.23_284.2942m/z	284.2942255	13.23251667	pos	3E,13Z-octadecadien-1-ol	LMFA05000048	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		38.7	0	M+NH4	C18H34O	-2.124571893	6309.086936	5928.186051	6240.097544	6307.005314	6147.017679	6940.490599	6675.436513	6036.578727	6274.565671
13.91_191.1555m/z	191.1554503	13.91423333	pos	Oxymonone	HMDB0015323	Benzenoids	Phenanthrenes and derivatives	Unclassified	*	C08019	38.7	0	M+H	C17H19NO4	0.719404837	391.5862628	990.6841114	354.2792915	449.9960314	0.001403199	344.9706037	497.6458555	343.3182385	677.1158763
14.34_316.2242m/z	316.2242189	14.34413333	pos	Val-Val-Val	HMDB0094676	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.7	0	M+H	C15H29N3O4	3.603089041	42318.07693	43899.03336	40400.90569	42079.50624	47346.75758	50076.20983	46340.52925	44059.51467	45589.07723
14.71_284.2942m/z	284.2941641	14.71186667	pos	octadecan-2E,13Z-dien-1-ol	75280	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		38.7	0	M+H	C18H34O	-2.355452646	3115.830223	3531.822952	1864.36029	2614.04433	2936.728536	2725.642186	2844.420837	2646.283219	2274.908811
14.79_208.1077m/z	208.1077334	14.78525	pos	Indole-3-acetaldoxime N-oxide	71605	Unclassified	Unclassified	Unclassified			38.7	0	M+NH4	C10H10N2O2	-1.682221216	8139.986617	7251.272389	7527.190027	8316.062471	8314.831938	7944.585663	8422.284111	7942.984168	8258.883984
14.95_167.1062m/z	167.1061684	14.95311667	pos	6-Pentyl-2H-pyran-2-one	87397	Organoheterocyclic compounds	Pyrans	Pyranones and derivatives	*		38.7	0	M+H	C10H14O2	-2.948083859	465.7855733	323.4425475	365.9149899	445.7730013	436.7853867	414.1154095	500.1063695	404.6386517	399.477716
15.15_208.1077m/z	208.1077334	15.13066667	pos	4-(Methylcarbamoyl)-1-(3-pyridyl)-1-butanone	HMDB0011603	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C16453	38.7	0	M+H	C10H13N3O2	-1.516610292	3872.205986	3287.467191	2969.893971	3174.559384	3123.846342	2962.883756	3225.564556	3375.611486	3239.945546
15.27_271.2413m/z	271.2413406	15.26638333	pos	ar-Artemisene	93751	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.7	0	M+H	C20H30	-2.541609573	1262.715254	883.5418062	758.6251151	387.1246907	601.5590118	371.5115575	732.2990738	390.3070766	500.0583254
15.29_264.0896m/z	264.0896121	15.29438333	pos	4'-(DIMETHYLAMINO)AZOXYBENZENE N-OXIDE	24046	Unclassified	Unclassified	Unclassified			38.7	0	M+K	C14H15N3	-0.637432824	255.8243931	214.7654081	137.3985437	525.5382057	358.7361002	166.4392867	3319.503036	313.319134	104.6358481
15.29_389.1107m/z	389.1107372	15.29438333	pos	N-Caffeoyltryptophan	HMDB0029830	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.7	0	M+Na	C20H18N2O5	-0.150744489	0.001403199	286.4458401	36.28619505	102.5180677	46.93548611	0.001403199	4037.210142	210.1889448	154.6276416
15.51_134.0594m/z	134.059403	15.50691667	pos	Diammonium sulfite	88579	Unclassified	Unclassified	Unclassified			38.7	0	M+NH4	H8N2O3S	0.123358307	12.06717556	47.42049405	0.001403199	12.59106742	47.90404839	32.4443553	294.4529327	8.643361568	10.45757467
2.14_159.0161m/z	159.0160685	2.1354	pos	Carbamoyl phosphate	HMDB0001096	Organic acids and derivatives	Organic phosphoric acids and derivatives	Unclassified	**	C00169	38.7	0	M+H	C2H6NO5P	-3.304896354	7257.645402	532.6784127	844.6805316	253.9224541	286.1758197	430.0373899	506.7359224	591.2390203	1275.611486
2.42_181.1101n	182.1173832	2.421616667	pos	cis-6-Nitro-p-mentha-1(7),2-diene	HMDB0035195	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		38.7	0	M+H, M+NH4	C10H15NO2	-0.949470841	516.771586	557.5652574	695.3589919	314.6336331	320.9491821	381.170086	297.2096912	537.6999193	425.2439483
2.48_174.9764m/z	174.9764013	2.484216667	pos	3-(Hydrohydroxyphosphoryl)pyruvate	63597	Unclassified	Unclassified	Unclassified			38.7	0	M+Na	C3H5O5P	-1.837456785	554.3870826	674.8155325	589.5009077	702.7972933	738.9763915	728.3703263	834.1108732	697.9892508	719.0232477
2.93_115.0503m/z	115.0502965	2.928333333	pos	N-Methylhydantoin	HMDB0003646	Organoheterocyclic compounds	Azolines	Imidazolines	**	C02565	38.7	0	M+Na	C4H6N2O2	0.81179669	537.4345351	451.6684082	562.8640286	553.5557221	623.1341041	649.1413557	640.7593324	591.2465061	578.3175321
3.11_163.0388m/z	163.0387874	3.112683333	pos	(E)-3-(2,3-Dihydroxyphenyl)-2-propenoic acid	HMDB0032057	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	**	C12623	38.7	0	M+H-H2O	C9H8O4	-1.017030679	2070.974647	1941.2185	1456.424519	1871.814612	1644.074214	1560.712045	1943.904747	1644.123672	1747.197152
3.24_221.1535m/z	221.1535025	3.238016667	pos	Glutinosone	67877	Unclassified	Unclassified	Unclassified			38.7	0	M+H	C14H20O2	-0.471421369	1347.196937	960.8813251	1450.588369	1509.827804	1581.964165	1106.197002	1496.401818	1335.071795	1008.358717
3.36_130.0862m/z	130.0861681	3.378983333	pos	Daunosine	HMDB0250880	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		38.7	0	M+H-H2O	C8H13NO3	0.591243364	807.2779256	618.9796585	425.9534589	538.8166296	642.993825	625.9534589	729.4076263	591.8060075	514.1519186
3.60_161.1322m/z	161.132194	3.596	pos	11-Methyl-7-oxatetracyclo[6.3.1.01,6.04,11]dodecane	HMDB0035055	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		38.7	0	M+H-H2O	C12H18O	-1.588528737	440.5349012	532.702744	253.1501111	428.4488164	277.2225256	424.8795881	552.4826313	469.3039932	508.1545108
3.69_224.1278m/z	224.1278454	3.6941	pos	Phenylmethylglycidic ester	HMDB0031729	Organoheterocyclic compounds	Epoxides	Oxirane carboxylic acids and derivatives	*		38.7	0	M+NH4	C12H14O3	-1.331512424	1389.705449	1465.508991	1412.6875	1604.375453	1207.537821	1218.08643	1173.046438	1382.556933	1181.065936
3.78_134.0599m/z	134.0599271	3.781933333	pos	Leukoaminochrome	HMDB0012992	Organoheterocyclic compounds	Indoles and derivatives	Indolines	*	C17756	38.7	0	M+H-H2O	C8H9NO2	-0.749120391	779.1850395	708.890509	895.1779595	319.2921527	436.6606176	333.352547	511.8281725	516.4539842	620.0724578
3.89_158.0577n	159.0650231	3.889633333	pos	Citraconic acid dimethyl ester	6495	Unclassified	Unclassified	Unclassified			38.7	0	M+H, M+Na, M+H-H2O	C7H10O4	-1.025509594	2220.588604	2108.147614	2429.931127	3209.823168	2627.661889	2707.609939	2578.440817	2843.903208	2754.164351
3.93_310.1395n	310.1394648	3.889633333	pos	(2S,4S)-Monatin	95722	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.7	0	M+NH4	C14H16N2O5	-0.966724464	711.7788619	780.9413979	895.2946409	1103.520661	968.8234282	1156.15894	983.1359537	1326.473007	1064.318734
3.93_160.1098n	183.0988637	3.9343	pos	5-Hydroxyajatyroic acid	HMDB0013898	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C16650	38.7	0	M+H-H2O, M+Na	C8H16O3	-0.825366349	4479.261545	4556.190114	4645.95463	4031.236103	3690.430435	3666.993011	4082.63831	4402.078286	4116.1148
4.02_304.0808m/z	304.0808473	4.024633333	pos	N6-Methyl-2'-deoxyadenosine	66047	Unclassified	Unclassified	Unclassified			38.7	0	M+K	C11H15N5O3	0.753758001	1064.36082	1338.734122	1277.456368	1504.903055	1506.47281	1545.151621	1065.162128	1327.659477	1402.503298
4.02_351.0116m/z	351.0116142	4.024633333	pos	Caftaric acid	HMDB0013680	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	***		38.7	0	M+K	C13H12O9	1.038772831	2122.79132	1636.658718	2151.304123	945.0499036	950.696148	1016.403651	3308.208824	3580.226422	3621.923677
4.11_325.1254m/z	325.12546	4.114783333	pos	Garcinia lactone dibutyl ester	HMDB0040462	Organic acids and derivatives	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives			38.7	0.0851	M+Na	C14H22O7	-1.084529452	5087.136952	5712.473867	5720.942867	5834.947775	5129.732276	5962.934432	4786.722761	5472.675833	5384.189797
4.25_352.1860m/z	352.1860268	4.249833333	pos	3'-N'-Acetylfusarochromanone	HMDB0037499	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans

5.59_209.1171m/z	209.1170772	5.590666667	pos	Isoelemicin	71476	Benzenoids	Phenol ethers	Anisoles	*	C16975	38.7	0	M+H	C12H16O3	-0.689916286	1830.440773	2030.736299	1903.001456	2941.647238	3224.978901	3124.77674	2207.852326	1832.939111	2476.991184
5.66_220.0342m/z	220.0342332	5.656316667	pos	FR 900098	63607	Unclassified	Unclassified	Unclassified			38.7	0	M+Na	C5H12NO5P	-1.505368848	3434.906054	3345.593047	3489.850971	5616.761579	5894.228974	5641.260432	3142.295208	3092.381553	3710.981724
5.70_227.2114m/z	227.2114267	5.69755	pos	Labienoxime	91209	Organic nitrogen compounds	Organonitrogen compounds	Oximes			38.7	0	M+NH4	C13H23NO	-1.736312132	640.4318856	1052.383584	712.6248488	1599.735554	1029.447842	935.4250474	706.8180769	605.6912389	1092.790657
5.77_289.0113m/z	289.0112784	5.7661	pos	2H-1-Benzopyran-6-acetic acid, 7-hydroxy-8-methoxy-2-oxo-	1210	Unclassified	Unclassified	Unclassified			38.7	0	M+K	C12H10O6	1.528876495	64746.26498	62425.29768	69313.68182	38338.90595	36209.04571	33206.05857	69467.15395	62827.6647	68152.99229
5.80_181.0718m/z	181.0717603	5.799666667	pos	Paraxanthine	HMDB0001860	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	**	C13747	38.7	0	M+H	C7H8N4O2	-1.341998029	1238.243626	1145.478368	1300.486676	2268.881141	1831.908058	1762.550661	1491.297182	1902.501184	1939.690129
5.82_182.0941n	183.1013769	5.821	pos	Amyl 2-furoate	HMDB0029456	Organoheterocyclic compounds	Furans	Furoic acid and derivatives	*		38.7	0	M+H-H2O, M+H	C10H14O3	-1.072833937	4542.388288	4068.94527	4642.49229	3659.335335	3755.319608	3846.864139	2805.329996	3521.176286	3589.08135
5.87_130.0650m/z	130.065034	5.8665	pos	INDOLE-3-CARBINOL	44445	Organoheterocyclic compounds	Indoles and derivatives	Indoles			38.7	0	M+H-H2O	C9H9NO	-0.623442017	4237.48908	2895.882024	2655.483002	2111.229577	2059.977885	2010.680894	2740.514598	2322.863146	2336.502267
5.91_113.0234m/z	113.0233768	5.9112	pos	Itaconic acid	44764	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C00490	38.7	0	M+H-H2O	C5H6O4	0.433293259	133.5637876	104.2693065	107.0225328	85.13660775	100.744408	114.2963266	190.6723288	108.9588703	164.957708
6.01_386.2533m/z	386.253258	6.01315	pos	20-hydroxy-PGE2	3814	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids	*		38.7	0	M+NH4	C20H32O6	-1.239089691	4660.014701	5795.859093	4760.619925	4424.243699	4103.351668	4203.057732	1670.33999	1895.678318	1783.470278
6.08_113.0234m/z	113.02338	6.084383333	pos	Mesaconic acid	LMFA01170116	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C01732	38.7	0	M+H-H2O	C5H6O4	0.458124975	212.2223871	205.2097269	206.1465437	164.5676762	206.0443812	178.1602364	210.4790207	251.102776	220.7565956
6.09_632.3632m/z	632.3632342	6.093533333	pos	Hydroxydestruxin B	94675	Organic acids and derivatives	Peptidomimetics	Depsipeptides			38.7	0	M+Na	C30H51N5O8	0.410024029	3973.661418	4235.252861	4629.633766	10258.15062	9186.074471	11601.10671	3842.878743	5463.441629	4556.564208
6.16_120.0808m/z	120.0808152	6.162416667	pos	p-Phenetidine	508	Unclassified	Unclassified	Unclassified			38.7	0	M+H-H2O	C8H11NO	0.288150949	2080.325966	1654.116039	1323.590021	773.0832018	707.5075328	722.5629528	1152.791612	1073.320581	934.7016672
6.18_171.0624m/z	171.0624205	6.182466667	pos	Pantoic acid	309	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C00522	38.7	0	M+Na	C6H12O4	-2.424834553	981.1545258	952.4781431	796.9425046	621.6761714	863.061572	626.5245797	738.0222157	859.906468	766.8058402
6.25_429.2265m/z	429.2265043	6.2535	pos	Austalide L	86764	Phenylpropanoids and polyketides	Flavonoids	Flavones	*		38.7	0	M+H	C25H32O6	-1.543308485	14536.71584	13222.79415	13203.9329	11831.77777	12458.79464	13201.33394	13376.95765	14333.83228	14651.65613
6.25_615.0746m/z	615.0745887	6.2535	pos	Myricetin 3-(2",3",4"-triacetylxyloside)	50883	Lipids and lipid-like molecules	Polyketides	Flavonoids			38.7	0	M+K	C26H24O15	-0.155226587	6438.156545	6767.666967	6870.060859	7467.91747	7356.785018	7837.899152	6249.040196	5605.641143	5502.365051
6.29_453.1725m/z	453.1725346	6.287516667	pos	Phenethyl rutinoside	88572	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		38.7	0	M+Na	C20H30O10	-1.358484979	9642.764333	12113.56883	10939.67679	11355.9123	10628.82097	11272.15251	7995.643169	7901.766748	8715.555905
6.64_465.2478m/z	465.2478146	6.638433333	pos	Testosterone glucuronide	2794	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	**	C11134	38.7	0	M+H	C25H36O8	-1.033757196	6616.631213	6451.172187	6933.88139	10156.69277	8302.619934	8389.228072	7988.312689	8676.504077	7484.15151
6.78_221.1534m/z	221.1533794	6.779133333	pos	Hexyl phenylacetate	HMDB0037714	Benzenoids	Benzene and substituted derivatives	Unclassified			38.7	0	M+H-H2O	C14H20O2	-1.03085588	8442.674702	8381.634273	8123.995673	9344.552469	9591.122804	8943.556513	7397.273358	7288.143596	7660.729839
6.79_534.3266m/z	534.3266175	6.7933	pos	L-Olivosyl-oleandolide	LMPK04000032	Lipids and lipid-like molecules	Polyketides	Macrolides and lactone polyketides	**	C11991	38.7	0	M+NH4	C26H44O10	-1.269923369	8427.518843	8001.100314	8200.859858	6729.813906	7030.804901	6120.985073	11002.13031	11369.3964	14190.75091
6.82_207.1379m/z	207.1379456	6.819833333	pos	2-Phenylpropyl butyrate	HMDB0034469	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.7	0	M+H	C13H18O2	-0.051657226	626.2838894	587.3008526	537.8786146	583.5361524	805.2211806	501.1178428	678.5886071	611.6665408	742.7261035
6.82_312.2165m/z	312.2164716	6.819833333	pos	Phytuberin	HMDB0035754	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*	C09709	38.7	0	M+NH4	C17H26O4	-1.574606179	3922.517863	3973.763096	3932.869234	6131.369625	6299.495001	5005.12701	3361.160302	3505.200714	3555.099219
6.92_296.1488m/z	296.1488191	6.919716667	pos	Marasmone	HMDB0036049	Organoheterocyclic compounds	Furofurans	Unclassified			38.7	0	M+NH4	C15H18O5	-1.546415742	1901.15222	2512.364076	2083.365134	4126.030789	2879.28901	3490.842287	2039.24796	3241.12637	3376.171172
7.13_149.0959m/z	149.0959084	7.131	pos	Dusf aldehyde	HMDB0032015	Benzenoids	Benzene and substituted derivatives	Benzenoid derivatives	*		38.7	0	M+H	C10H12O	-1.235745495	745.0758967	823.7763525	782.3860668	1077.856117	1041.464846	1037.661656	1090.551592	989.0554994	1055.578148
7.65_405.2630m/z	405.2629749	7.652983333	pos	7a,12a-Dihydroxy-3-oxo-4-cholenoic acid	5436	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	*	C15568	38.7	0	M+NH4	C24H36O5	-1.424321989	8481.866761	9032.747668	10209.9169	10406.51252	8865.73449	9070.214273	8836.734243	10941.03803	10604.23666
8.07_332.2191m/z	332.2190751	8.074933333	pos	Marimastat	HMDB0014924	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols			38.7	0	M+H	C15H29N3O5	3.253465443	3718.52439	3857.600534	4873.826412	4990.789275	5540.161806	4759.737887	4830.873983	4368.76818	5417.959263
8.13_310.2370m/z	310.2369875	8.13135	pos	(2'E,4'Z,7'Z,8E)-Colnelenic acid	HMDB0030996	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C16320	38.7	0	M+NH4	C18H28O3	-2.336798805	783.1894329	1491.708583	718.1590524	575.2248816	903.7044573	538.3145575	753.75625	1470.58414	695.5590536
8.28_455.2633m/z	455.2633048	8.280116667	pos	18-acetoxy-PGF2α-11-acetate	36162	Unclassified	Unclassified	Unclassified			38.7	0	M+H	C24H38O8	-1.408435541	4409.253638	4027.581496	4425.513254	4100.00584	3816.915687	3704.416494	3884.790511	3580.664382	5288.317921
8.41_271.0935m/z	271.0935452	8.405166667	pos	7-Hydroxy-6-(methoxyacetyl)-2,2-dimethyl-2H-1-benzopyran	HMDB0029774	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans	*		38.7	0	M+Na	C14H16O4	-2.315513069	5673.085546	5094.712125	5267.04354	5072.998785	5711.896356	5341.459884	6325.971652	5457.570307	5573.334019
8.97_410.2893m/z	410.2893878	8.97325	pos	20, 22-Dihydrodigoxigenin	HMDB0060730	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid lactones	*		38.7	0	M+NH4	C23H36O5	-1.814976695	4117.624992	5691.345744	5851.289718	4427.524976	4482.649224	4913.396473	2562.656296	3476.399719	3973.701009
8.98_203.1791m/z	203.179146	8.982066667	pos	(2-trans,6-trans)-farnesal	LMPR0103010012	Lipids and lipid-like molecules	Prenol lipids	Isoprenoids	**	C03461	38.7	0	M+H-H2O	C15H24O	-1.27695026	698.9413448	1330.517853	1234.825531	402.369851	438.1357897	423.8689192	519.6888635	713.4451203	611.3977932
9.16_437.2141m/z	437.2141352	9.158516667	pos	methyl 9,11-epidioxy-12,15-dihydroperoxy-5,7,13-eicosatrienoate	74992	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids			38.7	0	M+Na	C21H34O8	-1.09476919	2992.830201	3701.945013	4366.838785	1817.022397	1672.832016	2264.073747	2587.380108	2857.959641	2140.39521
9.73_354.2401m/z	354.2401702	9.72875	pos	C16 Sphinganine-1-phosphate	LMSP01050006	Lipids and lipid-like molecules	Sphingolipids	Sphingoid bases			38.7	0	M+H	C16H36NO5P	-0.611779584	2381.735415	3058.267052	1722.886031	2464.078184	1793.052024	2314.036025	1957.401293	2118.238925	2184.633497
9.81_235.1689m/z	235.1689264	9.806	pos	9-Pentadecene-12,14-dyne-1,11-diol	HMDB0034562	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		38.7	0	M+H	C15H22O2	-1.409124717	4237.833224	4816.722496	3367.682808	4075.174286	4138.67906	4248.541514	3819.565481	4509.867819	3822.211372
9.84_451.2993m/z	451.2993027	9.8393	pos	Methylarguacinosside A	93067	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			38.7	0	M+H	C19H42O10	-1.946806465	1240.7024	2494.60249	9861.132235	11036.5423	13582.70804	11932.31269	1280.694151	1140.75526	12148.5585
0.51_161.0817m/z	161.081681	0.51135	pos	Phenylethanolaminium	HMDB0062626	Organic nitrogen compounds	Organonitrogen compounds	Amines			38.6	0	M+Na	C8H12NO+	4.136916809	351.7837099	1855.631704	399.8453112	854.7465409	303.1433356	1333.350229	2540.664482	817.7604928	1300.344682
0.54_111.0917m/z	111.0916626	0.535	pos	Aniline	HMDB0003012	Benzenoids	Benzene and substituted derivatives	Aniline and substituted anilines	*	C00292	38.6	0	M+NH4	C6H7N	-0.131026855	216.0869994	520.7662361	224.3110343	307.2682592	174.08787	597.3598791	720.8178323	385.7323996	679.8576749
0.54_206.0204m/z	206.0204157	0.535	pos	Perflutren	HMDB0014696	Organohalogen compounds	Organofluorides	Unclassified			38.6	0	M+NH4	C3F8	-3.381148681	3752.152567	5893.028224	5526.76163	4177.211015	420.7915289	5095.845083	569.4226256	5475.957445	3790.265982
0.54_226.0116m/z	226.011637	0.535	pos	1-(Malonylamino)cyclopropanecarboxylic acid	HMDB0031700	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.6	0	M+K	C7H9NO5	2.173256117	4007.476936	4946.576789	4976.420143	4616.261285	2264.95653	5250.129723	1649.798616	5051.560936	5635.314288
0.72_202.0683m/z	202.0682609	0.7177	pos	Fructosamine	5808	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		38.6	0	M+Na	C9H15NO5	-1.85536801	5191.7	5936.398358	5870.186402	4831.253975	4659.475189	4602.225606	4363.917588	4289.228712	
0.72_206.0898n	206.0529628	0.7177166	pos	Seryltheronine	HMDB0029049	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.6	0	M+Na, M+K	C7H14N2O5	-2.171167724	22984.26905	23171.0347	28389.51891	34047.24118	36807.8239	35897.03489	27604.03817	28952.2338	28385.12201
0.72_260.1964m/z	260.1963741	0.7177166	pos	Leucyl-Lysine	HMDB0028934	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.6	0	M+H	C12H25N3O3	-1.905999852	5031.246817	5625.320755	6565.3264	7217.493478	7862.810559	7172.630402	4247.890454	4478.362992	4703.821267
0.74_117.1022m/z	117.1021542	0.73955	pos	1-Pyrrolidinecarboxaldehyde	90050	Organoheterocyclic compounds	Pyrrolidines	Unclassified			38.6	0	M+NH4	C5H9NO	-0.860746085	86.54502354	40.04420726	27.11239981	0.001403199	47.37678589	0.001403199	43.58583021	33.98181988	35.51525671
0.76_102.0551m/z	102.0551276	0.7586666667	pos	L-Threonine	HMDB0000167	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***	C00188	38.6	0	M+H-H2O	C4H9NO3	1.450354062	892.4275422	1164.12743	1126.058931	1354.885596	1734.47256	1645.555677	1206.61952	1165.68564	1177.943598
0.82_116.1071m/z	116.107051	0.818116667	pos	2-Methyl-4-pentenal	HMDB0030332	Organic oxygen compounds	Organic oxides	Unclassified			38.6	0	M+NH4	C6H10O	0.616715617	40776.102	42084.60354	43711.13288	47798.28398	47977.38296	46343.99654	33036.8513	39618.99961	35309.3589
0.84_178.0084m/z	178.0084281	0.8386	pos	Sodium fumarate	HMDB0030642	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C00116	38.6	0	M+H2Na2O4	C4H2Na2O4	-1.528433292	4114.237602	5126.920319	4135.164853	1185.519199	435.2329787	646.980097	1665.878176	922.9043882	1102.037148
0.86_231.1701m/z	231.1700509	0.859583333	pos	Leucyl-Valine	HMDB0028942	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***		38.6	0	M+H	C11H22N2O3	-1.16478004	2733.632791	2591.918883	2592.639703	1887.83164	1444.59538	1490.845292	1829.944255	1687.747284	1578.477202
0.86_261.0958n	262.1030886	0.859583333	pos	Asparaginylglutamic acid	HMDB0028730	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.6	0	M+H, M+Na	C9H15N3O6	-1.045708607	12068.56514	13541.14386	14601.37589	7515.336375	7166.711715	7125.220196	4949.758865	5010.0325	5239.490978
0.88_125.0345m/z	125.0345074	0.8802	pos	2-carboxy-Pyrimidine	45034	Unclassified	Unclassified	Unclassified			38.6	0	M+H	C5H4N2O2	-0.374499283	252.8353904	183.5449543	226.7340835	257.3368819	216.7773659	170.89465	120.6292709	195.4451866	242.1193404
0.96_171.0057m/z	171.0056757	0.962983333	pos	Dihydroxyacetone phosphate	HMDB0001473	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C00111	38.6	0	M+H	C3H7O6P	2.204163947	326.8608195	393.0046376	235.0741208	124.0450394	208.0895601	226.9606522	396.6629153	286.0156977	193.8438884
0.98_125.0345m/z	125.034489	0.9855	pos	Pyrimidine-4-Carboxylic Acid (sodium salt)	45027	Unclassified	Unclassified	Unclassified			38.6	0	M+H	C5H4N2O2	-0.522989929	47.22833565	85.05846135	97.40320199	27.25713323	73.3745995	0.001403199	0.001403199	39.97862291	39.99841818
1.07_153.1272m/z	153.1271967	1.072683333	pos	2-Octenyl acetate	HMDB0031297	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohol esters	*		38.6	0	M+H-H2O	C10H18O2	-1.145616367	1527.266791	1272.46338	1286.212295	1219.579856	1158.379198	1231.949205	1556.188792	1304.348924	1251.160154
1.09_103.0391m/z	103.0391325	1.09455	pos	Succinic acid semialdehyde	LMFA06000118	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C00232	38.6	0	M+H	C4H6O3	1.588229583	59.09018328	99.16950557	100.242642	71.82405654	81.54316586	62.45100191	47.7989162	95.96605691	110.0938078
1.16_129.0182m/z	129.0181544	1.157483333	pos	3-Oxoglutaric acid	HMDB0013701	Organic acids and derivatives	Keto acids and derivatives	Short-chain keto acids and derivatives	***		38.6	0	M+H-H2O	C5H6O5	-0.552141902	1985.618581	1829.083964	2285.178533	2907.73475	2440.860726	2596.195433	2184.492652	2483.194602	1853.8535
1.16_285.9843m/z	285.9843114	1.157483333	pos	Glyphosine	72874	Unclassified	Unclassified	Unclassified			38.6	0	M+Na	C4H11NO8P2	-3.417717917	6144.180563	5963.119547	6544.759217	7787.409257	6379.979308	6323.343053	6890.022802	6842.727383	6699.618417
1.22_288.1185m/z	288.1185365	1.22075	pos	Clavamycin E	71639	Unclassified	Unclassified	Unclassified			38.6	0	M+H	C11H17N3O6	-1.655026802	20785.88	21656.1167	22721.88384	22419.07688	19697.47863	22114.10551	16891.65376	21087.16076	19027.61931
1.31_221.1534m/z	221.1534005	1.306655	pos	3,4-Dihydro-2,2,5,7,8-pentamethyl-2H-1-benzopyran-6-ol	94748	Organic oxygen compounds	Benzopyrans	1-benzopyrans	*		38.6	0	M+H	C14H20O2	-0.934926775	2986.089476	3048.807808	2365.86264	2452.788466	2304.501082	2383.866923	2862.877524	2842.54588	2715.829646
1.42_238.9593m/z	238.959254	1.415933333	pos	Poppy acid	89480	Organoheterocyclic compounds	Pyrans	Pyranones and derivatives		C20209	38.6	0	M+K	C7H4O7	1.967160123	9153.581658	9672.883657	9406.225785	5531.749924	5131.048395	5002.579488	9188.946667	9669.755725	9460.225386
1.59_128.0342m/z	128.0341564	1.589283333	pos	5-Hydroxypyrrole-2-carboxylate	73317	Unclassified	Unclassified	Unclassified			38.6	0	M+H	C5H5NO3	-0.496190327	19.5932132	0.001403199	20.1974352	33.33556395	0.001403199	0.001403199	39.16176662	82.7045145	62.24665745
1.63_113.0234m/z	113.023403	1.633283333	pos	2,5-Dioxopentanoate	HMDB0060365	Organic acids and derivatives	Keto acids and derivatives	Short-chain keto acids and derivatives	**	C00433	38.6	0	M+H-H2O	C5H6O4	0.634896142	1433.0805	1407.481807	1352.659829	1217.019257	1251.741066	1262.421759	1217.880175	1320.030913	1285.233489
1.96_128.0341m/z	128.0341499	1.961133333	pos	Hydroxyminolaine	HMDB0034368	Organoheterocyclic compounds	Pyrroles	Pyrrole carboxylic acids and derivatives			38.6	0	M+NH4	C5H5NO3	-0.547841353	15.77409859	55.31564253	17.73551156	18.21318079	42.71289502	16.99732999	55.17440386	29.30192947	14.53226222
10.09_209.1997m/z	209.1996952	10.09966667	pos	Hypseric acid	LMFA01030248	Lipids and lipid-like molecules	Fatty Acyls	Lipids and lipid-like molecules	**	C08362	38.6	0	M+H	C14H28O2	-1.311489476	6973.803125	1920.573686	5131.825445	2946.169313	1545.430041	1550.229443	4796.104015	4796.102557	4723.668363
10.14_252.2085n	253.2157694	10.14475	pos	Palmitolinoleic acid	LMFA01030275	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C08362	38.6	0	M+H, M+NH4	C16H28O2	-1.7333607	6310.537398	4135.671014	9300.376279	5774.602542	4384.888686	4698.121979	8711.954011	5289.418248	3685.715017
10.16_112.0392m/z	112.0392403	10.16326667	pos	2,6-Dihydropyridine	63881	Unclassified	Unclassified	Unclassified			38.6	0	M+H	C5H5NO2	-0.581418199	54.76073249	101.0287101	95.83614962	46.80454243	71.53507365	84.57929061	100.7880813	84.80887222	20.1383987
10.43_235.1689m/z	235.1689299	10.4331	pos	Saussurea lactone	90173	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	*		38.6	0	M+H	C15H22O2	-1.394219393	5246.122954	3835.31164	3755.502102	3337.968711	3792.666758	3447.613345	4275.91024	4044.073672	4634.403397
10.46_257.2260m/z	257.2259586	10.45796667	pos	Androstenol	HMDB0005935	Lipids and lipid-like molecules	Steroids and steroid derivatives	Androstane steroids	*		38.6	0	M+H-H2O	C19H30O	-1.527027192	4415.427243	3049.853272	4541.664831	3780.271904	4155.855516	4657.408531	3592.326611	4595.852087	4512.240636
10.52_253.1703m/z	253.1703866	10.52125	pos	Apotriterpenol	90038	Organoheterocyclic compounds	Tetrahydrofurans	Unclassified	*		38.6	0	M+H-H2O	C19H24O3	-1.722696126	2229.715844	2276.215693	2041.328886	2229.718444	2451.406674	2457.075832	2224.882576	2423.668363	
10.81_327.0776m/z	327.0776129	10.8111	pos	TRIPHENYL PHOSPHATE	HMDB0259262	Unclassified	Unclassified	Unclassified			38.6	0	M+H	C18H15O4P	-1.407984007	5250.210419	4512.888454	4914.207384	6159.824526	5416.581539	5289.11032	6075.167065	5042.469123	4657.005247
11.21_365.1354m/z	365.1354224	11.21126667	pos	Hydroxygaleon	HMDB0031535	Organoheterocyclic compounds	Lactones	Gamma butyrolactones	*		38.6	0	M+Na	C20H22O5	-1.525818734	8694.986824	8226.284008	8094.946042	9641.312408	7707.86443	7939.472872	9637.053996	7810.27682	8498.327509
11.96_369.3511m/z	369.3511383	11.96068333	pos	5beta-cholestanone	LMST01010205	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C05844	38.6	0	M+H-H2O	C27H46O	-1.137549134	2395.105816	3497.380978	3381.532175	2573.170633	1215.642262	5557.210509	3322.293048	2839.288212	2596.721641
12.04_582.4334n	600.4672465	12.03775	pos	Polidocanol	HMDB0256665	Unclassified	Unclassified	Unclassified			38.6	0	M+NH4, M+Na	C30H62O10	-1.506164842	38478.80433	51995.74033	49029.6826	51840.64597	52456.90227	47429.91061	50152.32844	46567.18978	51791.22838
12.39_251.0464m/z	251.0464453	12.38798333	pos	(+)-cis-3,4-Dihydrophenanthrene-3,4-diol	66187	Unclassified	Unclassified	Unclassified			38.6	0	M+K	C14H12O2	-2.085912495	2895.437884	3410.55281	3033.887628	3308.041257	3784.624101	3560.043578	2974.581707	3052.905122	3352.354479
12.72_605.5494m/z	605.5494249	12.72343333	pos	PG(16:0/18:0/0:0)	62000	Unclassified	Unclassified	Unclassified			38.6	0	M+Na	C37H74O4	2.563421342	16554.09826	8615.593676	10247.30517	10387.94294	7633.711368	9351.14968	9041.254114	8716.700294	8900.239652
12.76_271.1661m/z	271.1661264	12.76383333	pos	2-Phenylethyl octanoate	HMDB0037719	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.6	0	M+Na	C16H24O2	-2.91841287	2745.202255	2044.213194	2431.96505	2478.073415	2215.390325	1938.672285	1957.820368	2089.294926	2087.588891
13.15_799.5445m/z	799.5445056	13.15121667	pos	PG(18:0/18:1(11Z))	HMDB0010603	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols	*		38.6	0	M+Na	C42H81O10P	-1.867874572	52749.37539	47525.74745	42949.48589	31654.4775	28375.49067	24885.26808	45503.06939	40995.14416	39113.0038
13.41_137.1072m/z	137.1071859	13.41138333	pos	5-Ethyl-2,3-dimethylpyrazine	HMDB0029727	Organoheterocyclic compounds	Diazines	Pyrazines	*		38.6	0	M+H	C8H12N2	-1.020759382	235.8071673	339.5887617	289.9521124	241.4490847	334.1315341	206.8672686	287.0632603	308.7610006	292.6484737
13.79_206.0664m/z	206.0664417	13.78933333	pos	(E)-3-(Methoxycarbonyl)pent-2-enedioate	69085	Unclassified	Unclassified	Unclassified			38.6	0	M+NH4	C7H8O6	2.809264353	551.9136069	532.8729082	536.0122733	559.3974183	616.6103833	591.133093	565.7627027	538.1188784	630.7709869
13.86_385.1776m/z	385.1776159	13.86473333	pos	Corticosterone	HMDB0001547	Lipids and lipid-like molecules	Steroids and steroid derivatives	Hydroxysteroids	***	C02140	38.6	0	M+K	C21H30O4	0.139801566	14059.75402	7253.244345	7074.584304	8239.676637	6817.733131	9576.413607	8062.934859	14058.96406	8254.741035
14.17_206.0665m/z	206.0665429	14.17256667	pos	(Z)-But-1-ene-1,2,4-tricarboxylate	63456	Organic acids and derivatives	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives	**	C04002	38.6	0	M+NH4	C7H8O6	3.347297966	6925.639952	6283.423405	6047.098576	6343.760903	6739.414905	6577.093047	6741.82757	6154.000971	6017.966152
14.75_228.1954m/z	228.1954113	14.75351667	pos	Propyl 2,4-decadienoate	LMFA07011001	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.6	0	M+NH4	C13H22O2	-1.875631969	895.4853002	1202.356161	745.7332618	766.0521735	848.6115724	828.4093309	1071.010021	964.0421534	658.5199745
15.51_135.0786m/z	135.0785847	15.5125	pos	3-Hepten-2-one	87713	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		38.6	0	M+Na	C7H12O	4.898476375	1250.418028	940.0645831	112.6490571	1424.807777	2985.598711	3622.736987	3418.447133	13.17319225	0.001403199
15.51_151.0740n	152.0812724	15.5125	pos	chondroitin sulfate E (GalNAc4,6diS-GlcA), precursor 5a	HMDB0062464	Benzenoids	Benzene and substituted derivatives	N-phenylureas	*		38.6	0	M+H-H2O, M+H	C7H9N3O	-3.493080025	1078.268424	1254.297429	127.2543697	1495.841874	3398.363554	3948.109935	3974.243639	29.33058211	10.63929565
2.00_112.0757m/z	112.0757231	2.004416667	pos	Arene oxide	65651	Unclassified	Unclassified	Unclassified			38.6	0	M+NH4	C6H6O	0.348648175	1001.507593	1004.976051	1029.793186	686.5361861	677.5340784	575.1617577	671.8982782	710.2157185	739.2947589
2.03_101.0600m/z	101.

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4.32_209.0687n	210.0759827	4.317083333	pos	3-Carbamoyl-2-phenylpropionic acid	HMDB0060367	Benzenoids	Benzene and substituted derivatives	Unclassified	**	C16591	38.5	0	M+H, M+Na	C10H11NO4	-0.485625934	1945.619042	2401.544207	2432.84602	1089.115492	1133.630839	901.282107	738.4119822	840.530065	868.3610096
4.34_197.0183m/z	197.0183416	4.33965	pos	3,5-Dinitroguaiacol	71560	Unclassified	Unclassified	Unclassified			38.5	0	M+H+H2O	C7H6N2O6	-4.467070033	8336.077635	8378.297761	9088.226421	9174.773866	8866.471207	9826.329158	8487.593487	9212.05894	8741.874331
4.41_296.1829n	319.1722686	4.4062	pos	S-Farnesyl Thioacetic Acid	43440	Unclassified	Unclassified	Unclassified			38.5	10.7	M+NH4, M+Na, M+H	C17H28O2S	6.308641918	7151.629046	21313.43356	5775.473679	93161.34199	211.7365482	852.7747724	1521.959034	13136.08351	558.8027963
4.41_300.1802m/z	300.1802156	4.4062	pos	dihydrophaseic acid	LMPR0103050005	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*	C15971	38.5	0	M+NH4	C15H22O5	-1.182781282	4804.929819	4978.197528	5253.891237	5175.164696	4603.365656	4883.990843	4292.728756	4651.046253	4493.371243
4.41_310.1757m/z	310.1757477	4.4062	pos	Fusarochromanone	89326	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans			38.5	0	M+NH4	C15H20N2O4	-1.317845945	3036.198716	3710.192096	4048.243391	2369.041238	1931.619041	2332.944137	3891.327857	4660.029751	4048.805638
4.41_376.1375n	377.1447796	4.4062	pos	(1x,2x)-Guaiacylglycerol 2-glucoside	89157	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			38.5	0	M+H, M+Na	C16H24O10	1.478803959	16881.4779	19348.08502	18925.40117	25417.2772	22076.20222	23246.89305	16124.61769	19617.50579	18424.32842
4.50_279.0837m/z	279.0836843	4.496783333	pos	Phenyl beta-D-glucopyranoside	69132	Unclassified	Unclassified	Unclassified			38.5	0	M+Na	C12H16O6	-0.876961481	331.0207573	945.5422533	1191.65514	821.9329199	1013.208642	669.6393572	942.6336543	1108.355758	922.7331853
4.50_294.0743m/z	294.0742765	4.496783333	pos	N-D-Glucosylarylamine	65913	Unclassified	Unclassified	Unclassified			38.5	0	M+K	C12H17NO5	1.74733944	857.4661922	967.1643307	1047.836273	2157.919892	2181.006374	2161.004116	2356.666697	2496.928768	2610.962589
4.52_391.0993m/z	391.0993524	4.51925	pos	3-O-Feruloylquinic acid	87130	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols	*	C02572	38.5	0	M+Na	C17H20O9	-1.708536231	1331.059668	1665.146315	1577.930324	113.2565559	65.05507063	99.97483148	3538.592559	3387.590708	3705.673513
4.54_254.0866m/z	254.0865873	4.542216667	pos	gamma-Glutamyl-2-aminobutyrate	HMDB0242176	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			38.5	0	M+Na	C9H15N2O5-	-3.15857298	2246.091724	2295.224492	2485.016085	22.1882813	0.001403199	41.50924486	323.3128208	241.9962188	242.8165102
4.54_312.2376m/z	312.2376347	4.542216667	pos	Margaric acid(d3)	LMFA01010048	Unclassified	Unclassified	Unclassified			38.5	0.873	M+K	C17H31D3O2	-0.856231898	3279.164369	3876.068233	2238.112028	4948.435618	29.5646549	650.6803856	1313.584992	2222.817625	916.2629072
4.57_265.1428m/z	265.1428453	4.565116667	pos	smpr0lum	4032	Unclassified	Unclassified	Unclassified			38.5	0	M+Na	C14H18N4	1.974100769	699.4157606	652.4076009	644.9810655	557.4057093	453.4116221	361.0074444	434.4224869	415.2253508	514.5304324
4.57_366.1705m/z	366.1705378	4.565116667	pos	Nequinate	87920	Organoheterocyclic compounds	Quinolines and derivatives	Quinolones and derivatives	*		38.5	0	M+H	C22H23NO4	1.514735601	3062.78484	2841.848721	2940.291417	2734.551436	2499.933956	2648.038778	4688.061333	4683.738981	4836.455536
4.61_223.0956m/z	223.0956609	4.610866667	pos	Hydralazine acetone hydrazone	HMDB0060606	Organoheterocyclic compounds	Diazanaphthalenes	Benzodiazines	*		38.5	0	M+Na	C11H12N4	0.959104031	1836.301774	1659.711893	1634.043767	2094.292715	2494.434625	1872.040306	2365.158188	2264.781031	2438.233547
4.63_319.1649m/z	319.1648917	4.63335	pos	Morphine N-oxide	69218	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.5	0	M+NH4	C17H19NO4	-1.13562497	1450.824089	1411.730187	1775.76302	2521.980242	2656.906461	2183.680936	1098.029641	903.5786163	1191.468104
4.75_195.1127m/z	195.1127217	4.7456	pos	Pilocarpidine	71960	Unclassified	Unclassified	Unclassified			38.5	31.1	M+Na	C10H14N2O2	-0.424633994	8585.424836	9653.557908	10257.52007	2158.63825	2313.983017	2426.520854	4336.73371	3746.567728	3782.163978
4.75_413.2654m/z	413.2654225	4.7456	pos	12alpha-hydroxy-3-oxo-5beta-cholan-24-oic Acid	HMDB0062742	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	*		38.5	0	M+Na	C24H38O4	-2.069988071	2512.191048	2598.377176	2694.002175	2307.962097	1553.663838	2199.408491	3949.850488	2443.478935	2498.86272
4.77_299.1462m/z	299.146216	4.768333333	pos	2'-O-Methyladenosine	58235	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	*	C04779	38.5	0	M+NH4	C11H15N5O4	-0.048085196	2160.026142	3251.601049	3315.178287	2374.238311	2109.126384	2403.741909	2529.366815	2897.888324	2825.928664
4.77_390.1572m/z	390.1571971	4.768333333	pos	GEMIFLOXACIN	44180	Organoheterocyclic compounds	Diazanaphthalenes	Naphthyridines			38.5	0	M+H	C18H20FN5O4	-0.030073832	130.7296946	177.7852712	34.67537857	973.8427035	1039.453907	1348.360193	72.50755168	168.1395741	76.15470661
4.79_318.1672m/z	318.1671953	4.7912	pos	Esmolol	2576	Benzenoids	Phenol ethers	Unclassified		C06980	38.5	0	M+Na	C16H25NO4	-1.299790658	3294.926185	3580.935558	4441.701972	2009.230214	1491.538836	1578.179739	2544.05177	3038.429469	2744.184859
4.84_163.0753m/z	163.0752688	4.836966667	pos	2-Phenyl-1,3-dioxolane-4-methanol	HMDB0031240	Benzenoids	Benzene and substituted derivatives	Unclassified	*		38.5	0	M+H-H2O	C10H12O3	-0.483937236	1369.633382	1371.79606	1635.661317	1206.276263	1140.524241	1112.549621	1485.233272	1594.565055	1638.300668
4.86_316.2115m/z	316.2115256	4.8596	pos	13,14-dihydro-15-keto-tetranor PGE2	941	Unclassified	Unclassified	Unclassified			38.5	0	M+NH4	C16H26O5	-1.08626649	2570.171237	2585.739575	2755.804473	2830.390096	2655.59234	2649.364219	2481.006342	2323.81246	2546.981687
4.96_402.1496m/z	403.1570289	4.8596	pos	Benzyl beta-primeveroside	95612	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			38.5	4.42	M+H, M+Na	C18H26O10	-7.073405536	105392.3765	106802.5266	122849.118	110754.7446	115391.9403	126123.052	131599.1694	127209.3489	
4.93_252.1225m/z	252.1225225	4.927016667	pos	Artemidiol	87116	Phenylpropanoids and polyketides	Isocoumarins and derivatives	Unclassified	*		38.5	0	M+NH4	C13H14O4	-2.187162591	433.7013575	646.9586678	507.1637845	965.4463498	678.4368207	571.30967	518.8239022	625.3457046	491.9572575
4.99_198.0888n	199.096048	4.991816667	pos	2,3-Methylene suberic acid	HMDB0059779	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.5	0	M+H, M+NH4	C10H14O4	-2.207865087	1160.068924	949.8555959	1103.981367	1279.963399	1158.287543	1152.895468	1120.515828	1089.173597	1247.1513
5.04_112.0394m/z	112.039429	5.035783333	pos	2,5-Dihydroxypyridine	63886	Unclassified	Unclassified	Unclassified			38.5	0	M+H	C5H5NO2	1.117980431	110.9330777	150.5944391	118.4849611	99.63724639	110.6285585	83.78887329	144.4286552	111.4371303	101.0067261
5.04_148.0391m/z	148.0390897	5.035783333	pos	4-Nitroacetophenone	65840	Unclassified	Unclassified	Unclassified			38.5	0	M+H-H2O	C8H7NO3	-1.303388773	810.8735812	787.2306886	837.2891258	1026.898787	1024.993991	969.8531509	872.8471764	884.736311	932.8698666
5.06_316.2114m/z	316.2114483	5.058233333	pos	Artemether	HMDB0015643	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.5	0	M+NH4	C16H26O5	-1.35723069	2916.516281	2864.72144	2933.360278	4004.815005	3752.039049	3838.382287	2348.612559	2865.070473	2514.340017
5.08_129.1022m/z	129.1021723	5.081	pos	5-Acetyl-3,4-dihydro-2H-pyrrole	87573	Organoheterocyclic compounds	Pyrrolines	Unclassified	*		38.5	0	M+NH4	C6H9NO	-0.6040743	588.4398889	503.1929181	562.7912455	510.8753861	587.235211	535.6117692	548.6022341	561.6655135	566.2974624
5.08_367.1359m/z	367.1358736	5.081	pos	Ethosuximide M3 glucuronide	2598	Unclassified	Unclassified	Unclassified			38.5	0	M+NH4	C13H19NO10	3.300630451	8119.059291	8754.505515	9047.563162	3697.755153	3255.011922	3631.975586	7559.356422	8637.426265	7851.152683
5.22_361.1388m/z	361.1388456	5.21595	pos	Avenanthramide 1s	HMDB0029285	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	*		38.5	0	M+NH4	C18H17NO6	-1.653056542	1909.137291	1979.931337	2177.379979	2115.546809	2287.148545	1953.893892	2048.302153	2243.222376	2293.920612
5.24_244.9852m/z	244.9851957	5.238683333	pos	Flaviolin	72004	Unclassified	Unclassified	Unclassified			38.5	0	M+K	C10H6O5	2.496446985	6163.424362	6169.658683	6617.472923	276.4574965	255.8034017	193.7453665	4596.428136	4952.496845	4880.450137
5.24_355.1723m/z	355.1723526	5.238683333	pos	6-oxo-famciclovir	HMDB0061100	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	*		38.5	0	M+NH4	C14H19N5O5	-0.331248398	3385.648419	3155.751437	3968.28138	1803.5394	1303.781208	1546.900301	2094.907608	2102.242443	2153.7501
5.26_299.1623m/z	299.1622557	5.26135	pos	N-Acetyl-9-O-lactoylneuraminic acid	HMDB0000768	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.5	0	M+NH4	C14H23N3O11	3.462493861	7154.072481	6924.013676	7724.69589	8699.427906	7477.388109	7295.899592	6010.443916	6989.575629	7205.906992
5.50_181.1221m/z	181.1220817	5.49815	pos	formyl 2Z,4E,6Z-decatrienoate	97205	Unclassified	Unclassified	Unclassified			38.5	0	M+H	C11H16O2	-1.246225435	707.4789426	956.8993572	758.7785815	632.3831461	699.6277002	599.4739136	891.1022164	906.7354627	767.9111468
5.52_231.0649m/z	231.0649436	5.5209	pos	Visnagin	LMPK13110003	Lipids and lipid-like molecules	Polyketides	Aromatic polyketides		C09049	38.5	4.16	M+H	C13H10O4	-1.050352763	1806.155425	2071.937502	1922.70923	654.0984128	771.0621059	591.5467472	1953.549863	1708.398877	1542.812513
5.54_171.0624m/z	171.0624236	5.543066667	pos	Abequose	3287	Unclassified	Unclassified	Unclassified			38.5	0	M+Na	C6H12O4	-2.403598397	951.7923279	943.5340006	1005.310938	815.5321669	826.2014061	821.7357689	1079.709829	876.676945	1057.019071
5.58_471.2369m/z	471.2368713	5.581883333	pos	Lucidenic acid D1	92933	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.5	0	M+H	C27H34O7	-1.825782754	1951.364859	2091.076642	1669.840132	2736.109573	2636.841895	2625.625739	1938.115393	1782.045337	1889.25128
5.59_482.2424m/z	481.2424368	5.590966667	pos	11-Deacetylvalitrate 11-(3-hydroxy-3-methylbutanoate)	HMDB0033654	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		38.5	0	M+NH4	C25H38O9	-1.608264871	3265.13729	2978.274115	2697.315008	4918.645284	4403.960683	5563.443372	3617.690947	4179.260967	4222.362784
5.70_393.2006m/z	393.2006176	5.69755	pos	3,3-Difluoro-5alpha-androstan-17beta-yl acetate	70090	Unclassified	Unclassified	Unclassified			38.5	0	M+K	C21H32F2O2	1.193574014	5.395785013	645.4116396	526.7059432	837.1600344	899.0689318	554.9771957	1488.622198	420.960782	323.0085114
5.93_452.2484m/z	452.2484228	5.933983333	pos	4,5-Dihydro-drospirenone-3-sulfate	HMDB0061126	Organoheterocyclic compounds	Lactones	Unclassified	*		38.5	8.64	M+NH4	C24H34O5S	4.380544705	18347.46546	18300.73749	19804.709	16551.92721	17485.78791	17362.27286	19941.1123	19811.88108	20399.98857
5.96_349.2371m/z	349.2371459	5.956833333	pos	3a,21-Dihydroxy-5b-pregnane-11,20-dione	LMST02030199	Lipids and lipid-like molecules	Steroids and steroid derivatives	Hydroxysteroids	**	C05478	38.5	0	M+H	C21H32O4	-0.545596531	1619.080688	1991.22134	1757.909953	1060.201585	1975.809566	2132.659039	1292.848878	1603.01461	1622.678843
5.98_429.1728m/z	429.1727688	5.97975	pos	pre-putrebactin	LMFA08020201	Lipids and lipid-like molecules	Fatty Acyls	Fatty amides			38.5	0	M+H	C16H30N4O7	-4.711872126	19355.37992	20232.87092	19752.43345	17831.19252	20956.04572	19792.23082	15263.45996	14624.59225	15759.67723
6.04_291.1197m/z	291.1197407	6.041083333	pos	N-Succinyl-L-diaminopimelic acid	388	Unclassified	Unclassified	Unclassified			38.5	0	M+H	C11H18N2O7	3.665377857	1790.655016	2780.959785	1768.101918	2357.994493	2574.540073	2934.733864	1964.923382	2825.892729	1918.890849
6.05_197.1534m/z	197.1534464	6.0535	pos	Hexamethylphosphoramide	72970	Unclassified	Unclassified	Unclassified			38.5	0	M+NH4	C6H18N3OP	4.868416524	4241.82148	4132.377617	3855.63626	3561.96122	3713.614527	3553.625761	3608.038928	3694.027496	3418.610775
6.11_211.1327m/z	211.1326873	6.113683333	pos	(±)-Jasmonic Acid	62988	Unclassified	Unclassified	Unclassified			38.5	0	M+H	C12H18O3	-0.873569414	2283.008189	2015.133772	2195.619348	2046.249497	2068.257647	1988.071406	1873.719565	2244.929694	2007.396395
6.17_371.1673m/z	371.1672923	6.17335	pos	(1S,2S,4R,5S,7S)-2,5,7-Fenchanetriol 2-O-b-D-glucoside	HMDB0033219	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		38.5	0	M+Na	C16H28O8	-0.994442832	4410.598677	3589.348351	4446.45715	2583.94641	2391.612591	2447.016669	2322.315865	3170.18628	2540.664931
6.31_479.1860m/z	479.1859523	6.308766667	pos	4-(2-Nitreothyl)phenyl primeveroside	87912	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		38.5	0	M+NH4	C19H27NO12	-2.599054043	8912.234231	13246.56297	11179.99397	12433.84388	11769.32098	11315.51299	11180.43373	9746.48376	12057.1053
6.42_129.1022m/z	129.102164	6.422383333	pos	N-Acetyl-2,3-dihydro-1H-pyrrole	87456	Organoheterocyclic compounds	Pyrrolines	Unclassified	*		38.5	0	M+Na	C6H9NO	-0.679070267	962.8416117	928.3740395	881.7957295	880.151267	897.0360336	782.9288496	1000.538114	840.922697	847.5208594
6.58_336.2162m/z	336.2162346	6.584266667	pos	Ubiquinone-2	HMDB0006709	Lipids and lipid-like molecules	Prenol lipids	Quinone and hydroquinone lipids	**	C00399	38.5	0	M+NH4	C19H26O4	-2.200903387	2605.440903	2588.171714	3379.67985	5386.575243	5665.958053	4507.498272	2295.488208	3290.715618	3123.674906
6.63_413.2656m/z	413.2656381	6.627483333	pos	9'-Carbory-alpha-chromanol	HMDB0012866	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans	*		38.5	0	M+Na	C24H38O4	-1.517547499	1902.749436	1913.372544	1873.814469	2907.215183	2176.16932	2289.588422	2573.462727	2319.979507	2249.834266
6.71_244.0520m/z	244.0520175	6.709016667	pos	S-methyl-L-Thiocitrulline (hydrochloride)	44315	Unclassified	Unclassified	Unclassified			38.5	0	M+K	C7H15N3O2S	1.763459232	0.001403199	0.001403199	0.001403199	1232.404749	1047.506375	1311.622472	0.001403199	0.001403199	0.001403199
7.18_454.1628m/z	454.1627714	7.182883333	pos	Alpinine	67607	Unclassified	Unclassified	Unclassified			38.5	0	M+K	C23H29NO6	0.302783344	11669.93712	12257.07588	12471.91359	13688.92565	12208.39594	12039.53598	10423.2714	10023.09301	12265.70127
7.45_312.1399m/z	312.1398754	7.448183333	pos	N-Glycosyl-L-asparagine	65973	Unclassified	Unclassified	Unclassified			38.5	0	M+NH4	C10H18N2O8	-0.903208833	779.9668448	822.0584016	1222.499642	48.21993311	197.9415279	105.3723825	396.3203673	562.9201813	339.5735491
7.47_113.1074m/z	113.1073941	7.465483333	pos	2,5-Dimethyl-1H-pyrrole	HMDB0032973	Organoheterocyclic compounds	Pyrroles	Substituted pyrroles			38.5	0	M+NH4	C6H9N	0.728492315	58.71286927	64.81209038	47.23104301	67.1108961	78.08454094	66.50078279	92.94842778	75.55594271	79.75979636
7.47_221.1533m/z	221.1533111	7.465483333	pos	2-Methyl-1-phenyl-2-propanyl butyrate	94757	Benzenoids	Benzene and substituted derivatives	Phenylpropanes			38.5	0	M+Na	C14H20O2	-1.340890232	1498.27831	1283.756239	1245.220685	1435.214876	1315.688418	1183.128397	1156.136955	1265.703712	1184.723811
7.49_205.1584m/z	205.1584173	7.4907	pos	2,6-Di-tert-butyl-1,4-benzenediol	HMDB0040178	Benzenoids	Benzene and substituted derivatives	Phenylpropanes			38.5	0	M+H-H2O	C14H22O2	-1.234949382	635.7567632	462.1259668	416.7543345	398.1754396	264.4853353	290.51902	383.2254017	341.9008548	309.1761076
7.69_469.1100m/z	469.1100179	7.690416667	pos	Glycitin	HMDB0002219	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavonoid O-glycosides	*		38.5	0	M+Na	C22H22O10	-1.119953697	4692.216477	4603.273327	4023.432396	5159.703787	4517.891352	4209.955422	3708.768944	4514.270924	3841.028868
8.07_335.2363m/z	335.2362677	8.074933333	pos	10Z-nonadecenoic acid	35026	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.5	0	M+K	C19H36O2	5.330322284	6310.329341	7743.440441	8905.189464	1494.920457	1436.602211	1287.744135	4096.428861	4401.77855	4822.926424
8.36_211.1326m/z	211.1325699	8.357283333	pos	Cyclen	HMDB0250623	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides			38.5	0	M+K	C8H20N4	3.572937363	1902.920556	2130.608151	1777.444554	1745.762195	1934.621041	1766.599008	1253.325639	1891.451834	2088.08593
8.50_448.3049m/z	448.3049267	8.497183333	pos	17-Deacetyl trinor PGF2α isopropyl ester	3619	Unclassified	Unclassified	Unclassified			38.5	0	M+NH4	C26H38O5	-1.913041954	1853.98541	1057.340999	529.9715468	517.2109873	4221.268877	2224.583445	519.5260681		
9.02_271.1453m/z	271.1452577	9.0248	pos	Ethyl 3-methyl-9H-carbazole-9-carboxylate	HMDB0032758	Organoheterocyclic compounds	Indoles and derivatives	Carbazoles			38.5	0	M+NH4	C16H15NO2	4.557192137	1952.401305	2018.300537	1877.121168	2139.243602	2145.258021	2577.844428	2142.571708	1888.391972	2436.975363
9.28_214.2526m/z	214.252633	9.281766667	pos	(E)-7-Tetradecene	HMDB0061833	Hydrocarbons	Unsaturated hydrocarbons	Unsaturated aliphatic hydrocarbons			38.5	0	M+NH4	C14H28	-1.495156635	4732.208532	4602.687804	6332.354871	6177.193323	4658.268975	4286.077846	5660.244089	4025.87378	4360.980811
9.37_219.1378m/z	219.1378428	9.36895	pos	Dimethylbenzyl carbinyl crotonate	88276	Benzenoids	Benzene and substituted derivatives	Phenylpropanes	*		38.5	0	M+H	C14H18O2	-0.520046371	806.4213448	1021.245563	740.7837719	1015.83371	1434.091331	888.2609245	1506.761671	1108.020163	1204.418016
9.47_350.2299m/z	350.2298697	9.466333333	pos	9-Nitrooleate	44827	Unclassified	Unclassified	Unclassified			38.5	0	M+Na	C18H33NO4	-0.945719829	2284.987763	2147.90597	2368.962834	3355.610557	2987.057547	3554.467331	2976.359481	2818.525031	2801.364205
9.53_120.0556m/z	120.0556296	9.529466667	pos	4-Aminocrotonamide	44444	Unclassified	Unclassified	Unclassified			38.5	0	M+H-H2O	C6H7N3O	0.04339093	1361.970877	414.0826942	1283.756237	493.9622059	488.7626279	433.1097737	539.2733201	1358.112	1629.750835
9.54_437.1929m/z	437.1929358	9.543266667	pos	Magnoshinin	68471	Unclassified	Unclassified	Unclassified			38.5	0	M+Na	C24H30O6	-1.263903264	9741.491372	6857.290115	14898.07816	11919.73912	5028.091169	12187.69134	6784.632966	4922.033405	14765.91027
9.94_505.1797m/z	505.1796862	9.942033333	pos	6alpha,9alpha-Difluoroprednisolone-17-butyrate	HMDB0060797	Lipids and lipid-like molecules	Steroids and steroid derivatives	Hydroxysteroids	*		38.5	0	M+K	C25H32F2O6	-0.358304662	4516.027296	2402.718425	3346.66185	6533.495086	3376.048417	2994.07948	2760.711498	2076.945288	4775.6811
0.51_190.1081m/z	190.1080897	0.51135	pos	4-Octenedioic acid	5451	Unclassified	Unclassified	Unclassified			38.4	0	M+NH4	C8H12O4	4.099037547	187.4506277	928.9680793	126.9656095	496.147286	155.6987654	594.5892755	1346.499052	388.4613158	503.1889977
0.54_218.1426n	261.1304325	0.535	pos	Pirimicarb	HMDB0256598	Unclassified	Unclassified	Unclassified			38.4	0	M+H-H2O, M+Na	C11H18N4O2	-1.552601799	815.9594041	1384.045427	1907.64802	723.5078871	901.043125	2131.515245	2407.456207	2324.491827	3223.913373
0.58_150.9955m/z	150.9954664	0.576333333	pos	4-Fluorophenol	71226	Unclassified	Unclassified	Unclassified			38.4	0	M+K	C6H5FO	-1.202475634	653.4263096	554.7193047	737.1715038	952.9749081	576.4079468	474.3216295	588.2328146	757.7366867	626.0784525
0.62_166.0708m/z	166.0707871	0.616683333	pos	3-(α-Hydroxyglutaric acid	45120	Unclassified	Unclassified	Unclassified			38.4	0	M+K	C5H8O5	-1.430834813	1021.140367	1224.489112	1243.274541	1365.788034	1271.432271	1307.231607	1484.072955	1639.752835	
0.66_113.0598m/z	113.0597994	0.657416667	pos	3-Methyl-2-oxovaleric acid	HMDB0000491	Organic acids and derivatives	Keto acids and derivatives	Short-chain keto acids and derivatives	*	C03465	38.4	0	M+H-H2O	C6H10O3	0.71878253	543.6364289	564.0410834	350.8580841	443.562223	404.2448235	478.3983285	492.635801	471.9274437	470.5615889
0.66_127.0389m/z	127.0388667	0.657416667	pos	3-hexenedioic acid	LMFA01170087	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.4	0	M+H-H2O	C6H8O4	-0.720577486	2617.007503	2610.115732	2306.523487	2373.484356	2268.992685	2363.215039	2608.28797	1992.732778	2103.026314
0.68_234.1444m/z	234.1444446	0.6788	pos	Lysylserine	HMDB0028960	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.4	0	M+H	C9H19N3O4	-1.663825248	1802.458865	2201.244415	1977.386974	2901.726936	3525.183582	4380.653366	1299.409384	1074.538895	1249.956218
0.72_102.0915m/z	102.0915234	0.717716667	pos	3-Methylcrotonaldehyde	62820	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*	C15604	38.4	0	M+NH4	C5H8O	2.176432702	176.4083547	147.4098539	120.3012816	381.5944168	246.991776	288.2122508	99.79046297	207.7498529	177.9204416
0.74_202.1426n	225.1317767	0.73955	pos	Arg-OEt	65589	Unclassified	Unclassified	Unclassified			38.4	0	M+Na, M+K	C8H18N4O2	-2.076889901	16727.43234	10312.72895	14485.62207	10041.28875	10240.02651	10557.63119	14694.57271	15353.34189	14192.92353
0.74_267.0950n	268.1022298	0.73955	pos	Neuraminic acid	3394	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C06469	38.4	0	M+H, M+Na	C9H17NO8	-1.733847785	6984.337863	4389.903715	5837.686885	4947.122473	4516.707682	4078.174247	6029.796896	4150.039101	4242.438857
0.82_210.9677m/z	210.9676905	0.818116667	pos	Calcium glycerophosphate	HMDB0303198	Unclassified	Unclassified	Unclassified			38.4	0	M+H	C3H7CaO6P	-0.959499971	30335.31198	30600.4985	28027.71241	25975.51339	29514.45078	28248.91082	28337.16039	29422.87754	30507.27906
0.82_221.0897n	204.0864395	0.818116667	pos	N-Acetylmannosamine	3357	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C00645	38.4	0	M+H-H2O, M+K, M+H	C8H15NO6	-0.947222302	24655.91153	24545.04091	26089.39496	28917.45261	27022.29411	26440.24297	24009.94609	23876.22841	24210.64705
0.82_334.1483n	335.1556188	0.818116667	pos	13-dimethylarsinoyl-tridecanoic acid	LMFA00000034	Lipids and lipid-like molecules	Fatty Acyls	Other Fatty Acyls			38.4	0	M+H, M+Na	C15H31AsO3	-1.71788559	5627.330192	6598.201755	6618.451107	7613.38943	8503.985828	7368.447447	5534.899277	6493.954446	6445.094055
0.84_129.0545m/z	129.0545217	0.8386	pos	2,2-Dimethyl Succinic acid	6473	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.4	0	M+H-H2O	C6H10O4	-0.67666837	1029.862433	626.3729894	685.2558663	568.1804319	562.7146912	573.1412877	776.7001306	550.532732	610.7918831
0.86_131.0701m/z	131.0701781	0.859583333	pos	Mevalonolactone	HMDB0006024	Organoheterocyclic compounds	Lactones	Delta valerolactones	*		38.4	0	M+H	C6H10O3	0.71156441	908.2201059	782.3382183	740.8112295	621.8386274	571.0208978	527.8388672	645.242644	691.2473425	691.2473425

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0.82_181.0329m/z	181.0329348	0.818116667	pos	Allantoin	89	Organoheterocyclic compounds	Azoles	Imidazoles	*	C01551	38.3	0	M+Na	C4H6N4O3	-1.746006503	386.238936	427.4073439	540.5651811	154.5835047	345.5027737	215.3533122	544.5049314	610.7267036	420.1300616
0.84_227.0634m/z	227.0633967	0.8386	pos	L-beta-aspartyl-L-alanine	62011	Organic acids and derivatives	Peptidomimetics	Hybrid peptides	*		38.3	0	M+Na	C7H12N2O5	-2.182942448	8674.297618	8784.584667	8429.730354	13303.63818	11730.01671	11486.4368	8269.48731	8799.389234	8485.243258
0.86_163.0301n	201.9906751	0.859583333	pos	tiopronin	HMDB0259104	Unclassified	Unclassified	Unclassified			38.3	0.722	M+H-H2O, M+K	C5H9NO3S	-1.264935463	89281.53572	87620.38742	82878.94396	98674.57601	105677.0441	99441.44593	85459.74063	82502.03154	84243.2047
0.86_375.0527m/z	375.0527327	0.859583333	pos	4-(4-Deoxy-α-D-gluc-4-enuronosyl)-D-galacturonate	63148	Unclassified	Unclassified	Unclassified			38.3	0	M+Na	C12H16O12	-1.885840125	4812.857375	4308.494143	4909.703663	9952.415573	9373.374441	9296.313471	4192.323189	4274.404849	3305.522561
0.88_127.0865m/z	127.0864512	0.8802	pos	NICOTINYL	44459	Unclassified	Unclassified	Unclassified			38.3	0	M+NH4	C6H7NO	-1.267209057	672.5394171	1141.640611	1153.130785	626.2590533	722.9197793	784.0659066	628.4919869	978.2359074	896.9637226
0.88_146.0445m/z	146.0445485	0.8802	pos	L-N-Carboxymethylserine	86941	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.3	0	M+H-H2O	C5H9NO5	-1.445445746	2771.069739	2778.681694	2590.63827	2179.21831	2232.437469	2251.252023	2446.071449	2644.933614	2413.815952
0.88_355.1240m/z	355.1240083	0.8802	pos	Flecainide meta-O-dealkylated	2702	Unclassified	Unclassified	Unclassified			38.3	0	M+Na	C15H19F3N2O3	0.031445464	3068.17932	3351.147108	3617.053696	3657.605629	2513.014201	3200.279706	3504.715092	2801.495864	2618.823224
1.09_143.0337m/z	143.0337324	1.09455	pos	2-Oxo-2,3-dihydrofuran-5-acetate	66005	Unclassified	Unclassified	Unclassified			38.3	0	M+H	C6H6O4	-1.075273943	1884.414776	1576.589129	1497.383969	1389.094958	1630.976571	1600.596458	1774.897216	1708.528592	1634.709972
1.12_157.0606m/z	157.0606355	1.115783333	pos	4-Imidazolone-5-propionic acid	HMDB0001014	Organoheterocyclic compounds	Azoles	Imidazoles	**	C03680	38.3	0	M+H	C6H8N2O3	-0.8526877	435.4924307	502.9711921	448.3501417	587.804511	484.4488843	498.851039	415.9551189	531.8342239	607.7920328
1.14_305.0075m/z	305.0074693	1.137683333	pos	2-O-p-Coumaroyltartronic acid	88855	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives			38.3	0	M+K	C12H10O7	6.234129384	11792.09899	9618.780551	10676.8392	11854.75718	8477.506847	6696.56647	10323.5607	10629.12337	11621.31582
1.16_318.1290m/z	318.1290325	1.157483333	pos	N-(1-Deoxy-1-fructosyl)histidine	HMDB0037839	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids			38.3	0	M+H	C12H19N3O7	-1.715065667	4393.570047	4815.653387	5010.989801	4798.40762	4268.548921	4382.993747	3801.132612	4814.553247	3716.40859
1.18_261.1442m/z	261.1442025	1.178066667	pos	Isoleucyl-Glutamate	HMDB0028906	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.3	0	M+Na	C11H20N2O5	-1.136448961	4424.033788	4730.658247	4674.682871	4740.079402	5172.581782	4910.510441	3560.201422	4970.090984	3976.403034
1.24_305.1215m/z	305.1214669	1.243033333	pos	Clitocine	89495	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			38.3	0	M+NH4	C9H13N5O6	3.686150753	3615.846698	3675.20878	3389.283646	2306.859871	2481.818906	2614.235005	3752.381365	3485.282317	3895.674693
1.35_156.0419m/z	156.04193	1.350266667	pos	2-Amino-2-methylbutanoate	66000	Unclassified	Unclassified	Unclassified			38.3	0	M+K	C5H11NO2	-1.765457029	107.3410861	184.8884834	123.6510913	152.8121802	150.4192028	100.8353803	156.2535099	168.6260444	57.64071133
1.35_227.1750m/z	227.1750438	1.350266667	pos	Isoleucyl-Isoleucine	85816	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.3	0	M+H-H2O	C12H24N2O3	-1.476743293	1411.088827	1177.276019	1354.643941	2495.004118	1815.111166	1839.605789	1188.298222	1443.594786	1153.316144
1.37_157.0719m/z	157.0718523	1.372566667	pos	N-Ethylammelide	66433	Unclassified	Unclassified	Unclassified			38.3	0	M+H	C5H8N4O2	-0.958604454	680.4474643	800.3603906	967.1830547	1211.971107	1130.075689	1258.395979	1059.236843	1385.685888	1151.833374
1.39_176.0655m/z	176.0655354	1.39465	pos	PROLI-NONOate	62983	Unclassified	Unclassified	Unclassified			38.3	0	M+H	C5H9N3O4	-5.979978962	869.5398796	885.7025973	876.3598211	1213.099777	1233.788148	1135.24021	1038.207313	983.9362987	1006.594772
1.44_185.0919m/z	185.0918586	1.438283333	pos	Serinyl-Proline	85940	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.3	0	M+H-H2O	C8H14N2O4	-0.985317213	4525.851807	4897.665059	4841.31307	3122.533143	2625.666458	2958.539973	2492.428411	3130.004085	2892.873255
1.52_244.9978m/z	244.9977572	1.52285	pos	(2E)-4-Hydroxy-3-methylbut-2-en-1-yl trihydrogen diphosphate	HMDB0242600	Lipids and lipid-like molecules	Prenol lipids	Isoprenoids	**	C11811	38.3	0	M+Na	C5H12O8P2	1.163730717	2559.100308	3159.116433	2909.629969	4111.809537	4545.832239	4637.119672	3082.994077	3524.42942	3434.812299
1.61_148.0966m/z	148.0966638	1.611133333	pos	3-Oxohexanoic acid	HMDB0010717	Organic acids and derivatives	Keto acids and derivatives	Medium-chain keto acids and derivatives	*	C02122	38.3	0	M+NH4	C6H10O3	-1.198555464	56.37645669	66.44962298	97.92573048	110.2585771	121.3420664	71.36841145	88.02713703	50.07606484	114.4003871
1.61_155.0812m/z	155.0812222	1.611133333	pos	p-Aminobenzoic acid	3261	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	**	C00568	38.3	0	M+NH4	C7H7NO2	-2.056174681	2067.492385	2538.949004	2661.166106	1673.057398	1717.082256	1645.617435	1528.865501	1718.799411	1561.087874
1.61_195.1127m/z	195.1126535	1.611133333	pos	MDAI	96729	Unclassified	Unclassified	Unclassified			38.3	0	M+NH4	C10H11NO2	-0.850470902	1180.944311	1211.121977	1278.41007	841.0763787	1090.716781	1060.680004	1070.681132	1304.260893	1353.363998
1.66_122.0600m/z	122.0599894	1.655616667	pos	2-Acetylpyridine	HMDB0035281	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds			38.3	0	M+NH4	C7H7NO	-0.34572642	1226.26	1734.153414	1507.663097	1169.481768	1241.655897	1151.398953	1403.887972	1455.691502	1472.450672
1.68_125.0596m/z	125.0596335	1.6764	pos	Mequinol	86430	Benzenoids	Phenols	Methoxyphenols	*		38.3	0	M+H	C7H8O2	-0.583671952	920.7892214	822.2723064	704.6209773	728.2156236	775.9207998	790.0916018	734.4715289	750.8348579	755.7945492
1.83_247.0743m/z	247.0742621	1.829866667	pos	N-Acetylcystathionine	HMDB0002381	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.3	0	M+H-H2O	C9H16N2O5S	-1.674947701	1067.352822	931.2021226	974.3312503	555.033179	570.4535957	518.6309864	948.7937393	1051.614645	988.3507742
1.85_145.0494m/z	145.0493663	1.8515	pos	(R)-2-ethylmalic acid	LMFA01050454	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C02488	38.3	0	M+H-H2O	C6H10O5	-1.042262716	851.9282766	780.5806561	746.8580961	760.5209561	765.6359708	774.143086	733.975086	725.8851628	469.1979272
1.92_132.1017m/z	132.1017288	1.916533333	pos	2-Methyl-3-pentenoic acid	HMDB0031562	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.3	0	M+NH4	C6H10O2	-1.545296113	1168.102658	1185.30368	1105.805937	1002.986206	1023.527504	903.9662954	1154.401782	1113.02413	1107.267209
1.94_229.1543m/z	229.1543285	1.938766667	pos	Mescaline	3346	Unclassified	Unclassified	Unclassified			38.3	0	M+NH4	C11H17NO3	-1.612543705	2347.871581	2375.12529	2372.679526	2639.293552	2572.38331	2515.866781	2522.470121	2392.79498	2400.239695
10.19_140.9954m/z	140.9953609	10.1851	pos	Acetylphosphate	HMDB0001494	Organic acids and derivatives	Organic phosphoric acids and derivatives	Phosphate esters	**	C00227	38.3	0	M+H	C2H5O5P	4.46143893	53685.39815	51645.99406	52434.73851	54425.82699	55563.62634	55250.43314	56520.92704	52493.3572	54242.00705
10.27_203.1430m/z	203.1429583	10.2673	pos	Feniculin	87223	Benzenoids	Phenol ethers	Unclassified	*		38.3	0	M+H	C14H18O	-0.412470457	1182.371745	919.1608259	1143.980803	1171.905588	917.2927478	1075.731184	1169.65135	1036.91533	1170.37129
10.42_209.1532m/z	209.1532438	10.41986667	pos	2,3,5,6,8,8a-Hexahydro-2,5,5,8a-tetramethyl-7H-1-benzopyran-7-	94764	Organoheterocyclic compounds	Benzopyrans	Unclassified	*		38.3	0	M+H	C13H20O2	-1.74155064	2337.267714	1996.299939	1472.041902	1672.437172	1516.715784	1478.450887	1228.833668	1571.306044	1561.426629
10.46_221.1170m/z	221.1170219	10.45796667	pos	1-(5-Acetyl-2-hydroxyphenyl)-3-methyl-1-butanone	HMDB0032589	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		38.3	0	M+H	C13H16O3	-0.903681695	3213.314517	2011.088481	2417.464745	2215.219653	2486.43377	2464.889875	2549.627586	2402.632838	2766.137753
10.74_247.1661m/z	247.1661486	10.73778333	pos	Linalyl butyrate	HMDB0030427	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		38.3	0	M+Na	C14H24O2	-3.131712484	968.3677302	1081.62887	907.9421558	964.9264934	1171.032946	1079.086842	892.5923623	1369.72691	1188.09367
10.91_840.5727m/z	840.572717	10.91385	pos	PS(16:1(9Z)/22:0)	HMDB0112364	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoserines	*		38.3	0	M+Na	C44H84NO10P	0.259056025	3243.58301	2261.422664	16738.78488	13964.01463	13796.80859	11442.5538	20604.00598	19699.24427	11256.346
11.46_261.0165m/z	261.0165073	11.45555	pos	SQ 26180	71381	Unclassified	Unclassified	Unclassified			38.3	0	M+Na	C6H10N2O6S	5.585850935	4127.641312	3943.66851	4581.566128	4923.392219	4514.118375	5594.81672	4886.211098	4588.289747	5651.325466
11.69_136.1120m/z	136.1119794	11.688	pos	2,4,6-Trimethylaniline	73217	Unclassified	Unclassified	Unclassified			38.3	0	M+H	C9H13N	-0.714267857	455.8597042	260.2762505	273.3468064	342.0635806	340.089722	367.019852	309.1116317	352.3101374	363.2449062
12.34_384.2347m/z	384.2346755	12.34246667	pos	6alpha,9-Difluoro-11beta-hydroxypregn-4-ene-3,20-dione	70851	Unclassified	Unclassified	Unclassified			38.3	0	M+NH4	C21H28F2O3	0.542740563	905.0321838	904.202037	1091.305929	794.3796781	1010.961638	761.383274	943.6813508	1059.321062	1034.759085
13.53_206.0665m/z	206.0665571	13.525	pos	(2E)-3-(methoxycarbonyl)pent-2-enedioic acid	LMFA07010698	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters			38.3	0	M+NH4	C7H8O6	3.422960215	422.6356228	363.1939297	647.0850861	646.766116	562.0702316	685.1743314	563.2752977	640.5607135	698.2105506
13.60_149.1071m/z	149.1071468	13.59691667	pos	Norcotinine	64431	Organoheterocyclic compounds	Pyridines and derivatives	Pyridinylpyridines	*	C06524	38.3	0	M+H	C9H12N2	-1.203672053	885.1208697	823.507237	596.7686997	550.0384048	431.0333916	458.2469761	735.9722501	648.2804448	
13.70_123.0916m/z	123.0916172	13.69921667	pos	Trimethylpyrazine	HMDB0031844	Organoheterocyclic compounds	Diazines	Pyrazines	*		38.3	0	M+H	C7H10N2	-0.471637423	1424.962172	1435.403245	1263.818189	2002.022365	1677.291721	1721.214344	1499.108941	1681.882607	1505.247611
14.64_878.744m	901.7236565	14.63885	pos	TG(16:0/18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))	HMDB0005391	Lipids and lipid-like molecules	Glycerolipids	Triradylglycerols	**	C00422	38.3	0	M+NH4, M+Na	C57H98O6	-2.237019436	99147.13567	111974.2303	119937.7598	150785.2491	207754.3403	206284.9168	156333.0014	156157.1862	168957.7985
14.97_312.3254m/z	312.3254369	14.96678333	pos	6Z,9Z-Eicosadien-11-ol	LMFA05000532	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols			38.3	0	M+NH4	C20H38O	-2.223769008	3089.965213	920.5828258	1558.637615	2019.092602	1462.488821	1699.135469	2223.796726	1679.618114	2681.132185
15.29_448.1166m/z	448.1165933	15.29438333	pos	Pigment A aglycone	HMDB0029250	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	*		38.3	0	M+H	C25H19O8+	2.961889063	81.83821894	1218.120412	441.8499349	857.2094957	1005.653714	192.6192616	24275.60845	914.536454	521.1027453
15.52_150.1019m/z	150.1019161	15.51933333	pos	2-Dimethylamino-5,6-dimethylpyrimidin-4-ol	68685	Unclassified	Unclassified	Unclassified			38.3	0	M+H-H2O	C8H13N3O	-3.936071698	3509.289728	3147.541484	345.3340342	3954.244869	8703.800385	11326.82149	11997.60762	45.83606009	11.6705949
15.52_166.0749m/z	166.0748756	15.51933333	pos	Cytomazine	HMDB0029862	Organoheterocyclic compounds	Triazines	Aminotriazines	*	C14147	38.3	0	M+H-H2O, M+H	C6H10N6	4.271400433	6845.602932	3134.317539	998.5233748	5243.580392	12700.41024	15071.26062	16384.48115	19.02467769	17.62111455
15.52_219.1112m	202.1078867	15.51933333	pos	Zeatin	HMDB0012204	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	**	C00371	38.3	0	M+H-H2O, M+H	C10H13N5O	-3.811299831	10914.43556	10465.37174	1234.231028	14183.94239	36372.5051	41765.66489	40367.74547	264.991375	14.54814541
2.05_290.0318m/z	290.0317837	2.048466667	pos	Histamine Phosphate	85412	Unclassified	Unclassified	Unclassified			38.3	0	M+H-H2O	C5H15N3O8P2	5.322764627	9872.854961	10785.78527	11448.96694	7339.312777	6593.687891	6605.581638	8174.635593	10101.25893	9519.077498
2.07_129.1021m/z	129.102105	2.069933333	pos	L-Lysine	HMDB0000182	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***	C00047	38.3	0	M+H-H2O	C6H14N2O2	-0.920073105	396.8394091	256.4656416	320.3791208	269.9058762	242.1887216	298.5521519	313.3931348	299.2198435	252.534006
2.16_156.0419m/z	156.0419207	2.157266667	pos	Pentanoic acid, 4-amino-, (R)-; Valeric acid, 4-amino-, (R)-(+)-; (	74874	Unclassified	Unclassified	Unclassified			38.3	0	M+K	C5H11NO2	-1.844907707	154.1392557	187.3918372	108.2646232	177.3265463	170.9228136	257.1043467	39.68789037	152.4808429	231.9828656
2.24_157.0469m/z	157.0468665	2.240783333	pos	(9S)-2,3-Dihydrovomifoliol-isovalerate	LMFA01050453	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C04272	38.3	0	M+NH4	C5H10O4	-1.961761345	96.69928204	26.39571043	0.001403199	0.001403199	11.58724739	12.07655924	20.70856092	0.001403199	38.03109804
2.26_121.0648m/z	121.0648062	2.260566667	pos	4-Hydroxystyrene	7012	Benzenoids	Benzene and substituted derivatives	Styrenes	*	C05627	38.3	0	M+H	C8H8O	0.124054176	566.1799711	360.3572896	405.7936246	378.0452831	334.0137811	371.950674	361.662497	377.0453402	358.3380965
2.32_194.0434n	217.0324622	2.32085	pos	Galacturonic acid	HMDB0002545	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C08348	38.3	0	M+H, M+Na	C6H10O7	3.686185611	3220.041422	3244.638642	3208.876045	0.001403199	0.001403199	0.001403199	82.86778103	79.16301346	0.001403199
2.45_217.0325m/z	217.0324888	2.450033333	pos	3-Dehydro-L-gulonate	58394	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C00618	38.3	0	M+Na	C6H10O7	3.171792418	4196.690558	5354.707822	5098.281777	0.001403199	0.001403199	0.001403199	179.0509871	367.567604	240.9751855
2.66_194.034n	217.0325701	2.655183333	pos	L-Iduronic acid	63648	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C06472	38.3	0	M+H, M+Na	C6H10O7	3.911795702	3073.329134	3295.987344	3230.212672	0.001403199	0.001403199	0.001403199	30.88332616	73.44126129	105.6064854
2.72_140.0341m/z	140.0340526	2.721583333	pos	6-Hydroxynicotinic acid	3264	Organoheterocyclic compounds	Pyridines and derivatives	Pyridinecarboxylic acids and derivatives	**	C01020	38.3	0	M+Na	C6H5NO3	-1.20046654	128.9572087	147.9720484	179.4493914	121.2147378	200.513788	198.3626613	197.7593086	198.3626613	131.3447274
2.79_171.0623m/z	171.0622824	2.79025	pos	Digitoxose	44745	Unclassified	Unclassified	Unclassified			38.3	0	M+Na	C6H12O4	-3.357251172	675.9041407	834.1519096	1030.679691	817.546923	757.5088608	811.6135638	923.8746976	749.4660438	748.813276
2.82_230.1014m/z	230.1013852	2.821016667	pos	DPTA NONOate	62980	Unclassified	Unclassified	Unclassified			38.3	0	M+K	C6H17N5O2	0.011930449	712.664601	653.1889386	653.0279043	708.2849145	606.3970771	713.1471823	773.4188333	699.1942817	689.558574
2.96_144.0653m/z	144.0653558	2.9608	pos	3-Amino-2,3-dideoxy-scyllo-inosose	71790	Unclassified	Unclassified	Unclassified			38.3	0	M+H-H2O	C6H11NO4	-1.140849831	1316.462174	1448.709912	1609.345416	1568.417944	1795.882837	1738.235858	1912.591064	1599.856098	1789.387578
2.96_221.1535m/z	221.1535105	2.9608	pos	2-[3]-ladderane ethanoic acid	LMFA01140082	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			38.3	0	M+H	C14H20O2	-0.435405376	3213.86575	2971.920945	3470.877525	3512.127113	3567.394098	3719.716152	4070.437673	3991.363422	3487.520844
3.03_277.0267m/z	277.0266694	3.027516667	pos	3-Hydroxyflavone	HMDB0031816	Phenylpropanoids and polyketides	Flavonoids	Flavones	***	C01495	38.3	0	M+K	C15H10O3	2.172393408	21173.38923	23637.70092	24905.33096	23127.086254	1692.228173	1529.376265	18021.49443	18255.49636	18573.72365
3.11_187.0938m/z	187.0937582	3.112683333	pos	Thetyxene Glycol Monomethyl Ether	HMDB0062666	Organic oxygen compounds	Organooxygen compounds	Ethers			38.3	0.0858	M+Na	C7H16O4	-1.959112695	1273.22647	1244.743931	1273.22647	1192.047716	11920.47716	14653.83908	1754.217599	1754.217599	1304.53948	1472.242266	
3.38_221.1534m/z	221.153447	3.378983333	pos	rosafuline	LMFA05000696	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols			38.3	0	M+H	C14H20O2	-0.723456409	2666.025029	2003.068127	1565.842064	1642.102394	2284.198222	1935.234064	2491.272367	1876.244709	1912.701776
3.43_308.0099m/z	308.0099198	3.431116667	pos	Sulfamethoxazole N4-hydroxylamine	HMDB0013852	Benzenoids	Benzene and substituted derivatives	Benzenesulfonamides	*		38.3	0	M+K	C10H11N3O4S	-0.985303224	4332.405843	3795.556613	3901.684977	1949.41246	2012.154466	1910.958995	3205.165043	3299.884946	3368.370553
3.53_203.1155n	226.1045621	3.530816667	pos	L-Glutamic acid n-butyl ester	3544	Unclassified	Unclassified	Unclassified			38.3	0	M+H-H2O, M+H, M+Na	C9H17NO4	-1.200125028	3338.345234	4689.163146	4175.273982	2076.855671	2529.022038	2564.10999	4153.404008	4357.228028	4111.717582
3.55_102.0552m/z	102.0551656	3.552233333	pos	L-Homoserine	HMDB0000719	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00263	38.3	0	M+H-H2O	C4H9NO3	1.769610997	313.9938858	292.7889259	273.1501587	226.9298047	294.8224579	243.6777306	382.5524502	329.3590541	348.5180856
3.52_125.0961m/z	125.0960751	3.568016667	pos	3,5,5-Trimethyl-2-cyclopenten-1-one	HMDB0040246	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds			38.3	0	M+H	C8H12O	-0.131594487	1388.082026	1324.716501	1473.224072	1368.34243	1564.999107	1940.203968	1827.766021	1940.203968	1827.766021
3.57_141.0181m/z	141.0180531	3.568016667	pos	cis-4-Carboxymethylenebut-2-en-4-olide	66181	Organoheterocyclic compounds	Dihydrofurans	Furanones	*	C04431	38.3	0	M+H	C6H4O4	-1.299736044	128.05662	118.1376156	78.54501886	50.47227121	91.99990115	98.56071456	131.1477239	129.2781615	99.54473443
3.57_313.0890m/z	313.0889917	3.568016667	pos	Osmundalin	87571	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		38.3	0	M+Na	C12H18O8	-1.366815379	1967.623704	2631.660154	1448.843281	908.6903368	867.3761396	1225.074698	1496.291427	1838.145628	1483.33583
3.65_213.1231m/z	213.1230571	3.648783333	pos	2-Phenyl-1,3-propanediyl monocarbamate	2657	Unclassified	Unclassified	Unclassified			38.3	0	M+NH4	C10H13NO3	-1.597812986	815.6623254	960.0621884	881.279457	401.8436367	317.8953584	356.8967557	258.3974802	294.184627	410.3621598
3.74_291.0950n	274.0916786	3.73775	pos	2-Deoxy-2,3-dehydro-N-acetylneuraminic acid	66213	Unclassified	Unclassified	Unclassified			38.3	0	M+H-H2O, M+H	C11H17NO8	-1.544666724	3376.577212	3712.417399	3771.175784	3536.372025	3308.130229	3178.831441	2888.641796	3454.038848	2986.97011
3.87_300.1801m/z	300.1800941	3.866916667	pos	Pisumic acid	HMDB0039241	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.3	0	M+NH4	C15H22O5	-1.613340249	612.8967755	551.258128	753.958898	1934.285578	1907.632275	1243.408806	1040.032447	1181.433471	964.9723808
3.89_213.1228m/z	213.1228305	3.889633333	pos	n-acetylglopamine	96187	Benzenoids	Phenols	Benzenediols	*		38.3	0	M+NH4	C10H13NO3	-2.759362828	1043.292507	527.3755862	1106.476352	304.1475738	191.7967275	492.8845752	437.0217541	198.8077577	613.6763491
4.05_134.0963m/z	134.0963081	4.04663333	pos	N-Methylphenylethanolamine	HMDB0001387	Organic nitrogen compounds	Organonitrogen compounds	Amines	*	C03711	38.3	0	M+H-H2O	C9H13NO	-0.778642019	285.2921533	275.0818947	267.2338302	252.5548323	241.9301012	241.9458788	236.6019068	223.0361604	223.6334205
4.09_354.1542m/z	354.1542289	4.091916667	pos	Diethylpropion (metabolite XI Glucuronide)	2025	Unclassified	Unclassified	Unclassified			38.3	0	M+H-H2O	C17H25NO8	-1.346040435	1484.17121	724.4434885	1548.050729	740.2564688	1199.734602	1179.55495	739.0401126	885.4453669	442.6281029
4.14_189.0737m/z	189.0736872	4.136716667	pos	(Z)-1-(Methylthio)-5-phenyl-1-penten-3-yne	HMDB0032688	Benzenoids	Benzene and substituted derivatives	Unclassified	*		38.3	0	M+H-H2O	C12H12S	2.336392177	246.821788	364.7238893	296.7882943	498.5529126	588.1227003	595.5823705	375.8901448	435.6145043	429.6646709
4.32_327.0950n	328.102249	4.317083333	pos	Acetaminophen glucuronide	HMDB0010316	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		38.3	0	M+H, M+Na	C14H17NO8	-1.357171013	3336.993285	3249.227581	3369.724964	4132.020527	3360.732938	2786.048049	3138.400539	3552.154225	3723.171966
4.36_141.0181m/z	141.0180931	4.3623	pos	2-Maleylacetate	HMDB0060348	Organic acids and derivatives	Keto acids and derivatives	Medium-chain keto acids and derivatives	**	C02222	38.3	0	M+H-H2O	C6H6O5	-0.89803343	536.7361901	531.0598783	70.64210656	118.114803	52.04432642	67.81761611	49.74482489	57.40656489	55.25727233
4.41_266.1154n	267.122683	4.4062	pos	Sapidolide A	HMDB0041582	Organoheterocyclic compounds	Lactones	Gamma butyrolactones			38.3	0	M+H, M+Na	C14H18O5	-0.064135664	31516.7706	32827.53318	33713.79064	23241.85091	21325.49675	21266.29996	31894.63241	36567.82934	33665.71597
4.43_340.1749m/z	340.1749376	4.42815	pos	Tetraneurin A	67802	Unclassified	Unclassified	Unclassified			38.3	0	M+NH4	C17H22O6	-1.633801707	1873.93361	2207.13658	2531.048209	5744.296662	4994.110625	5615.184458	2872.711522	3825.228317	3617.119397
4.45_248.1854m/z	248.1853829	4.451133333	pos	Talaromycin A	86753	Organic oxygen compounds	Organooxygen compounds	Ethers			38.3	0	M+NH4	C12H22O4	-1.094248775	1048.070585	962.3055102	1080.181377	1164.94643	1096.053011	1088.757874	912.5449794	1117.145626	1032.035741
4.54_223.1414m/z	223.1413704	4.542216667	pos	Spermine dialdehyde	HMDB0013076	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		38.3	0	M+Na	C10H20N2O2	-1.63948271	1630.015706	1613.943663	1597.05945	1743.307677	1614.3897	1549.632396	1828.677148	1559.700761	1578.613227
4.61_383.1995m/z	383.1994572	4.610866667	pos	9-Fluoro-16alpha-methylpregn-4-ene-3,11,20-trione	70638	Unclassified	Unclassified	Unclassified			38.3	0	M+Na	C22H29FO3	0.45393608	1461.597562	1807.68847	1597.584435	1279.580552	1081.758331	1102.400094	1091.913627	1191.848925	1060.302954

6.41_546.1369n	569.1257536	6.406516667	pos	Biochanin A 7-(6-methylmalonylglucoside)	87109	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavonoid O-glycosides	*		38.3	0	M+H, M+Na	C26H26O13	-0.766821832	12816.40605	13319.13695	14120.9823	6093.362938	6890.828966	5528.708503	1736.949507	3129.594474	1875.622558
6.44_144.0654m/z	144.065406	6.43815	pos	Alanopine	65929	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		C03210	38.3	0	M+H-H2O	C6H11NO4	-0.70518959	653.5027866	424.3372846	415.3485353	419.3950733	272.3414241	408.7872394	550.5375756	521.7989452	429.909745
6.65_269.2108m/z	269.2107657	6.647516667	pos	2,2,4-Trimethyl-1,3-pentadienol diisobutyrate	HMDB0059777	Organic acids and derivatives	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives			38.3	0	M+H-H2O	C16H30O4	-1.242082859	986.6569917	626.8868595	650.1636708	972.7232712	800.6832554	682.9932406	1021.593773	1026.892728	979.4307313
6.71_198.1486m/z	198.1486218	6.709016667	pos	2-tert-Butyl-4-hydroxyanisole	HMDB0059926	Benzenoids	Phenols	Methoxyphenols			38.3	0	M+NH4	C11H16O2	-1.296175058	972.4551537	969.5707645	831.7625384	646.4666805	675.9623316	781.9959975	915.7341212	831.9208816	830.7770472
6.73_235.1689m/z	235.1688987	6.729133333	pos	Oxysolavetivone	90327	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.3	0	M+H	C15H22O2	-1.527269123	2985.607594	2822.733236	2849.543856	2498.667743	2598.54206	2503.23961	2688.114407	3044.522717	2738.783182
6.75_111.0805m/z	111.0805322	6.748833333	pos	γ-heptenoic acid	34705	Unclassified	Unclassified	Unclassified			38.3	0	M+H-H2O	C7H12O2	0.709048575	186.9139353	143.4204875	200.582386	153.2271573	128.5935568	100.2704482	180.9870983	148.5928384	150.9988438
6.82_368.2402m/z	368.2402171	6.811983333	pos	4,4-Difluoropregn-5-ene-3,20-dione	70642	Unclassified	Unclassified	Unclassified			38.3	0	M+NH4	C21H28F2O2	1.870263086	44182.99007	39970.37438	39414.35534	40497.20868	43624.33026	38020.71048	45969.9219	41112.51902	45897.52264
6.93_207.1376m/z	207.1375887	6.928783333	pos	2-Phenylethyl 3-methylbutanoate	HMDB0035017	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.3	0	M+H	C13H18O2	-1.783148536	879.4176575	842.2126708	539.8785777	637.590404	465.3908052	476.6343149	531.7633176	608.6939611	720.4991422
7.03_111.0805m/z	111.0805361	7.025516667	pos	δ-heptenoic acid	34706	Unclassified	Unclassified	Unclassified			38.3	0	M+H-H2O	C7H12O2	0.739608573	267.0605167	196.7814466	214.8197444	183.9345924	228.1569554	173.8302908	186.5520201	196.1575213	218.4356322
7.16_111.0805m/z	111.0805284	7.16055	pos	β-heptenoic acid	34704	Unclassified	Unclassified	Unclassified			38.3	0	M+H-H2O	C7H12O2	0.679792433	124.164811	164.0147736	173.8495992	183.1228198	169.0656785	138.352192	253.7182363	181.7091932	182.379993
7.16_183.1014m/z	183.1013892	7.16055	pos	Furfuryl pentanoate	HMDB0037727	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.3	0	M+H	C10H14O3	-0.997208959	464.1087258	547.0752524	565.5584402	560.0977827	670.2397265	608.0872377	722.1432093	670.0399813	669.9632651
7.88_199.1802m/z	199.1802243	7.876666667	pos	5-Ethyl-4-methyl-2-pentyloxazole	HMDB0037889	Organoheterocyclic compounds	Azoles	Oxazoles		0.726	M+NH4	C11H19NO	-1.465572692	6110.8649	4852.776445	5243.466549	5987.848363	5772.593669	5318.895513	6622.536182	5558.604337	5474.356018	
7.92_255.2103m/z	255.2103336	7.915266667	pos	5a-Androst-3-en-17-one	HMDB0006046	Lipids and lipid-like molecules	Steroids and steroid derivatives	Androstane steroids	*		38.3	0	M+H-H2O	C19H28O	-1.446275618	1930.812883	2045.148078	2395.158689	3166.340695	2538.952771	2829.759817	2127.920159	2388.854579	2061.109704
7.95_250.1774m/z	250.1773845	7.950883333	pos	Threoninyl-Isoleucine	85957	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.3	0	M+NH4	C10H20N2O4	5.392470604	17188.8526	14099.48121	14175.20535	15105.1323	15525.4009	13711.48209	16681.28073	15124.31539	13786.10148
7.97_344.2249m/z	344.224886	7.9736	pos	4-Dodecylbenzenesulfonic Acid	HMDB0059915	Benzenoids	Benzene and substituted derivatives	Benzenesulfonic acids and derivatives			38.3	0.107	M+NH4	C18H30O3S	-1.549184021	9003.182096	9394.992367	9420.771599	12187.29498	11594.40932	9319.107172	8577.748024	8774.493865	8151.011136
8.29_163.0387m/z	163.0387315	8.292383333	pos	trans-2,3-Dihydroxycinnamate	63527	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	**	C12623	38.3	0	M+H-H2O	C9H8O4	-1.327264325	937.1033827	567.6023734	541.8508675	712.5953791	606.5799213	416.7834392	629.9974791	554.4313037	720.6032618
8.34_250.1774m/z	250.1773501	8.3362	pos	Isoleucyl-Threonine	85822	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.3	0	M+NH4	C10H20N2O4	5.244308964	132650.5971	151746.6907	137209.5693	143653.7773	132218.0638	132450.0112	136837.8487	127379.0225	153572.3283
8.60_455.2631m/z	455.2631163	8.602816667	pos	Rhodopsonin IV	67493	Unclassified	Unclassified	Unclassified			38.3	0	M+H	C24H38O8	-1.82351808	6654.431218	7214.451543	8709.241656	9086.184004	9644.309244	9384.30396	6912.210393	8024.624805	8740.76091
8.68_586.3576m/z	586.3576369	8.6834	pos	Fumonisin AK1	89237	Organic acids and derivatives	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives	*		38.3	0	M+H-H2O	C30H53NO11	-1.551864215	6491.924055	6122.952763	7189.358619	8398.092949	844.4689335	500.5663054	2895.475235	3406.351504	3254.160724
8.94_111.0805m/z	111.0805064	8.939166667	pos	2,4-Dimethyl-2-pentenoic acid	HMDB0039819	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.3	0	M+H-H2O	C7H12O2	0.508064446	244.4536856	271.031966	187.4381432	254.6987145	223.3966691	243.244227	252.709305	196.1802263	267.9552168
9.84_299.1058m/z	299.105763	9.8379	pos	PS-5	71644	Unclassified	Unclassified	Unclassified			38.3	0	M+H	C13H18N2O4S	-0.810069193	15686.50612	15636.90841	13944.18984	14631.31432	17410.95996	18884.38452	15683.34011	15392.57596	17541.62037
0.54_124.0755m/z	124.0755399	0.535	pos	Benzaldehyde	HMDB0006115	Benzenoids	Benzene and substituted derivatives	Benzoyl derivatives	***	C00261	38.2	0	M+NH4	C7H6O	-1.418288551	219.615083	445.861152	288.5167994	244.3574718	118.9201349	303.6522745	78.157362177	307.988847	398.33193
0.54_138.9798m/z	138.9798472	0.535	pos	Phosphoglycolic acid	5780	Organic acids and derivatives	Organic phosphoric acids and derivatives	Phosphate esters	**	C00988	38.2	0	M+H-H2O	C2H5O5P	4.878351652	888.6913128	873.3515348	864.8362628	914.5291338	432.2552126	742.4743442	443.8958053	718.5770912	836.3226069
0.54_184.0017n	185.0070416	0.535	pos	2-Pyrone-4,6-dicarboxylate	66020	Unclassified	Unclassified	Unclassified			38.2	0	M+H-H2O, M+H	C7H4O6	4.842368791	1827.247576	1868.529799	2319.495375	2258.064112	878.3819609	2073.152417	1118.032087	2288.471378	1832.32121
0.54_207.0172m/z	207.017168	0.535	pos	2,3-Diaminosalicylic acid	HMDB0013159	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*		38.2	0	M+K	C7H8N2O3	3.080863024	23120.61529	35606.76059	33830.71784	32189.55142	3267.015052	33716.85376	5778.983429	33223.83855	25738.72298
0.54_210.0166m/z	210.0165628	0.535	pos	α-D-Glutamyl phosphate	3366	Unclassified	Unclassified	Unclassified			38.2	0	M+H-H2O	C5H10NO7P	1.598058304	444.4561971	643.1084674	534.2332723	568.914596	0.001403199	557.5679588	48.38144511	767.673475	437.3174905
0.56_196.0165m/z	196.0164609	0.555633333	pos	3-Indoxyl phosphate	103478	Unclassified	Unclassified	Unclassified			38.2	0	M+H-H2O	C8H8NO4P	3.073667818	107475.8159	94157.10834	92036.74685	93747.12098	82323.06351	91925.48378	84414.02964	88289.17786	85550.29536
0.58_121.0648m/z	121.0648183	0.576333333	pos	4-Ethoxyphenol	HMDB0032036	Benzenoids	Phenols	4-alkoxyphenols	*		38.2	0	M+H-H2O	C8H10O2	0.195687144	226.1509484	165.1701914	160.6068642	93.18333904	134.2933375	132.0446827	130.1362397	215.5164088	91.42313378
0.64_144.0427m/z	144.0426749	0.63815	pos	2-Hydroxyethylphosphonate	63584	Unclassified	Unclassified	Unclassified			38.2	0	M+NH4	C2H7O4P	5.190402094	1713.300768	1026.098293	1233.063644	1405.773321	1197.673026	1833.51847	1264.977246	1245.918598	1270.681459
0.66_127.1229m/z	127.1228643	0.657416667	pos	1-(3-Aminopropyl)-4-aminobutanal	62806	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		38.2	0	M+H-H2O	C7H16N2O	-0.7674349	478.8612778	1388.064273	1391.17833	1300.043487	765.1183193	655.2049624	785.562022	1348.246826	1352.19517
0.68_244.1287m/z	244.1286986	0.6788	pos	Aspartyl-Lysine	85672	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.2	0	M+H-H2O	C10H19N3O5	-1.852872597	3544.048966	3349.558696	2982.434749	3324.391977	3306.368878	3306.940057	3609.524675	3242.497136	3842.281376
0.74_164.0915m/z	164.0915044	0.73955	pos	Dimethyl succinate	HMDB0033837	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.2	0	M+NH4	C6H10O4	-1.574407491	1133.093604	733.3941807	1135.704867	927.4020711	780.1587326	1065.787184	1162.255719	865.8765316	688.2498019
0.74_209.0587m/z	209.058726	0.73955	pos	Serylcysteine	HMDB0029036	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.2	0	M+H	C6H12N2O4S	-1.57796458	6285.881397	4463.677934	4630.420048	10736.28719	13086.9461	14096.88902	5305.40803	4077.697968	4648.245305
0.74_225.1229m/z	225.1229574	0.73955	pos	3-Phenylpropionylglycine	HMDB0002042	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		38.2	0	M+NH4	C11H13NO3	-1.986420987	2250.765588	2757.808654	2757.808654	3665.452249	2068.982447	1478.863861	1656.614317	1648.018988	1813.933535
0.74_237.0844n	260.0736377	0.73955	pos	N-Acetyl-D-glucosaminate	65562	Unclassified	Unclassified	Unclassified			38.2	0	M+H, M+Na	C8H15NO7	-1.880419498	14002.77945	10487.98441	12846.12851	12822.65884	10244.82033	10370.52848	12051.69835	11955.33344	10429.2332
0.74_271.1032m/z	271.1032277	0.73955	pos	Histidylaspartic acid	HMDB0028881	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.2	0	M+H	C10H14N4O5	-1.733838644	3310.764933	4073.259926	4357.987171	4747.577216	4196.968983	4216.49854	2507.450846	1970.927961	2717.664163
0.74_290.1221n	291.1292878	0.73955	pos	Argininosuccinic acid	HMDB0000052	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***	C03406	38.2	0	M+H-H2O, M+H, M+Na	C10H18N4O6	-1.76065807	16584.09898	14777.07699	15186.57842	18907.59285	20671.75051	21054.07406	12521.88236	11015.98699	10561.28572
0.78_135.0649m/z	135.0648661	0.776966667	pos	D-Xylitol	HMDB0002917	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	***	C00379	38.2	0	M+H-H2O	C5H12O5	-2.098588836	487.4616602	456.4930406	548.8496716	414.4709317	249.3275656	333.35031	306.5788055	423.1756592	543.7834598
0.84_181.0969m/z	181.0969308	0.8386	pos	Hydroxy-3,4-dihydrocarbostyril	1550	Unclassified	Unclassified	Unclassified			38.2	0	M+NH4	C9H9NO2	-1.369267364	1332.537261	2531.886011	2625.680057	194.1381096	401.5662575	351.3504119	609.8421329	629.9156131	419.2874233
0.84_199.9952m/z	199.9952485	0.8386	pos	2-(hydroxyimino)- Pentanedioic acid	6691	Organic acids and derivatives	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives	*		38.2	0	M+K	C5H7NO5	-2.061032944	2536.217022	2335.90108	2150.440749	3065.079023	3432.12802	3166.896412	2645.12781	2671.393124	2384.841005
0.84_257.1604m/z	257.1604206	0.8386	pos	Glutaminyllysine	HMDB0028802	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.2	0	M+H-H2O	C11H22N4O4	-1.445548949	1767.096347	1422.225256	1799.642249	734.5193622	478.002645	435.9557312	378.7576723	749.2658884	458.4647106
0.88_158.0446m/z	158.0445572	0.8802	pos	trans-4-Carboxymethylenebut-2-en-4-olide	69495	Organoheterocyclic compounds	Dihydrofurans	Furanones			38.2	0	M+NH4	C6H4O4	-1.620959274	1487.477934	1519.846773	1651.751031	2496.794248	2325.42124	2453.876082	2229.95305	2293.675613	2145.669484
0.88_194.1024m/z	194.1024164	0.8802	pos	3-propylmalic acid	LMFA01170064	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates	**	C02123	38.2	0	M+H-H2O	C7H12O5	0.666924909	0.001403199	53.04920374	78.1552919	0.001403199	0.001403199	0.001403199	318.1743355	117.1812429	
0.88_199.0323m/z	199.032251	0.8802	pos	N-Carbamoyl-DL-aspartic acid	337	Unclassified	Unclassified	Unclassified			38.2	0	M+Na	C5H9N2O5	-1.653293983	881.8593413	1144.520177	834.363224	665.1486801	874.7384277	1004.423318	1069.107126	972.0605087	1015.283768
0.90_284.1963m/z	284.1963309	0.898483333	pos	Alanolol	1128	Benzenoids	Benzene and substituted derivatives	Phenylacetamides	C13235		38.2	0	M+H	C14H22N2O3	-2.018153298	16433.66484	17107.90806	18922.20554	3756.220173	2339.49579	3143.110281	1586.889387	2667.115397	
0.92_213.1231m/z	213.1231213	0.91985	pos	O-BENZYL-L-SERINE	44267	Unclassified	Unclassified	Unclassified			38.2	0	M+NH4	C10H13NO3	-1.268907786	1675.1178	1528.045537	1809.272504	2205.268743	1850.463817	1970.797713	1803.244486	1713.003224	1524.480029
0.92_218.0901n	219.0973299	0.91985	pos	Hydroxyprolyl-Serine	HMDB0028872	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.2	0	M+H, M+Na	C8H14N2O5	-1.000094624	4185.930356	4631.143511	4622.684254	4812.610952	3997.047241	4157.710257	4090.112022	5905.525763	4836.397299
0.94_111.0806m/z	111.0805502	0.941583333	pos	Dihydro-5-propyl-2(3H)-furanone	HMDB0031681	Organoheterocyclic compounds	Lactones	Gamma butyrolactones			38.2	0	M+H-H2O	C7H12O2	0.849863879	287.3432317	170.7875348	237.7256376	236.6319288	266.5381657	310.5627819	290.9802583	178.325511	229.0456194
0.98_125.0960m/z	125.0960442	0.98445	pos	trans-alpha-octenoic acid	LMFA01030018	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.2	0	M+H-H2O	C8H14O2	-0.3323282189	1794.653329	1459.955344	1333.693383	1345.951799	1253.045515	1141.618746	1662.901758	1268.357144	1602.956328
0.98_145.0493m/z	145.0492982	0.98445	pos	3-Hydroxyadipic acid	5334	Organic acids and derivatives	Hydroxy acids and derivatives	Hydroxy acids and derivatives	*		38.2	0	M+H-H2O	C6H10O5	-1.462593557	2141.020969	2239.865804	2018.841737	1588.4194217	1482.577559	1355.059644	1784.630477	1672.851139	
1.01_209.1534m/z	209.1534016	1.006283333	pos	(3R,8E)-3-Hydroxy-5,8-megastigmadien-7-one	96000	Organic oxygen compounds	Carbonyl compounds				38.2	0	M+H	C13H20O2	-0.983623039	2412.113016	1780.781885	1562.46731	1538.222773	1512.109384	1355.540097	1883.511397	1625.491364	1450.536841
1.16_185.0303m/z	185.0303091	1.157483333	pos	5-Hydroxyisourate	63393	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	**	C11821	38.2	0	M+H	C5H4N4O4	-1.206188911	2842.230459	2580.957892	2646.369903	3431.500111	2966.615959	2999.015921	2842.660458	2342.673456	2199.306346
1.16_244.1055n	227.1022008	1.157483333	pos	Glutamylproline	HMDB0028827	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.2	0	M+H-H2O, M+H	C10H16N2O5	-1.772127682	9751.550059	11710.36131	11341.97406	10960.32746	10969.99518	11422.40656	8422.447753	10174.97601	8745.596258
1.18_143.0813m/z	143.0813097	1.178066667	pos	4-Acetamido-2-aminobutanoic acid	HMDB0031411	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C06442	38.2	0	M+H-H2O	C6H12N2O3	-1.213845253	1346.609365	1695.096091	1641.93073	1454.875236	1507.640339	1501.349092	1305.978818	1423.809898	1390.27063
1.18_145.0970m/z	145.0969684	1.178066667	pos	GUVACINE	44304	Unclassified	Unclassified	Unclassified			38.2	0	M+NH4	C6H9NO2	-1.460842976	661.5129968	946.0202613	734.3550939	1216.531822	1180.709463	1050.054104	681.3231464	762.790102	765.6289099
1.20_197.0653m/z	197.0653492	1.197066667	pos	Dehydrosporic acid	342	Organoheterocyclic compounds	Lactones	Gamma butyrolactones	**	C05422	38.2	0	M+NH4	C8H8O5	-1.777890389	4681.631719	5293.939569	5870.205843	4695.222066	4421.613276	4502.0181	4753.489067	5277.279021	4613.233397
1.20_225.0867m/z	225.0866941	1.199716667	pos	5-Hydroxykynurenine	63541	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C05651	38.2	0	M+H	C10H12N2O4	-1.290546476	2430.242759	2722.67834	2727.098967	1840.755758	2400.339917	1753.435169	3039.060095	3180.00695	3068.60491
1.22_111.0806m/z	111.0805685	1.22075	pos	ε-heptenoic acid	34707	Unclassified	Unclassified	Unclassified			38.2	0	M+H-H2O	C7H12O2	0.992828908	300.9080227	177.8734187	217.3189997	246.7435538	220.3524826	208.9387891	293.9164049	289.1718956	287.7642159
1.24_287.1113n	270.1079641	1.243033333	pos	n-Ribosylhistidine	6481	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.2	0	M+H-H2O, M+Na	C11H17N3O6	-1.682174564	2589.856517	3770.438175	3304.484167	2647.404413	2912.401316	2598.269406	1830.774795	3213.908772	2754.664706
1.29_206.1020m/z	206.1020467	1.285033333	pos	N-Acetyl-D-quinovosamine	70939	Unclassified	Unclassified	Unclassified			38.2	0	M+H	C8H15NO5	-1.229994964	2086.775661	2138.290832	1859.867067	1271.010952	1377.623836	1425.850119	1658.127363	1862.887721	1818.049524
1.29_263.1639m/z	263.1362978	1.327966667	pos	1-dimethylsiloxy-decane	LMFA11000719	Lipids and lipid-like molecules	Fatty Acyls	Hydrocarbons			38.2	0	M+H	C12H27NO	4.70915446	21909.11727	23251.65113	20547.76424	19513.79287	21673.59518	20156.05196	19288.15239	21673.79354	20410.79504
1.46_113.0962m/z	113.096218	1.458683333	pos	Isopentyl acetate	HMDB0031528	Organic acids and derivatives	Carboxylic acids and derivatives	Carboxylic acid derivatives	*	C12296	38.2	0	M+H-H2O	C7H14O2	0.972580991	137.0050206	148.0514197	139.849907	132.572484	137.3328285	133.1443883	96.15027191	99.77479315	103.3532468
1.54_111.0806m/z	111.0805934	1.544616667	pos	4-Methyl-5-hexanolide	HMDB0031174	Organoheterocyclic compounds	Lactones	Delta valerolactones			38.2	0	M+H-H2O	C7H12O2	1.186561089	209.4357151	253.853614	217.9063504	213.3123071	256.1012124	227.3425125	260.4496566	243.1740685	199.4853977
1.54_153.0545m/z	153.0545027	1.544616667	pos	Vanillin	HMDB0012308	Benzenoids	Phenols	Methoxyphenols	***	C00755	38.2	0	M+H	C8H8O3	-0.775002601	1179.473894	1126.578141	1131.030536	1014.839389	1176.579686	1160.694032	1378.905349	917.1293783	1171.071875
1.59_147.0650m/z	147.0649707	1.589283333	pos	L-Fuculose	HMDB0060267	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	**	C01721	38.2	0	M+H	C6H12O5	-1.307682332	229.2716751	257.1870459	254.0762164	165.4571467	207.6206222	186.0229704	178.2679535	281.0719795	199.4494035
1.70_324.0021m/z	324.0021284	1.697866667	pos	Riccionidin A	LMPK12010445	Lipids and lipid-like molecules	Polyketides	Flavonoids		4.88	M+NH4	C15H9O6+	-3.307317943	9651.250246	9368.933076	10694.5409	10188.82035	10139.70134	10183.46115					
1.76_157.0606m/z	157.0605656	1.76405	pos	Imidazolelactic acid	HMDB0002320	Organoheterocyclic compounds	Azoles	Imidazoles	*	C05132	38.2	0	M+H	C6H8N2O3	-1.300677328	200.1898113	193.3265046	217.3988161	112.3980301	19.13214062	27.20755997	183.5890634	161.1945234	189.2375539
1.79_111.0806m/z	111.0805729	1.7859	pos	beta-EMGBL	69656	Unclassified	Unclassified	Unclassified			38.2	0	M+H-H2O	C7H12O2	1.026856186	367.2400483	324.0902439	278.7160666	275.1355634	268.1730265	264.1212838	301.2290038	265.7423028	227.8542838
1.92_221.9845m/z	221.9844712	1.916533333	pos	8-Hydroxythioguanine	HMDB0060804	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	*		38.2	0	M+K	C5H5N5OS	-0.916127731	2035.817436	2534.762743	2487.726048	480.2768376	399.5880781	369.4694219	1721.765006	1991.988716	1806.944362
10.29_156.9904m/z	156.9904497	10.28965	pos	Methylmalonic acid	3712	Organic acids and derivatives	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives	**	C02170	38.2	0	M+K	C4H6O4	5.786030648	3001694.836	2979027.77	2892698.175	2990649.312	3100580.091	3075927.635	3111124.14	2969944.075	3077250.515
11.11_810.5970m/z	810.5970242	11.11425	pos	PC(14:0/22:1(13Z))	HMDB0007887	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	**	C00157	38.2	0	M+Na	C44H86NO8P	-1.652832983	36323.76246	31491.54831	20176.35401	8588.177682	5302.819972	4759.976629	18701.60313	14109.91824	9199.543847
12.23_297.2396m/z	297.2396963	12.2313	pos	12,13-epoxy-9-octadecenoic acid	35862	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C14826	38.2	6.26	M+H	C18H32O3	-0.198850938	24811.88529	20989.09694	24409.09169	25462.04213	24225.14158	28627.73456	28410.87023	28503.27847	
12.37_605.5493m/z	605.5492841	12.37401667	pos	DG(14:1(9Z)/22:0/0:0)	HMDB0007057	Lipids and lipid-like molecules	Glycerolipids	Diradylglycerols	*		38.2	0	M+NH4	C39H74O5	-1.69167127	18075.571	17608.4802	16576.84634	17511.8436	13495.79614	15260.82993	16975.39344	16129.98844	15425.80179
12.62_256.2630m/z	256.2630206	12.62173333	pos	Hexadecenal	HMDB0060482	Lipids and lipid-like molecules	Fatty Acyls	Fatty aldehydes	*	C06123	38.2	3.12	M+NH4	C16H30O	-1.975041443	126836.6876	119875.5208	111542.2466	109266.5531	123734.2109	129099.3368	123673.9792	114278.9816	118150.9479
12.79_649.6266m/z	649.6265638	12.78523333	pos	19:0 Cholesteryl ester	41699	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid esters	**	C02530	38.2	0	M+H-H2O	C46H82O2	-2.444851311	2361.22103	3011.273415	4076.320137	3349.030464	4403.676526	4204.543544	2832.717433	3362.18134	4198.8677
13.55_322.0771m/z	322.0771261	13.54818333	pos	7-aminoflunitrazepam	96150	Organoheterocyclic compounds	Benzodiazepines	1,4-benzodiazepines	*		38.2	0	M+K	C16H14FN3O	6.6322839	11984.59433	603.0665828	0.001403199	64.82943288	101.7849642	0.001403199	97.82991778	28.88481571	29.24684636
13.73_100.0760m/z	100.0759578	13.73403333	pos	5-Aminopentanoic acid	HMDB0003355	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00431	38.2	0	M+H-H2O	C5H11NO2	2.456837455	173.1643125	175.7939502	193.3695883	144.7921001	195.285289	148.4692781	184.4117524	184.0356432	206.500906
14.29_313.1765m/z	313.1765131	14.29098333	pos	MG(i-12:0/0:0/0:0)	HMDB0072860	Lipids and lipid-like molecules	Glycerolipids	Monoradylglycerols	*		38.2	0	M+K	C15H30O4	-3.845414425	3076.833145	3101.920149	2871.16444	3144.95144	3259.755314	3352.209926	1348.039179	3164.279617	3428.683155
14.70_223.0632m/z	223.0631742	14.70206667	pos	2,4'-Diphenyldiamine	73114	Unclassified	Unclassified	Unclassified			38.2	0	M+K	C12H12N2	-0.175378978	55402.51836	3125.874261	6055.013913	2120.976429	2579.677238	1827.183968	1955.574997	2626.73902	2370.318219
14.79_172.1117m/z	172.1116956	14.79195	pos	Rasagiline	HMDB0015454	Benzenoids	Indanes	Unclassified			38.2	0	M+H	C12H13N	-2.2225577449	4003.285398	3700.254116	4046.977592	4144.4287	4375.423795	4257.910561	4446.911691	4262.33192	3934.847566
14.94_154.1223m/z	154.12234	14.93678333	pos	1-Phenyl-1-propanol	87821	Benzenoids	Benzene and substituted derivatives	Phenylpropanes	*		38.2	0	M+NH4	C9H12O	-2.208301257	262.7561665	230.8256323	223.7597981	226.3788281	210.1098054	238.6161168	276.5239128	236.271126	176.3938262
15.32_111.0918m/z	111.0918468	15.31646667	pos	3-Methylpyridine	HMDB0061887	Organoheterocyclic compounds	Pyridines and derivatives	Methylpyridines			38.2	0	M+H	C6H7N	1.849278499	53.7852622	41.71274393	54.3200094	137.0405337	53.90339083	36.84070365	55.62390685	48.60739434	42.94581512
15.50_155.0918m/z	155.0917833	15.50085333	pos	1-Nitrohexane	HMDB0013812	Organic

3.87_284.2064m/z	284.2063789	3.866916667	pos	Pentadecylic acid(d3)	LMFA01010045	Unclassified	Unclassified	Unclassified		38.2	1.01	M+K	C15H27D3O2	-0.773379505	5355.40191	4770.109424	3588.719787	7206.543096	2741.128115	2283.082118	3177.822055	3969.154759	3747.262331
3.89_101.0600m/z	101.0600252	3.889633333	pos	2-Methyl-3-hydroxybutyric acid	HMDB0000354	Fatty Acyls	Fatty acids and conjugates	*		38.2	0	M+H-H2O	C5H10O3	2.704586309	225.9565112	202.7046427	173.8589856	189.0495144	196.5730372	147.3976027	219.8592742	210.5662188	215.5889705
3.91_163.0753m/z	163.0752965	3.911966667	pos	1-(2,4-Dihydroxyphenyl)-1-butanone	88210	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*	38.2	0	M+H-H2O	C10H12O3	-0.330357143	927.1298706	1014.194569	920.5979168	823.9641215	720.3387032	672.0631561	1348.56074	1086.666228	1020.24814
3.98_281.1493m/z	281.1492813	3.979183333	pos	Valyl-Tyrosine	86031	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	38.2	0	M+H	C14H20N2O4	-1.079064736	1013.751007	994.0489947	1039.586164	1419.5788	1308.699027	1172.563872	953.2711953	1056.029465	1101.387018
4.05_125.0961m/z	125.0960702	4.040633333	pos	3Z-Hexenyl acetate	LMFA07010181	Organic acids and derivatives	Carboxylic acids and derivatives	Carboxylic acid derivatives	**	C19757	38.2	M+H-H2O	C8H14O2	-0.149345052	900.7314089	830.7698344	799.5566561	712.3807101	773.5872571	815.6472634	811.4608228	733.995677	884.222796
4.09_289.0372m/z	289.0371995	4.091916667	pos	5-Methoxycanthin-6-one	HMDB0030227	Alkaloids and derivatives	Indolonaphthyridine alkaloids	Unclassified		38.2	0	M+K	C15H10N2O2	-0.744473195	436.4291799	372.8721746	524.6356144	456.574375	439.629514	336.1355505	1869.065893	1898.861052	1945.746565
4.14_276.0840m/z	276.0839675	4.138716667	pos	N-Acetylvanillalanine	HMDB0011716	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	38.2	0	M+Na	C12H15NO5	-1.089709984	844.5830414	965.6620012	872.1477373	663.3250537	646.3168661	532.9247493	874.1811167	979.4244232	960.5921155
4.18_363.0681m/z	363.0680624	4.182316667	pos	D-1-Deoxy-erythro-hexo-2,3-diulose	86599	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	38.2	0	M+K	C12H20O10	-2.291085374	1981.841808	1929.276338	1993.677733	594.8541638	522.2799376	541.5854867	1152.533888	1226.377514	1263.278153
4.29_111.0806m/z	111.0805624	4.294383333	pos	2-Hexenyl formate	92996	Organic acids and derivatives	Carboxylic acids and derivatives	Carboxylic acid derivatives		38.2	0	M+H-H2O	C7H12O2	0.945132011	307.3661837	264.7162242	227.950997	268.5795082	223.2151889	225.6702473	264.5344407	222.0478579	299.7023122
4.29_316.2115m/z	316.2115063	4.294383333	pos	Tetranor-PGD1	74980	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids		38.2	0	M+NH4	C16H26O5	-1.150961159	1608.094394	1969.34617	1975.811637	1839.46828	1658.789253	1923.096825	1954.874464	1891.506035	1573.562974
4.34_147.0803m/z	147.0802537	4.33965	pos	3-Phenylbutyric acid	HMDB0001955	Phenylpropanoids and polyketides	Phenylpropanoic acids	Unclassified	*	38.2	0	M+H-H2O	C10H12O2	-1.143465929	978.9249763	989.4661704	931.9106623	716.6772656	551.4608127	519.1577771	788.6611931	842.0120082	849.8457443
4.34_231.1126m/z	231.1125921	4.33965	pos	1,2-Didroxyactarine	2628	Unclassified	Unclassified	Unclassified		38.2	30.3	M+H	C13H14N2O2	-0.921627076	2786.438476	2761.372384	2464.493029	2564.706616	2441.052611	2268.353454	2035.202182	2529.895248	2620.621941
4.36_143.0701m/z	143.070146	4.3623	pos	2-Methyladipic acid	HMDB0029167	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*	38.2	0	M+H-H2O	C7H12O4	-0.778755891	425.526293	460.0386622	561.065794	540.6897165	405.3385367	437.9235504	410.180239	315.7071477	460.4863634
4.36_366.0978m/z	366.0977675	4.3623	pos	6-Methylpretetramine	63773	Unclassified	Unclassified	Unclassified		38.2	0	M+H	C20H15NO6	1.517089147	487.9808953	1797.050662	1875.842812	1008.979361	713.5131665	457.4042756	1279.531452	1685.91505	1334.456053
4.38_311.1462m/z	311.146155	4.384366667	pos	Galactosyl 4-hydroxyproline	86214	Alkaloids and derivatives	Rhoeadine alkaloids	Unclassified	*	38.2	0	M+NH4	C11H19NO8	4.308611886	14905.67208	15397.44413	16016.86289	12103.48522	11616.29411	10881.64622	10019.41059	11029.67979	10386.66816
4.38_316.0736m/z	316.0735554	4.384366667	pos	Glutaminylmethionine	HMDB0028803	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	38.2	0	M+K	C10H19N3O4S	2.779498259	3609.270985	4329.137704	4217.52589	3366.370445	2943.117955	3004.827375	4365.360898	4247.207988	4673.471819
4.38_341.1703m/z	341.1702584	4.384366667	pos	Acremoauxin A	67000	Unclassified	Unclassified	Unclassified		38.2	0	M+NH4	C16H21NO6	-1.406732441	6649.786037	5299.011148	4969.953036	3870.113985	2751.905636	4503.270024	1916.950759	1870.902403	3311.948965
4.38_344.1702m/z	344.1701809	4.384366667	pos	Hinokitiol glucoside	70917	Unclassified	Unclassified	Unclassified		38.2	0	M+NH4	C16H22O7	-0.606187308	371.1415501	1872.492184	1809.944036	125.7643892	199.8684765	0.001403199	186.7072025	150.1924744	354.5985504
4.47_121.0648m/z	121.064828	4.473983333	pos	1,2-Dimethoxybenzene	HMDB0032139	Benzenoids	Benzene and substituted derivatives	Methoxybenzenes	*	38.2	0	M+H-H2O	C8H10O2	0.265751737	361.6570295	278.4304572	272.3665495	259.9436732	255.2474998	267.0683892	280.715306	292.4929236	251.8417891
4.52_190.0709m/z	190.0709222	4.51925	pos	2-Oxohept-3-enedioate	63518	Unclassified	Unclassified	Unclassified		38.2	0	M+NH4	C7H8O5	-0.445531953	157.5333319	102.1951739	108.1678975	109.3746362	184.8779367	154.1727821	182.0068048	115.3603909	111.9073165
4.66_156.0419m/z	156.0418587	4.656183333	pos	Pentanoic acid, 4-amino-, (S)-; (S)-4-Aminopentanoic acid; (S)-4	74875	Unclassified	Unclassified	Unclassified		38.2	0	M+K	C5H11NO2	-2.374154041	27.7817205	12.37646697	91.14367613	0.001403199	54.77228221	95.86557617	36.37918014	75.41962957	32.36928626
4.72_110.0733n	128.10692?1	4.723666667	pos	2-Propylfuran	HMDB0040277	Organoheterocyclic compounds	Heteroaromatic compounds	Unclassified		38.2	0	M+H, M+NH4	C7H10O	1.153378224	3245.034697	3100.033667	3191.043476	3206.654756	3116.783204	2924.977888	3592.172011	3087.652102	3067.89651
4.72_411.1255m/z	411.1255483	4.723666667	pos	4-eoclopone	HMDB0304482	Lipids and lipid-like molecules	Prenol lipids	Isoprenoids	**	C01852	38.2	M+H	C17H24O10	1.595772918	1236.177	2432.626353	2460.289656	1395.944707	1924.013279	2059.188884	1977.043238	1898.187068	2146.375199
4.79_186.1408n	209.1283355	4.7912	pos	7-Ethyl-5,6-dihydro-1,4-dimethylazulene	91006	Hydrocarbons	Unsaturated hydrocarbons	Branched unsaturated hydrocarbons	*	38.2	0	M+H, M+Na	C14H18	-0.31770143	1567.109834	2131.370271	2418.850299	591.7588638	720.6054626	765.8684491	1039.640607	1008.050755	1102.181234
4.84_392.1546m/z	392.1546305	4.836966667	pos	Geniposidic acid	64052	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*	C11673	38.2	M+NH4	C16H22O10	-1.314865825	2459.326467	2696.233923	2639.51325	3416.668299	3332.543792	3094.832588	3763.964284	4544.668091	3963.448277
4.86_306.1368m/z	306.1367859	4.8596	pos	Elaeocarpidine	68411	Unclassified	Unclassified	Unclassified		38.2	0	M+K	C17H21N3	0.299999784	4016.332129	3841.87847	5020.248037	4843.407165	4289.972565	5181.059704	3372.440984	3861.578869	4359.234238
4.95_144.0653m/z	144.0653266	4.948983333	pos	Glutamic acid gamma-methyl ester	HMDB0061715	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		38.2	0	M+H-H2O	C6H11NO4	-1.198440302	640.5754859	717.4207417	673.7039955	636.7407846	638.3710152	605.8021162	709.268281	593.5136349	598.522248
4.97_569.1776m/z	559.1775935	4.970833333	pos	5-Hydroxy-6,7,3',4',5'-pentamethoxyflavanone 5-O-rhamnoside	LMPK12140634	Unclassified	Unclassified	Unclassified		38.2	0	M+Na	C26H32O12	-1.871869545	7658.408841	8210.058723	8627.589134	2742.152654	2247.026181	2198.621341	4604.678599	5545.215401	5294.488273
4.99_125.0960m/z	125.0960377	4.991816667	pos	2-Butyrfuran	HMDB0040272	Organoheterocyclic compounds	Heteroaromatic compounds	Unclassified		38.2	0	M+H	C8H12O	-0.432661032	1017.535519	1088.994341	947.4409081	949.8328682	977.2481666	1012.045015	1007.490829	1030.393269	999.1803948
5.01_155.0579m/z	155.0578767	5.013433333	pos	1,1,3,3-tetramethylurea	HMDB0062789	Organic acids and derivatives	Organic carbonic acids and derivatives	Ureas		38.2	0	M+K	C5H12N2O	-2.105324592	160.0762591	152.8271834	97.03432744	127.0690297	46.83144613	123.8029344	58.74939621	169.7204843	196.3755082
5.04_141.0180m/z	141.0180387	5.035783333	pos	2-Methylene-4-oxopentanedioic acid	HMDB0037759	Organic acids and derivatives	Keto acids and derivatives	Gamma-keto acids and derivatives		C06035	38.2	M+H-H2O	C6H6O5	-1.24241844	35.57510937	79.64111603	83.08237535	36.61313855	38.73725102	17.63793401	97.63216256	18.70377064	71.70839778
5.10_242.1384m/z	242.1384298	5.103066667	pos	Vanillin 1,2-butylene glycol acetal	HMDB0032552	Benzenoids	Phenols	Methoxyphenols	*		38.2	M+NH4	C12H16O4	-1.13675286	1973.069994	2181.369803	2087.854603	2110.280644	2256.128983	2113.840386	2629.61122	2212.321946	1954.742246
5.22_141.0180m/z	141.0180381	5.21595	pos	2-methylene-4-oxo-pentanedioic acid	74922	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			38.2	M+H-H2O	C6H8O5	-1.246171891	396.6967461	461.0901676	413.7386127	243.209766	261.7507965	268.0208624	358.6520166	407.5736589	350.4599645
5.26_446.2453m/z	446.2452805	5.26135	pos	Stemoafen-9-carboxylic acid	2452	Unclassified	Unclassified	Unclassified			38.2	M+H-H2O, M+H	C25H36O7	-1.822189641	4233.639991	4875.287753	4854.004624	2384.662142	2540.338713	2467.373329	3962.541024	4261.167172	
5.28_129.1273m/z	129.1273335	5.284233333	pos	(Z)-5-Octen-1-ol	87566	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		38.2	M+H	C8H16O	-0.453212688	98.69714263	105.9771692	58.86945317	64.60005592	73.82346183	71.66118518	75.9519495	88.35162057	102.2722514
5.28_360.2375m/z	360.237488	5.284233333	pos	2,3-Dinor-TXB2	LMFA03030003	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids	*		38.2	M+NH4	C18H30O6	-1.683728154	1746.952923	1517.534369	2061.365262	1885.323498	1716.472744	1801.561905	743.8635154	980.0544758	838.3876107
5.40_264.1359n	265.1431364	5.396716667	pos	Abscisic acid	HMDB0036093	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	***		38.2	M+H-H2O, M+H	C15H20O4	-1.070147812	4451.794507	4887.788137	4807.24146	5955.402857	6096.229644	6075.380409	4108.961475	4736.559174	4025.91809
5.42_188.1048n	171.1014861	5.419283333	pos	(+/-)-Methyl 5-acetoxyhexanoate	HMDB0032387	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.2	M+H-H2O, M+Na	C9H16O4	-0.44979115	2427.280367	2267.539713	2624.242785	1760.89843	2049.749882	2038.089689	2218.717564	2108.600422	2010.123096
5.46_414.2304m/z	414.2304569	5.481066667	pos	3beta-Hydroxypregn-5-en-20-one sulfate	HMDB0060382	Lipids and lipid-like molecules	Steroids and steroid derivatives	Sulfated steroids	**	C18044	38.2	M+NH4	C21H32O5S	-1.0441965	3174.010256	3825.531095	3362.335893	3297.104549	3028.244015	2956.691044	3829.980441	3352.418223	3690.341279
5.52_436.0684m/z	436.0684006	5.5209	pos	S-Adenosyl-4-methylthio-2-oxobutanoate	3518	Unclassified	Unclassified	Unclassified			38.2	M+K	C15H19N5O6S	-0.911284297	2543.531363	2685.684291	3196.696338	607.1598988	785.3447985	795.0999459	2731.066701	2343.648814	2461.924447
5.61_249.0730m/z	249.0730023	5.613933333	pos	Genipin	HMDB0035830	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*	C09780	38.2	M+Na	C11H14O5	-1.51238738	2509.617502	2517.423543	2162.304267	2487.479089	2343.884024	3054.854025	2497.758556	2421.968794	3166.188552
5.66_207.1378m/z	207.1377576	5.656316667	pos	2-Phenylethyl pentanoate	HMDB0035016	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		38.2	M+H	C13H18O2	-0.963489898	3345.447804	2666.834241	2758.037554	3026.591254	2925.182235	2606.130413	2946.627314	2570.447584	2618.609396
5.71_301.0632m/z	301.0631799	5.7661	pos	1,6-Dimethoxypyrene	HMDB0060337	Benzenoids	Pyrenes	Unclassified		C18260	38.2	M+K	C18H14O2	2.449806646	1458.944582	1462.02702	1734.159498	704.3488494	659.2973112	686.158493	1696.871458	1426.449926	1582.340156
5.82_219.1378m/z	219.1378048	5.821	pos	Isoamyl cinnamate	92527	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Cinnamic acid esters			38.2	M+H	C14H18O2	-0.694380099	1186.848545	1111.889053	1169.125397	1357.779829	1163.529786	1279.207722	835.3496874	1217.092103	1141.47387
5.82_219.0575m/z	219.0574981	5.821	pos	N-Acetyl-L-leucine	HMDB0033519	Organic acids and derivatives	Organic carbonic acids and derivatives	Organosulfonic acids and derivatives			38.2	M+H	C7H17NO4S	1.518256857	0.001403199	0.001403199	0.001403199	4270.220327	4258.575307	4741.085458	0.001403199	0.001403199	0.001403199
5.84_111.0806m/z	111.0805523	5.843716667	pos	1,3-Diacetylpropane	86057	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds			38.2	M+H-H2O	C7H12O2	0.866376067	2469.00363	1952.898411	2125.380518	2227.410156	2335.303603	2222.403184	2629.363093	2191.996266	2403.718649
5.84_141.0180m/z	141.0180353	5.843716667	pos	2-Hydroxymuconate	65778	Unclassified	Unclassified	Unclassified			38.2	M+H-H2O	C6H6O5	-1.263777854	49.33391634	57.63926276	25.78531507	46.33711456	25.67998941	46.3933534	15.01091672	55.17979656	53.3002812
6.04_219.1741m/z	219.174104	6.041083333	pos	Nookatone	HMDB0013687	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		38.2	M+H	C15H22O	-1.089919634	1415.496389	1598.509157	1171.959681	993.7859255	1188.337072	1301.353205	1420.643249	1467.293936	1386.235517
6.16_111.0806m/z	111.0805616	6.162416667	pos	alpha-EMGBL	69653	Unclassified	Unclassified	Unclassified			38.2	M+H-H2O	C7H12O2	0.93870992	836.04409	893.9141331	824.7301501	734.7657142	808.3426117	771.762673	903.6683681	758.7841706	872.2352171
6.48_246.1073m/z	246.1073181	6.476883333	pos	Cabulosine	96475	Unclassified	Unclassified	Unclassified			38.2	M+NH4	C14H20N2O5	-4.949766062	3174.010256	3688.54951	2668.594569	4460.502137	4600.14647	5188.990972	3933.17302	3554.475904	3588.688915
6.78_136.0213m/z	136.0213277	6.779133333	pos	Thiobenzamide S-oxide	71172	Unclassified	Unclassified	Unclassified			38.2	M+H-H2O	C7H7NOS	-1.430750364	578.1227491	480.6324751	344.7017791	480.9608335	383.5386499	379.9477929	544.8686675	316.4870134	507.0828485
6.84_225.1846m/z	225.184588	6.8409	pos	Linalyl isobutyrate	86967	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		38.2	M+H	C14H24O2	-1.420507302	3107.998578	2960.396401	2939.508613	3999.705641	4069.5098	3618.787753	3453.006282	3402.293135	3923.966866
6.90_315.1864n	316.1936664	6.8951	pos	(E)-Piperolein A	86778	Organoheterocyclic compounds	Benzodioxoles	Unclassified	*		38.2	4.35 M+H, M+Na	C19H25NO3	9.3479945	38156.3528	40771.2236	42997.60607	52612.3719	46720.5993	48627.00581	25936.75465	30008.64072	31270.7035
7.29_323.1957m/z	323.195693	7.294266667	pos	Perindoprilat	HMDB0060574	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.2	M+H-H2O	C17H28N2O5	-2.47126708	519.1720892	669.0013699	682.1060182	651.0096722	696.8635719	524.7272661	496.7261313	777.0139082	691.0808728
7.31_235.1689m/z	235.1688775	7.305883333	pos	Dihydromyoporone	LMFA05000650	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		38.2	M+H-H2O	C15H24O3	-1.502429886	6398.120913	5889.970749	5227.427057	6119.165577	5578.24416	5482.098064	5748.578687	5759.940212	5536.787674
7.48_512.2414m/z	374.2413839	7.480483333	pos	Endoxifen-2-glucuronide	HMDB0060622	Phenylpropanoids and polyketides	Stilbenes	Stilbene glycosides	*		38.2	M+H-H2O	C15H17NO8	0.446382194	2120.500059	2029.655553	3263.614298	904.4856947	484.8665394	368.1045191	1113.788003	1073.715828	1154.053729
7.58_441.2089m/z	441.2088883	7.5833	pos	Merodesmosine	86951	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.2	M+K	C18H34N4O6	-5.232205503	16637.56203	15436.92658	14800.61566	17552.45719	16406.23453	17563.63801	15703.97394	16577.9628	16102.50338
7.76_435.1983m/z	435.1982871	7.759183333	pos	Fluocinolone acetonide	2741	Lipids and lipid-like molecules	Steroids and steroid derivatives	Hydroxysteroids			38.2	M+H-H2O	C24H30F2O6	1.172466398	3478.498992	5863.358098	4451.750522	1684.18885	2130.74611	2055.126217	3827.446853	4183.636001	3630.925262
8.48_348.2139m/z	348.2139268	8.4786	pos	10-Nitrolinoleic acid	HMDB0005049	Lipids and lipid-like molecules	Fatty Acyls	Lineolic acids and derivatives	*	C13800	38.2	M+Na	C18H31NO4	-1.852071751	5607.740191	6159.840584	5226.879202	5859.565241	6614.949443	5886.296274	6427.645254	5952.673401	6127.056042
8.57_177.1271m/z	177.12711	8.5719	pos	(2S,4R)-p-Mentha-1(7),5-dien-2-ol acetate	91031	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		38.2	M+H-H2O	C12H18O2	-1.450361673	497.7303756	460.7040911	376.952286	352.2472467	384.7844518	336.0391289	493.2432517	426.0383115	356.0605468
8.79_476.1569m/z	476.1568973	8.772583333	pos	3-Methylbutanoyl-(7Z, 10Z,13Z,16Z,19Z)-heneicosapentaenoic	LMFA04000028	Lipids and lipid-like molecules	Fatty Acyls	Other Fatty Acyls	**		38.2	M+H	C29H37NO3	-4.876650747	6424.351	7887.876725	4617.467804	3579.867786	1544.959858	1299.107974	1359.066717	1391.491498	1295.174389	
9.05_250.1775m/z	250.177492	9.0492	pos	Threoninyl-Leucine	85958	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.2	M+NH4	C10H20N2O4	0.855482535	1251.55415	1068.87278	1062.031188	712.0952801	1157.403274	986.1861027	1270.746986	1164.11031	1414.232411
9.07_121.0648m/z	121.0648259	9.072833333	pos	2-Methoxy-4-methylphenol	HMDB0032136	Benzenoids	Phenols	Methoxyphenols	*		38.2	M+H-H2O	C8H10O2	0.250529592	321.3937459	313.88536	344.9755804	207.704152	217.6520842	274.9276618	352.7654971	242.6537759	295.933088
9.40_369.3105m/z	369.310539	9.399783333	pos	alpha-N-(3-hydroxyhexadecanoyl) L-ornithine	LMFA08020242	Lipids and lipid-like molecules	Fatty Acyls	Fatty amides			38.2	M+H-H2O	C21H42N2O4	-1.632214969	13279.25465	15218.09577	13052.46167	12928.00609	12880.90698	12633.42037	15024.77315	13076.43086	13311.91604
0.51_140.1178m/z	140.1177631	0.51135	pos	Desmethyl-betahistine(2-(2-aminoethyl)pyridine)	1307	Unclassified	Unclassified	Unclassified			38.1	M+NH4	C7H10N2	-3.774107984	255.5459829	624.7870369	117.1075855	381.7032822	245.4391358	643.7275177	1387.945751	903.1307354	663.7239788
0.53_120.0807m/z	120.0807335	0.535	pos	1-(p-Hydroxyphenyl)ethylamine	65983	Unclassified	Unclassified	Unclassified			38.1	M+H-H2O	C8H11NO	-0.30826131	443.1636752	582.3660376	295.5260094	80.20022113	84.06877842	295.5268021	174.2753387	276.9286257	198.9566634
0.68_145.0493m/z	145.0492845	0.6788	pos	3-Hydroxymethylglutaric acid	HMDB0000355	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*	C03761	38.1	M+H-H2O	C6H10O5	-1.546861917	358.914596	966.0632111	755.2503123	291.9208887	487.1769596	613.9533822	606.3239356	656.06555	754.5279745
0.68_198.0870m/z	198.0870177	0.6788	pos	HC Red No. 3	73130	Unclassified	Unclassified	Unclassified			38.1	M+H	C8H11N3O3	-1.521966993	2365.712483	2218.291978	2016.177111	1915.076862	1786.515604	2608.838335	2777.919874	2617.420314	2837.369551
0.72_486.0051m/z	486.0051192	0.717716667	pos	Deoxyuridine triphosphate	HMDB0001191	Nucleosides, nucleotides, and analogues	Pyrimidine nucleotides	Pyrimidine deoxyribonucleotides	**	C00460	38.1	M+NH4	C9H15N2O14P3	-4.956150434	6320.041674	5902.028013	7384.029602	4134.352903	5032.456333	4937.753848	5745.372295	4660.603271	4458.93384
0.76_192.0500m/z	192.0499919	0.758666667	pos	Nitrilotriacetic acid	70268	Unclassified	Unclassified	Unclassified			38.1	M+H	C6H9NO6	-1.421138468	3483.709465	2807.937344	3075.933246	4226.091445	4480.755348	4182.350976	1665.075886	1242.130554	1909.093752
0.82_127.0502m/z	127.0501635	0.818116667	pos	Thymine	290	Organoheterocyclic compounds	Diazines	Pyrimidines and pyrimidine derivatives	**	C00178	38.1	M+H	C5H6N2O2	-0.320610711	3171.570816	3463.16565	3272.771477	4305.034299	3830.036524	4652.773832	3279.786798	2966.049717	3244.391019
0.86_138.0911m/z	138.091149	0.859533333	pos	Lentianin	LMFA05000672	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		38.1	M+NH4	C8H8O	-1.594538656	1216.019	963.2106386	1189.216695	663.6335883	676.9018048	570.4496592	683.8711539	570.4496592	683.8711539
0.86_246.1446m/z	246.144552	0.859583333	pos	Prolyl-Hydroxyproline	85915	Unclassified	Unclassified	Unclassified			38.1	M+NH4	C10H16N2O4	-1.22965494	2716.41271	2608.030538	3028.198869	2856.397341	2735.838097	2557.372986	2111.795388	2606.847267	2663.827832
0.88_260.1479n	283.1395187	0.8802	pos	Asparaginyl-Lysine	85651	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.1	M+H-H2O, M+Na	C10H20N4O4	-2.020545785	7181.377764	7975.345747	7799.674133	8097.229736	7097.835329	7338.454376	6162.027345	7096.146251	7410.344282
0.88_273.1076m/z	273.1076329	0.8802	pos	Nicotinate D-ribonucleoside	58552	Unclassified	Unclassified	Unclassified			38.1	M+H	C11H13NO6	-1.88103976	3572.824698	4150.156019	4173.786734	7120.087764	6707.040207	7049.896681	4689.270897	5296.274556	5147.016474
0.90_341.0467m/z	341.0467266	0.898483333	pos	1,3-Glyceryl dinitrate glucuronide	1584	Unclassified	Unclassified	Unclassified			38.1	M+H-H2O	C9H14N2O13	1.19077923	5227.269379	6311.783979	6765.65427	8258.135506	7550.539165	7758.529653	5959.771264	7194.195825	6437.939154
0.95_143.0701m/z	143.0700887	1.0504	pos	Diethyl malonate	86354	Organic acids and derivatives	Dicarboxylic acids and derivatives	Dicarboxylic acids and derivatives	*		38.1	M+H-H2O	C7H12O4	-1.136154566	507.1087016	461.637288	419.2770833	452.5744599	510.4847444	455.4938573	516.3468316	461.9774685	436.4633365
1.05_166.0499m/z	166.0498504	1.0504	pos	3,5-Dihydroxy-phenylglycine	63854	Unclassified	Unclassified	Unclassified			38.1	M+H-H2O	C8H9NO4	-0.104519768	172.3221383	220.3179151	307.2203795	150.2922575	226.5258895	219.8166482	64.3950465	207.3614903	108.7811744
1.18_147.0649m/z	147.0649346	1.178066667	pos	1,5-Anhydrosorbitol	HMDB0002712	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C07326	38.1	M+H-H2O	C6H12O5	-1.527871815	85.1931137	209.9943564	125.8490575	36.52817591	129.9906541	119.4617542	149.345688	118.1758741	43.71506985
1.24_188.0350m/z	188.0349639	1.243033333	pos	DL-Methionine sulfoxide	6428	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C02989	38.1	M+Na	C5H11NO3S	-1.338852812	1199.832965	1193.871624	1248.254542	820.1527428	879.719439	927.1219325	1289.139042	1300.432948	1161.521604
1.31_175.0842n	198.0732974	1.30655	pos	N-Carboxyethyl-g-aminobutyric acid	HMDB0002201	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.1	M+H, M+Na	C7H13NO4	-1.403333476	6263.086911	7144.962236	7464.843224	6030.561634	5725.741434	5893.417505	5938.440018	6112.9676	6112.549083
1.39_129.1273m/z	129.1273013	1.39465	pos	(±)-(E)-2-Octen-4-ol	HMDB0031300	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols	*		38.1	M+H	C8H16O	-0.704568135	146.8402891	126.3193156	76.41630764	82.41979042	81.26462791	52.94422602	94.55429063	104.2945589	71.46598701
1.47_180.0879m/z	180.0878645	1.441593333	pos	3-Methoxymatic acid	3799	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.1	M+H-H2O	C11H14O4	-0.452023029	1305.187358	1348.682862	854.9487662	832.0088969	1242.612433	1124.845577	1238.235715	595.6499713	521.8585757
1.48_122.0271

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1.79_181.0971m/z	181.0970826	1.7859	pos	p-Acetaminobenzaldehyde	2829	Unclassified	Unclassified	Unclassified				37.9	0	M+NH4	C9H9NO2	-0.438478532	309.1774479	302.4046609	357.2526555	54.18257517	34.10630092	65.10720426	91.90913561	192.3398609	225.2743746
10.46_166.9984m/z	166.9983809	10.45796667	pos	4-Oxoproline	HMDB0304793	Unclassified	Unclassified	Unclassified				37.9	0	M+K	C5H6NO3-	3.551764808	613.7481079	407.6194556	490.3138386	389.0442498	423.5568782	434.4141734	411.533635	463.7587369	474.5735342
10.46_495.2322m/z	495.2321751	10.45796667	pos	Dihydrocodeine-6-glucuronide	2096	Unclassified	Unclassified	Unclassified				37.9	0	M+NH4	C24H31NO9	-3.210332276	9611.100616	6404.560625	10296.33839	7949.23354	8318.445637	9354.495225	7085.926572	10022.69083	10345.81315
10.63_347.2187m/z	347.2187034	10.63171667	pos	Europine	68230	Unclassified	Unclassified	Unclassified				37.9	0	M+NH4	C16H27NO6	3.160135226	2591.049996	4456.638498	1457.410975	873.2747691	1759.226366	932.1071213	736.2513632	2786.271281	546.4287152
11.36_771.5138m/z	771.5137642	11.35961667	pos	PG(16:0/18:1(11Z))	LMGP04010008	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols	*			37.9	0	M+Na	C40H77O10P	-1.191346393	4114.500617	5990.51867	3249.300726	790.4929139	0.001403199	0.001403199	4866.772554	2677.658408	968.28113
11.67_271.1662m/z	271.1661687	11.67456667	pos	4,7,11,14-hexadecatetraenoic acid	LMFA01030164	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates				37.9	0	M+Na	C16H24O2	-2.748104486	760.7952454	838.5199614	537.4901291	834.2850699	713.5560253	1023.219241	694.0028802	745.6784454	641.9129537
11.75_810.5971m/z	810.5970759	11.7471	pos	PC(14:1(9Z)/22:0)	HMDB0007919	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	*			37.9	0	M+Na	C44H86NO8P	-1.570588	170851.4515	135849.2722	105645.2844	36488.24725	31267.61599	21810.75403	89334.70985	64038.86587	52470.85076
11.96_605.5492m/z	605.5492369	11.96068333	pos	DG(18:0/18:1(9Z)/0:0)	HMDB0007160	Lipids and lipid-like molecules	Glycerolipids	Diradylglycerols	*			37.9	0	M+H-H2O	C39H74O5	-1.76742142	26551.74293	28929.47847	28643.89708	25048.97297	22935.8089	23706.18125	31045.2326	25681.42124	27516.30127
11.99_271.1661m/z	271.1660919	11.98863333	pos	4,8,12,16-hexadecatetraenoic acid	34835	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates				37.9	0	M+Na	C16H24O2	-3.057558122	1100.078465	1548.711191	1195.328956	1479.268236	1194.922273	1359.179839	1352.477286	1413.397392	1344.761837
12.37_271.1660m/z	271.1660022	12.37401667	pos	16:4(4Z,7Z,10Z,13Z)	73857	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates				37.9	0	M+Na	C16H24O2	-3.41906073	1199.464544	1226.490211	1307.045647	1242.921873	1314.352177	1041.692164	1016.984338	994.4611147	1143.735416
12.67_427.2452m/z	427.2451733	12.66695	pos	3β-Hydroxy-7,12-dioxo-5β-cholan-24-oic Acid	42779	Unclassified	Unclassified	Unclassified				37.9	0	M+Na	C24H36O5	-0.795503783	1734.605145	950.7672773	1061.749674	1144.699218	1116.71289	1385.22214	1804.712013	979.651875	1824.892522
13.33_271.1603m/z	271.1602058	13.33273333	pos	[2-(Dimethoxymethyl)-1-heptenyl]benzene	91367	Benzenoids	Benzenoids	Benzene and substituted derivatives				37.9	0	M+Na	C16H24O2	-3.40443291	1831.968851	1477.021779	1503.473919	1984.311063	1637.011588	1736.414868	1393.933732	1863.392357	1512.64963
13.46_704.5663m/z	704.5663181	13.46155	pos	1-O-(alpha-D-galactopyranosyl)-N-tetracosanyl-2-aminononane-	LMFA13010062	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides				37.9	0	M+H	C39H77NO9	-1.124865863	3921.095214	5621.354604	5665.133203	7052.352371	8538.359764	8143.493406	7992.948915	7107.67452	8624.910341
13.72_686.5558m/z	686.5557532	13.72123333	pos	GlcCer(d15:1/18:0)	LMSP0501AA46	Lipids and lipid-like molecules	Sphingolipids	Neutral glycosphingolipids				37.9	0	M+H	C39H75NO8	-1.154656346	8274.334581	8302.185088	7842.515728	13441.184	14605.2654	12986.32076	11178.79346	11447.16924	12400.71508
14.12_232.1192m/z	232.1191567	14.11671667	pos	QUINAMIDE ISOPROPYLIDENE	43826	Unclassified	Unclassified	Unclassified				37.9	0	M+H	C10H17NO5	5.225459177	1496.849359	1457.79804	1747.870582	1489.07955	1869.558958	1543.508361	1726.441429	1649.94901	1774.124069
14.26_178.0352m/z	178.0352423	14.26028333	pos	Sulforaphane	HMDB0005792	Organosulfur compounds	Sulfoxides	Unclassified				37.9	0	M+H	C6H11NOS2	-1.356078034	1387.135889	1298.226396	1207.176108	1227.044795	1419.555386	1361.287207	1454.455332	1333.876111	1402.745113
14.63_167.1062m/z	167.1061561	14.62908333	pos	1,6,6-Trimethyl-2,7-dioxabicyclo[3.2.2]nonan-3-one	64049	Unclassified	Unclassified	Unclassified				37.9	0	M+H-H2O	C10H16O3	-2.716073854	200.1601236	462.1425212	425.3252429	479.0869008	456.0586907	412.8960858	542.4405258	479.8665728	540.765954
15.51_136.0502m/z	136.0502165	15.50691667	pos	1,2-Diamino-4-nitrobenzene	73087	Unclassified	Unclassified	Unclassified				37.9	0	M+H-H2O	C6H7N3O2	-2.102248868	207.6105891	163.7324155	25.51831993	229.9418458	552.5082064	484.7178983	510.4677571	2.082224483	0.001403199
2.03_169.0970m/z	169.0969582	2.026633333	pos	PHENYLACETOHYDROXAMIC ACID	44449	Unclassified	Unclassified	Unclassified				37.9	0	M+NH4	C8H9NO2	-1.296723523	134.7385791	102.5446443	121.3171253	119.9457248	126.0678113	126.5658863	112.7552499	169.3190193	178.3612489
2.07_152.0562m/z	152.0562446	2.069933333	pos	2-Hydroxyadenine	HMDB0000403	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	*			37.9	0	M+H	C5H5N5O	-2.923928645	679.9955058	882.2519606	730.1943767	942.6159184	844.1321947	762.6490766	753.8772506	924.2877407	713.4806515
2.09_173.1171m/z	173.1171176	2.0913	pos	4-hydroperoxynonenal	LMFA06000253	Unclassified	Unclassified	Unclassified				37.9	0	M+H	C9H16O3	-0.599789491	1387.246294	1297.464113	1281.146428	1188.074005	1191.178436	1033.759169	1315.982115	1180.980292	1265.222724
2.09_185.0919m/z	185.0918821	2.0913	pos	4-Hydroxy-L-phenylglycine	43209	Unclassified	Unclassified	Unclassified				37.9	0	M+NH4	C8H9NO3	-1.11680352	386.9083315	509.0162994	498.6847951	380.8699567	387.4844828	504.835934	322.2338153	386.1181721	508.9180837
2.22_167.0702m/z	167.0701651	2.220616667	pos	Phenylacetol	HMDB0000779	Phenylpropanoids and polyketides	Phenylpropanoic acids	Unclassified	***	C01479		37.9	0	M+H	C9H10O3	-0.635190798	519.5691283	431.0743783	250.0474225	528.2024358	424.4041514	431.9258563	327.475506	476.6357916	381.8250113
2.54_133.0647m/z	133.0646803	2.53565	pos	3,4-Dimethylbenzoic acid	HMDB0002237	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*			37.9	0	M+H-H2O	C9H10O2	-0.739584897	192.7996485	242.2076879	203.1708685	206.2441155	175.6967821	157.8687783	305.8231944	206.7726079	
2.90_133.0647m/z	133.0646725	2.904316667	pos	2-Phenylpropionic acid	34507	Phenylpropanoids and polyketides	Phenylpropanoic acids	Unclassified	*			37.9	0	M+H-H2O	C9H10O2	-0.791667835	104.9772486	127.7171975	173.8946205	179.0270655	217.0604355	284.7837072	200.7161008	212.195709	229.3687652
2.93_166.0834m/z	166.0834472	2.928333333	pos	3beta,6beta-Dihydroxynortropane	93560	Alkaloids and derivatives	Tropane alkaloids	Unclassified				37.9	0	M+Na	C7H13NO2	-2.810228391	1610.569518	2024.424515	2006.639129	1816.132862	2144.032563	2109.941571	1711.034092	1829.193518	1873.692347
2.95_171.1126m/z	171.1126297	2.950733333	pos	Vanillylamine	HMDB0012309	Benzenoids	Phenols	Methoxybenzenes	**	C16666		37.9	0	M+NH4	C8H11NO2	-1.139671347	23.10381372	102.4924127	90.77337293	180.806768	181.8902437	142.2609009	120.3041937	135.0336056	114.2694849
3.03_315.0633m/z	315.0632979	3.027516667	pos	Ascochitine	HMDB0030145	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*			37.9	0	M+K	C15H16O5	1.326251079	1572.704221	1666.243221	2411.015851	5124.590812	4156.488854	4246.556002	2978.058986	3100.235234	3435.002751
3.06_185.0919m/z	185.0919086	3.060433333	pos	3-Hydroxy-4-methylanthranilate	66092	Unclassified	Unclassified	Unclassified				37.9	0	M+NH4	C8H9NO3	-0.96834046	290.9617608	312.4007587	170.0595426	301.7304455	224.3197438	202.0593293	264.5578982	154.5506216	298.0079557
3.41_156.1382m/z	156.1381778	3.414066667	pos	5-Isopropylbicyclo[3.1.0]hexan-2-one	HMDB0035229	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds				37.9	0	M+NH4	C9H14O	-0.816697839	284.6879883	362.7332337	272.9045709	303.3377573	264.674781	245.7561939	305.3608818	287.4010724	298.5944306
3.43_288.0428m/z	288.0428143	3.431116667	pos	Dubamine	68473	Unclassified	Unclassified	Unclassified				37.9	0	M+K	C16H11NO2	2.720498129	591.1988557	643.3751491	524.4293538	330.8650936	156.1710781	202.5699883	434.5918516	616.592287	498.6242946
3.45_141.0543m/z	141.0543102	3.446883333	pos	2,4,6-Trihydroxytoluene	71189	Unclassified	Unclassified	Unclassified				37.9	0	M+H	C7H8O3	-2.216237464	514.2837514	486.2113088	523.7779235	521.0108581	533.7207626	469.4840185	570.4296808	446.8783179	608.9306283
3.53_157.0833m/z	157.0832988	3.530816667	pos	Polypropylene glycol (m w 1,200-3,000)	HMDB0032478	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols	*			37.9	3.98	M+Na	C6H14O3	-1.60495952	8027.502144	7686.280563	6442.224015	5572.88796	7628.976887	9042.57118	8752.764306	7375.440066	8695.564694
3.54_149.1072m/z	149.1072067	3.5398	pos	Benzenopyranemirine	HMDB0034236	Benzenoids	Benzene and substituted derivatives	Unclassified				37.9	0	M+NH4	C9H9N	-0.90142201	3305.38852	2581.705831	1978.729715	1139.392478	1195.720987	1139.860059	2150.915278	1600.015705	1608.592726
3.60_391.2309m/z	391.2309132	3.604716667	pos	Rehmaionoside B	71698	Unclassified	Unclassified	Unclassified				37.9	0.0193	M+H	C19H34O8	-4.43662481	9113.650526	12873.5194	14234.74968	16622.49172	12933.13007	12651.18673	8857.724331	13214.68894	10717.69301
3.67_379.0442m/z	379.0442366	3.671416667	pos	Cichoriin	67515	Phenylpropanoids and polyketides	Coumarins and derivatives	Coumarin glycosides	*			37.9	0	M+K	C15H16O9	4.841196665	3446.243829	3985.010816	4003.364424	5693.325135	4568.85429	3967.155991	3513.33716	4355.165327	3967.491426
3.72_440.0269m/z	440.026879	3.716333333	pos	5-Hydroxylansoprazole sulfone	923	Unclassified	Unclassified	Unclassified				37.9	0	M+K	C16H14F3N3O4S	-4.963475149	4920.212949	4680.641469	4695.116762	1101.29867	1043.355201	1045.719409	2859.472986	3573.511664	3908.149708
3.89_295.0373m/z	295.0373444	3.889633333	pos	4-[(2,4-Dihydroxyphenyl)azo]benzenesulfonic acid	HMDB0037835	Organoheterocyclic compounds	Azobenzenes	Unclassified				37.9	0	M+H	C12H10N2O5S	-3.314104602	1394.556198	1381.922312	1293.495434	1748.71462	1860.831313	1584.731234	1518.232672	1803.65935	1698.132223
3.91_163.0389m/z	163.0388652	3.911966667	pos	3-Hydroxycoumarin	6512	Phenylpropanoids and polyketides	Coumarins and derivatives	Hydroxycoumarins	*			37.9	0	M+H	C9H6O3	-0.649794377	1.2E+06	816.6289243	864.0293991	794.947689	870.6817168	616.4721546	898.1720588	825.7885	604.8549609
3.91_198.0760m/z	198.0759998	3.911966667	pos	cis-Caffeic acid	HMDB0003501	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	*	C01481		37.9	0	M+NH4	C9H8O4	-0.46937284	293.4358578	328.0537785	257.9493839	187.6131558	121.3604793	186.0640954	257.7906555	224.4080519	207.3958107
4.02_155.0446m/z	155.0445666	4.024633333	pos	4-Amino-2-nitrophenol	73033	Unclassified	Unclassified	Unclassified				37.9	0	M+H	C6H6N2O3	-3.582606079	149.6035867	196.3406601	105.8093192	212.7632365	218.9376784	175.6642883	154.7706497	146.4080108	158.8858275
4.07_184.0576m/z	184.0576316	4.069116667	pos	N-Acetylthreonine	HMDB0062557	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues				37.9	0	M+Na	C6H11NO4	-2.464284365	878.5707129	901.9071986	827.1179948	739.0576414	846.6864891	940.5636286	943.4481216	887.9044685	1026.018142
4.11_153.0544m/z	153.054424	4.114783333	pos	2',3'-Dihydroxyacetophenone	HMDB0029658	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*			37.9	0	M+H	C8H8O3	-1.292841936	863.0744138	843.3428316	880.7975793	619.2095709	661.6597382	922.7786205	685.8790018	734.2698021	828.0656763
4.18_237.1483m/z	237.1483301	4.182316667	pos	4-Heptyloxybenzoic acid	69931	Unclassified	Unclassified	Unclassified				37.9	0	M+H	C14H20O3	-0.808260995	1143.11415	853.3082075	991.7967314	755.0466413	778.5290321	870.7998459	843.9203955	851.1002073	779.3268488
4.20_207.1378m/z	207.1378452	4.204866667	pos	alpha-Methylmethyl butyrate	HMDB0036391	Benzenoids	Benzene and substituted derivatives	Phenylpropanes	*			37.9	0	M+H-H2O	C13H18O2	-0.538610111	1839.624557	1393.499551	1333.59496	952.6383333	1122.892765	1144.16373	1496.215135	1324.432527	1446.859942
4.20_277.0268m/z	277.0268296	4.204866667	pos	2'-Hydroxyflavone	LMPK12110080	Phenylpropanoids and polyketides	Flavonoids	Flavones	*			37.9	1.33	M+K	C15H10O3	2.845241623	5706.072093	5604.563389	6110.695399	925.9855945	601.6933424	959.9436919	5248.613628	5197.911048	5162.57369
4.23_139.1228m/z	139.1228005	4.2272	pos	Phenylethylamine	HMDB0012275	Benzenoids	Benzene and substituted derivatives	Phenethylamines	***	C05332		37.9	0	M+NH4	C8H11N	-1.439805249	110.0786532	57.475721	157.4994675	107.9176855	88.30554347	81.98319436	125.1698897	133.4786967	91.05256383
4.23_301.0848m/z	301.0847972	4.2272	pos	Sudan Brown RR	73207	Unclassified	Unclassified	Unclassified				37.9	0	M+K	C16H14N4	-0.791177283	1019.314478	793.2568577	1078.840866	1150.601099	1110.342548	796.6367086	839.684053	1095.645088	984.2736911
4.27_272.0323m/z	272.03233	4.272416667	pos	2-Hydroxy-6-oxo-(2'-aminophenyl)-hexa-2,4-dienoate	66796	Unclassified	Unclassified	Unclassified				37.9	0	M+K	C12H11NO4	1.562056849	1697.495368	1419.976891	1241.268629	0.001403199	0.001403199	0.001403199	1081.437563	1191.654302	1263.373163
4.34_153.0544m/z	153.054423	4.33965	pos	4',6'-Dihydroxyacetophenone	HMDB0029660	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*			37.9	0	M+H	C8H8O3	-1.299377296	604.3491126	451.0167255	472.3094399	442.035963	451.5595895	430.7451881	515.6570338	468.6856664	467.7862012
4.38_182.0562m/z	182.0562425	4.384366667	pos	(S)-Isowillardine	HMDB0030376	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C08289		37.9	0	M+H-H2O	C7H9N3O4	1.130107157	202.2596432	147.0821989	179.9156702	128.0217903	236.0195943	152.6418197	312.3251597	350.7458458	232.4923556
4.50_232.1000m/z	232.0999923	4.496783333	pos	Ethyl 3-[(2-furanylmethyl)thio]propanoate	94596	Organoheterocyclic compounds	Heteroaromatic compounds	Unclassified				37.9	0	M+NH4	C10H14O3S	-0.927256042	402.6813255	563.2105479	609.9070991	1163.185833	1196.272206	995.1257416	1607.250583	1655.913469	1519.486303
4.72_173.1171m/z	173.1171353	4.723666667	pos	Butyl 3-hydroxy-2-methylidenebutanoate	94736	Organic acids and derivatives	Hydroxy acids and derivatives	Beta hydroxy acids and derivatives				37.9	0	M+H	C9H16O3	-0.496661258	328.7292281	292.1597475	266.2803551	289.6922316	296.6476476	271.9006922	279.8772644	294.585946	285.5739268
4.75_387.1256m/z	387.1255754	4.7456	pos	1-O-Sinapoyl-β-D-glucose	64184	Unclassified	Unclassified	Unclassified				37.9	5.15	M+H	C17H22O10	-7.764346821	3917.96293	4202.007639	4463.508113	5896.553425	5827.347814	5530.773365	4063.655674	4571.667916	4637.17509
4.77_230.1021m/z	230.102055	4.768333333	pos	Linamarin	HMDB0033699	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C01594		37.9	0	M+H-H2O	C10H17NO6	-0.987414858	834.5413061	827.2585875	873.7023942	711.8445256	688.1560418	694.741693	840.2091291	706.2741543	817.6113703
4.79_406.0216m/z	406.0215567	4.7912	pos	Ketoprofen lysine B sulfate	HMDB0038486	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*			37.9	0	M+NH4	C12H17NO10S	2.947511707	460.9737503	719.7502535	679.650457	1317.37534	1111.593046	1378.972925	638.5564017	1011.85307261	1016.702589
4.84_484.1843m/z	484.1842805	4.836966667	pos	AM-toxin I	71340	Unclassified	Unclassified	Unclassified				37.9	0	M+K	C23H31N3O6	-0.366881132	5783.892283	6535.828526	7438.177674	8601.750297	7700.785429	8329.499055	5551.579593	6050.960776	5804.056483
4.90_301.1133m/z	301.113345	4.904516667	pos	Tebupirimfos	HMDB0258766	Unclassified	Unclassified	Unclassified				37.9	0	M+H-H2O	C13H23N2O3PS	-0.210517205	2782.439578	3265.240605	3585.075579	4952.079873	4884.283576	4393.542959	3181.601579	3512.603733	3162.183685
5.06_559.1416m/z	559.1416119	5.058233333	pos	Citrusin F	HMDB0039235	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates				37.9	0	M+K	C22H32O14	-1.445441742	4583.272136	5409.088954	4857.747642	90.71817023	183.832326	181.4618584	2292.77849	2875.796937	2260.581364
5.08_153.0544m/z	153.0544384	5.081	pos	p-Anisic acid	58021	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*	C02519		37.9	0	M+H	C8H8O3	-1.197636679	1736.736754	1757.166645	1707.339154	1793.926205	1749.606916	1855.296442	1751.973665	1689.310709	1906.018685
5.21_201.1271m/z	201.1271208	5.1758	pos	Cinnamylvalerate	HMDB0041318	Benzenoids	Benzene and substituted derivatives	Styrenes				37.9	0	M+H-H2O	C14H18O2	-1.241497397	391.9599104	253.7226885	352.9300807	399.015781	321.5727301	428.4229623	244.7212145	308.3609243	
5.22_151.0388m/z	151.0387887	5.21595	pos	PHLORACETOPHENONE	44660	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*			37.9	0	M+H-H2O	C8H8O4	-1.082000556	581.3426648	521.5495851	511.0839634	8.522816746	25.28899469	0.804772849	381.6114188	477.0172051	411.818603
5.22_159.1165m/z	159.1165184	5.21595	pos	4-Methyl-1-phenyl-2-pentanone	HMDB0031569	Benzenoids	Benzene and substituted derivatives	Unclassified	*			37.9	0	M+H	C12H16O	-1.751408853	811.7748819	797.5680205	843.109903	831.1021461	803.567202	811.1797312	806.7513055	786.9862372	847.3484266
5.54_249.1070m/z	249.1069947	5.543066667	pos	N2-Succinyl-L-glutamic acid 5-semialdehyde	HMDB0001180	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C05932		37.9	0	M+NH4	C9H13NO6	-4.837937484	2205.170168	2252.746903	2456.84124	2198.224544	2083.479198	2157.865928	2336.026384	2302.588333	2114.820255
6.14_287.1251m/z	287.1250638	6.140733333	pos	(S)-(+)-Abscisic acid	53364	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	**	C06082		37.9	0	M+Na	C15H20O4	-1.196184393	479.1745065	548.0637599	667.560341	151.02823	167.4917134	279.0631771	263.4658227	294.8799406	368.4960126
6.20_249.1847m/z	249.1847243	6.1979	pos	4,5-Dimethyl-5-propyl-2-furanheptanoic acid	HMDB0112089	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates				37.9	0	M+H-H2O	C16H28O3	-0.594257644	1258.063674	1159.060471	1165.098947	840.1153211	1018673	688.8240751	602.533234	1047.194738	883.3614348
6.36_153.0544m/z	153.0544372	6.355166667	pos	2',4'-Dihydroxyacetophenone	HMDB0029659	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*	C03663		37.9	0	M+H	C8H8O3	-1.205855168	460.0422392	578.211404	591.4762722	455.0036763	506.5566232	480.9456146	473.8246877	448.9276187	550.8762005	
6.69_280.1669n	298.2008497	6.690566667	pos	3,4,4-Trimethyl-1,2-cyclopentanedione	95017	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*			37.9	0	M+H, M+NH4	C16H24O4	-2.126152461	2907.57067	3384.19471	3156.726578	3575.069988	3105.951	3721.943456	3224.343777	4056.067133	3618.46944
6.71_153.0908m/z	153.0907943	6.709016667	pos	2,6,6-Trimethyl-2-cyclohexene-1,4-dione	HMDB0040216	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*			37.9	0	M+H	C9H12O2	-1.392292337	1466.178255	1367.615605	1294.905303	1179.45206	1075.899658	1162.031488	1404.868102	1346.300587	1329.141931	
6.82_156.0652m/z	156.0652453	6.819833333	pos	(2S,5S)-trans-Carboxymethylproline	71640	Unclassified	Unclassified	Unclassified				37.9	0	M+H-H2O	C7H11NO4	-1.584573433	197.2925019	161.5471627	141.8178968	167.1977243	201.1927164	186.5016062	224.5693718	186.4067777	209.8293968	
7.02_211.1326m/z	211.1326227	7.01515	pos	Dihydro-3-(2-octenyl)-2,5-furandione	88993	Organic acids and derivatives	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives				37.9	0	M+H	C12H18O3	-1.180871755	2839.094621	2850.156126	3064.589236	2807.44826	3055.383543	2869.290512	2750.636928	2589.362275	2668.157603
7.03_329.1496m/z	329.1495865	7.025516667	pos	Phenylalanyl-Tyrosine	85905	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*			37.9	0	M+H	C18H20N2O4	0.009008408	1191.618233	1065.417533	1279.814285	1003.156399	1222.692836	1102.699739	923.8904076	1180.87235	1213.568331
7.04_153.0544m/z	153.0544236	7.03765	pos	2,4'-Dihydroxyacetophenone	HMDB0029657	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*	C13635		37.9	0	M+H	C8H8O3	-1.295589371	606.1760646	529.7203601	588.0959334	491.455721	492.5782039	456.7688535	634.3767511	517.9333841	548.8444623
7.16_185.0919m/z	185.0919063	7.16055	pos	2-Amino-3-methoxy-benzoic acid	43207	Unclassified	Unclassified	Unclassified				37.9	0	M+NH4	C8H9NO3	-0.971868959	175.8072828	103.084158	229.7852895	198.9202074	241.5250795	234.6334817	168.801292	159.8529163	245.4324122	
7.23_156.1382m/z	156.1381571	7.230183333	pos	(R)-Cryptone	91122	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds				37.9	0	M+H	C9H14O	-0.966844612	364.2697372	336.4480774	276.283896	380.7382585	322.832136	328.3852674	322.7952975	310.464984	381.7196015
7.69_488.2975m/z	488.2975111	7.690416667	pos	PG(15:0/0:0)	LMGP04050034	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols				37.9	0	M+NH4	C21H43O9P	-1.66745936	5809.307727	6006.23546	8849.853644	2040.880344	1819.568598	1944.053791	3262.086696	3639.394077	3649.514919
7.84_589.2974m/z	589.2974415	7.837283333	pos	Arbekacin	1113	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates				37.9	0	M+K	C23H46N4O9	3.009711333	3706.228153	3349.393766	3354.892978	2203.747131	1684.032441	1647.410172	1917.585224	1957.333709	2175.194842
8.07_271.1689m/z	271.1688694	8.074933333	pos	Estrone	264	Lipids and lipid-like molecules	Steroids and steroid derivatives	Estrane steroids	**	C00468		37.9	0	M+H	C18H22O2	-1.432225425	677.1950761	828.754906	859.4451895	166.154132	162.1798562	170.0300066	317.2874074	422.7978144	393.4057234
8.09_144.1381m/z	144.1380826	8.085633333	pos	2-Octen-4-one	87568	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*			37.9	0	M+NH4	C8H14O	-1.649023081	497.7900287	619.1744466	562.5054405	592.7125519	589.8537039	781.1560467	641.9451187	621.607824	820.1108968
8.09_265.1583m/z	265.1582784	8.085633333	pos	1,7-Diphenyl-4-hepten-3-one	HMDB0031873	Phenylpropanoids and polyketides	Diarylheptanoids	Linear diarylheptanoids	*			37.9	0	M+H	C19H20O	-1.564450553	2539.185929	3189.195672	3791.972092	1198.886017	1338.667903	1418.733878	2099.999264	2389.179654	2375.579771
8.85_173.1171m/z	173.1171456	8.84705	pos	4-hydroperoxy 2-Nonenal	44823	Unclassified	Unclassified	Unclassified				37.9	0	M+H	C9H16O3	-0.437075378	587.3919979	426.8689854	632.4998601	600.3490885	439.2722706	703.4793072	621.0846674	518.6436186	568.4216405
9.09_178.1071m/z	178.1070533	9.09375	pos	Ethyl methyl_ succinate	HMDB0059893	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*			37.9	0	M+NH4	C7H12O4	-2.06818767	204.2364639	97.07482711	136.8298355	130.9109862	159.9316758	129.3901333	199.7497469	198.3725177	193

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0.68_246.0299n	269.0189646	0.6788	pos	Fonofos	72746	Unclassified	Unclassified	Unclassified			37.2	0	M+H, M+Na	C10H15OPS2	-1.042860191	2093.319392	2065.96579	2191.273702	5613.922114	5900.638904	5657.731837	3436.016515	4303.798653	3622.140899
0.70_278.1515n	301.140685	0.698133333	pos	alpha-CEHC	HMDB0001518	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans	*		37.2	0	M+Na, M+K	C16H22O4	-1.239899659	8676.029445	9675.650474	9764.603981	7061.278237	8025.406024	6997.350003	9846.386153	9055.051302	7997.909845
0.70_395.0383m/z	395.0382732	0.698133333	pos	Caffeic acid 3-O-glucuronide	96063	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		37.2	0	M+K	C15H16O10	2.157958943	2739.961126	3022.438129	2864.699856	6174.80031	5048.680965	5719.726402	4696.617813	4373.389678	4522.244444
0.80_182.0480m	182.0479604	0.796983333	pos	Acamprosate	753	Organic acids and derivatives	Organic sulfonic acids and derivatives	Organosulfonic acids and derivatives			37.2	0	M+H	C5H11NO4S	-1.076488245	1934.701016	1850.458842	1815.161454	2343.398926	2152.490022	2203.012276	1669.497327	2312.917194	2246.748978
0.80_261.1077m/z	261.1077171	0.796983333	pos	L-alpha-glutamyl-L-hydroxyproline	62010	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		37.2	0	M+H	C10H16N2O6	-1.520653812	4228.098718	3948.844091	4249.710738	6885.487735	6618.000854	6484.517103	3405.698554	3823.062264	3378.279237
0.84_336.0549m/z	336.0549253	0.8386	pos	Triazophos	72443	Unclassified	Unclassified	Unclassified			37.2	0	M+Na	C12H16N3O3PS	2.253842297	1198.301355	1912.451487	1773.874112	3548.251832	2591.195235	2602.319051	1505.916044	2140.730684	1801.496454
0.92_244.1542m/z	244.154216	0.919185	pos	3,7-Dimethyl-2E,6E-decadien-1,10-dioic acid	96875	Unclassified	Unclassified	Unclassified			37.2	0	M+NH4	C12H18O4	-0.524514891	393.8384726	444.8837484	282.0019298	609.1186155	536.6121891	441.7799433	324.5139897	256.9417233	557.4148959
0.96_215.0075m/z	215.0075402	0.962983333	pos	3-(Carboxycarbonylamino)-L-alanine	66139	Unclassified	Unclassified	Unclassified			37.2	0	M+K	C5H8N2O5	0.025695959	0.001403199	0.001403199	0.001403199	92.52057037	32.77791477	0.001403199	39.20624193	59.56071575	0.001403199
1.03_240.1087m	240.10871	1.028516667	pos	Tetrahydroneopterin	5890	Organoheterocyclic compounds	Pteridines and derivatives	Pterins and derivatives	*		37.2	0	M+H+H2O	C9H15N5O4	-1.578146161	569.2352407	1058.537545	1106.059393	1311.671366	1039.835478	843.7317289	768.9841261	1223.211037	1492.423377
1.05_173.0005m/z	173.0005438	1.0504	pos	6Z-Octene-2,4-diynoic acid	74334	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			37.2	0	M+K	C8H6O2	4.523348862	19135.61071	18285.58075	18276.14237	16611.04074	17156.45959	17330.60122	18964.14376	18239.74258	18352.18758
1.09_387.0074m/z	387.007394	1.09455	pos	Ribavirin 5'-diphosphate	2298	Unclassified	Unclassified	Unclassified			37.2	0	M+H+H2O	C8H14N4O11P2	-6.802518438	7094.688223	8301.322092	9007.873519	8605.504728	8967.386055	9649.92259	5798.114363	9494.391911	8192.745423
1.16_247.1396m/z	247.1395601	1.157483333	pos	Octopine	3377	Unclassified	Unclassified	Unclassified			37.2	0	M+H	C9H18N4O4	-2.118263623	7028.941269	5146.166563	5224.868563	5706.925373	2933.468576	3093.64089	4773.495231	5929.404821	4314.176059
1.18_182.0672m/z	182.0671803	1.178066667	pos	2-Dehydro-D-xylonate	65865	Unclassified	Unclassified	Unclassified			37.2	0	M+NH4	C5H8O6	7.722743536	14235.59183	17744.11542	15304.37885	15797.45148	16647.32314	16954.03476	13911.22739	15554.27013	14588.22221
1.26_300.1073m	300.107287	1.264483333	pos	Arginyl-Serine	85633	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		37.2	0	M+K	C9H19N5O4	1.626791138	724.3586459	1141.893244	1288.767976	313.8140563	366.84041	385.5505542	87.31610822	316.3352119	268.7709814
1.72_198.1485m/z	198.1485233	1.7202	pos	7E,10-undecadien-4-olide	LMFA07040065	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters			37.2	0	M+NH4	C11H16O2	-1.84306422	85.10508971	118.4436639	46.54197511	99.99005203	45.77738181	37.61273569	37.74877261	30.30368137	108.7215255
1.81_143.9966m/z	143.996582	1.807733333	pos	Cyanopyrazine	65702	Organoheterocyclic compounds	Diazines	Pyrazines		C02018	37.2	0	M+K	C5H3N3	6.919615965	1546.65946	1444.502698	1501.851244	1413.491822	1550.48576	1539.498642	1642.811341	1431.680923	1323.973782
1.98_227.0471m/z	227.0471269	1.982566667	pos	(E)-3-(2-Methylpropylidene)-1(3H)-isobenzofuranone	88130	Organoheterocyclic compounds	Isocoumarans	Isobenzofuranones	*		37.2	0	M+K	C12H12O2	1.271574607	1082.737874	1855.360688	1422.255478	643.3771233	651.8269132	614.5802015	662.3753957	757.6383652	489.9242134
1.98_248.1002m/z	248.1001994	1.982566667	pos	alpha-[3-[(Hydroxymethyl)nitrosoamino]propyl]-3-pyridinemethanol	HMDB0062444	Organoheterocyclic compounds	Pyridines and derivatives	Unclassified	**	C19580	37.2	0	M+Na	C10H15N3O3	-1.610737484	1455.219176	1181.639128	1307.140697	1164.579611	1366.452718	1512.713557	1334.648105	1685.291098	1297.796721
10.00_605.5484m/z	605.5483792	10.00346667	pos	DG(20:0/16:1(9Z)/0:0)	58899	Lipids and lipid-like molecules	Glycerolipids	Diradylglycerols	*		37.2	0	M+H+H2O	C39H74O5	-3.145087395	5348.164836	6434.457951	3093.207538	3791.949547	3241.215826	3446.122628	4942.049976	3431.390469	3834.90659
10.19_463.1887m/z	463.1887322	10.1851	pos	PA(8:0/8:0)	40919	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphates	*		37.2	0	M+K	C19H37O8P	6.999530599	5194.711	5593.420071	3627.750254	5475.663514	5454.943899	5487.419766	3926.912531	5164.436033	5555.894018
10.23_130.0347m/z	130.0347209	10.22606667	pos	N-Methyl-N'-nitro-N-nitrosoguanidine	70187	Unclassified	Unclassified	Unclassified			37.2	0	M+H+2O	C2H5N5O3	-8.364158058	361.8055256	287.7069776	211.8627512	337.9743995	404.1595029	373.908755	300.6209536	305.7827798	418.9544867
10.23_170.0962m/z	170.0961855	10.22606667	pos	4-Biphenylamine	471	Benzenoids	Benzene and substituted derivatives	Biphenyls and derivatives	**	C10998	37.2	0	M+H	C12H11N	-1.421251384	7039.429679	6812.004752	6362.520437	6802.158372	6730.751471	6471.943147	7088.777031	6497.960963	6862.325334
10.47_605.5489m/z	605.5489112	10.40298333	pos	DG(20:1(11Z)/16:0/0:0)	HMDB0007388	Lipids and lipid-like molecules	Glycerolipids	Diradylglycerols	*		37.2	0	M+H+H2O	C39H74O5	-2.290671066	3305.021097	2599707597	28223.45846	21279.77723	20463.84027	19644.44492	28167.45153	29910.23835	26601.26593
10.45_295.1512m/z	295.1512176	10.4464	pos	S-(2-Methylpropionyl)-dihydrolipoamide-E	58573	Lipids and lipid-like molecules	Fatty Acyls	Fatty amides	*	C04424	37.2	0	M+NH4	C12H23NO2S2	1.339210197	4577.72295	1785.15889	1329.861325	2057.363279	4074.847018	4755.514373	2423.205735	2350.218729	5035.266125
10.69_790.5577m/z	790.5576682	10.68925	pos	PG(16:0/20:3(5Z,8Z,11Z))	61854	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols	*		37.2	0	M+NH4	C42H77O10P	-2.061542431	712598.4243	634663.5947	597298.5043	505091.7397	475951.368	466349.351	625044.8753	559451.982	543694.5084
10.91_199.0203m/z	199.0203331	10.91385	pos	Propane-1,2,3-tricarboxylate	73371	Organic acids and derivatives	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives	*		37.2	0	M+Na	C6H8O6	-5.542122099	1498.331577	1421.405786	1313.296704	1471.801751	1432.527578	1567.19328	1447.925937	1338.804665	969.9082353
11.58_603.5332m/z	603.533166	11.58235	pos	DG(14:0/22:2(13Z,16Z)/0:0)	HMDB0007030	Lipids and lipid-like molecules	Glycerolipids	Diradylglycerols	*		37.2	0	M+H+2O	C39H72O5	-2.451278458	2341.257766	3157.541671	2056.474862	1625.002041	2188.528501	1157.237622	2134.851332	1652.378024	1450.004367
11.93_836.5411m/z	836.5411202	11.92588333	pos	PS(18:1(9Z)/20:2(11Z,14Z))	77998	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoserines	*		37.2	0	M+Na	C44H80NO10P	-0.104274913	13133.06576	7916.877332	7220.959386	5403.957357	3375.55845	4832.99984	6879.031591	5871.878822	4314.977083
12.21_760.5834m/z	760.5833598	12.20523333	pos	PC(14:1(9Z)/20:0)	59361	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	**	C00157	37.2	0	M+H	C42H82NO8P	-2.26680488	5726.823988	5188.564954	4095.662582	3682.663073	2897.579733	4995.482397	5870.322087	4400.666797	4906.153312
13.07_810.5965m/z	810.5965488	13.07185	pos	PC(16:0/20:1(11Z))	LMGP01011468	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	*		37.2	0	M+Na	C44H86NO8P	-2.256532355	663121.3983	536597.1694	395263.16	139793.4924	116960.9592	96196.22407	312144.1111	227646.3744	186064.2763
14.48_333.1516m/z	333.1515516	14.48083333	pos	Eremopetasin sulfoxide	HMDB0032003	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		37.2	0	M+H+2O	C19H26O4S	-0.972387279	975.4041889	1269.245229	1289.792208	1448.700548	1368.801905	1373.124969	1259.4482	1205.332538	1130.950329
15.50_159.0660m/z	159.0660347	15.50008333	pos	(±)-Glycerol 1,2-diacetate	HMDB0031712	Lipids and lipid-like molecules	Glycerolipids	Diradylglycerols	*		37.2	0	M+H+2O	C7H12O5	4.824821744	733.9072891	777.3353476	72.80357389	1129.125089	1781.475688	2277.923851	2146.827121	0.001403199	0.001403199
15.51_133.0630m/z	133.0630127	15.50691667	pos	2-Isopropylfuran	94803	Organoheterocyclic compounds	Heteroaromatic compounds	Unclassified			37.2	0	M+Na	C7H10O	5.696622762	334.688231	284.2200139	39.20223897	509.9123578	950.304851	1036.808857	1159.157635	0.001403199	0.001403199
15.51_199.0825m	199.0922056	15.5125	pos	2-Acetyl-1,5,6,7-tetrahydro-6-hydroxy-7-(hydroxymethyl)-4H-azepin-4-one	90504	Organoheterocyclic compounds	Azepines	Unclassified	**		37.2	0	M+H+2O, M+H	C9H13NO4	-9.945093121	2551.59009	2187.614459	340.1882414	2849.804027	6434.480619	7457.228962	7451.506599	9754.6257	0.001403199
15.52_176.1175m/z	176.1174576	15.51933333	pos	Debrisoquine	58453	Organoheterocyclic compounds	Tetrahydroisoquinolines	Unclassified	*	C13650	37.2	0	M+H	C10H13N3	-4.376097281	1151.08819	1118.600883	128.3488809	1639.393961	3498.173825	4719.445915	4769.844815	8.728639631	
2.00_223.0634m/z	223.0634134	2.004416667	pos	Benzidine	71201	Benzenoids	Benzene and substituted derivatives	Biphenyls and derivatives		C16444	37.2	0	M+K	C12H12N2	1.124227458	458.4930206	162.7097978	221.2596841	222.4487823	130.462489	209.3543632	281.5994841	180.6121186	208.1280494
2.05_285.0529m/z	285.0528655	2.048466667	pos	Dihydrowyerone acid	HMDB0039493	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		37.2	0	M+K	C14H14O4	2.025672841	2471.538425	2512.200623	2422.183427	1647.086456	1615.335253	1729.870561	2077.375268	2338.737645	2013.941289
2.11_203.9909m/z	203.9908694	2.113216667	pos	8-oxoguanine	96151	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	*	C20155	37.2	0	M+K	C5H3N5O2	-5.835302574	65.24619446	133.0569433	121.6133239	0.001403199	30.12285921	57.03156682	50.01318043	76.68185234	66.35398754
2.26_188.1152m/z	188.1152656	2.260666667	pos	Inmepip	71954	Unclassified	Unclassified	Unclassified			37.2	0	M+Na	C9H15N3	-2.982970208	3874.278224	3165.108743	3137.795852	3178.8201369	308.685579	319.4613144	1130.130458	1387.730286	
2.36_219.0601m/z	219.0601217	2.360916667	pos	Zileuton	43372	Organoheterocyclic compounds	Benzothiophenes	1-benzothiophenes			37.2	0	M+H+2O	C11H12N2O2S	6.190184825	328.7500743	332.0901938	279.3160615	457.6781998	524.6307902	556.3907072	456.7891441	396.2932204	287.6337778
2.74_187.1324m/z	187.1324231	2.743533333	pos	(5S)-6-Hydroxy-5-isopropenyl-2-methylhexanoate	64065	Unclassified	Unclassified	Unclassified			37.2	0	M+H	C10H18O3	-2.40573962	152.8853258	231.9958404	158.2285369	149.1005644	326.9715858	252.4230142	199.4943572	225.4405823	253.3301098
2.82_117.0573m/z	117.0572688	2.821016667	pos	Dihydropteridine	6249	Organoheterocyclic compounds	Pteridines and derivatives	Unclassified	*	C05649	37.2	0	M+H+2O	C6H6N4	9.778297795	366.6854666	278.0180257	242.3724779	179.9004728	144.4786601	118.7699502	293.6323046	176.2565723	163.0661825
2.84_203.0812m/z	203.0811869	2.839933333	pos	alpha,beta-Didehydrotryptophan	66511	Unclassified	Unclassified	Unclassified			37.2	0	M+H	C11H10N2O2	-1.569692908	257.568129	338.2432043	255.5963183	351.8321557	340.62112	233.3652302	247.8602301	341.78948	320.8302598
2.90_194.0782m/z	194.0781735	2.904316667	pos	L-3-Amino-2-(oxalylamino)propanoic acid	93325	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			37.2	0	M+NH4	C5H8N2O5	5.831320484	491.3546926	288.3621646	233.8527555	303.9839854	371.5770011	321.8459558	343.1357573	304.1401147	399.5821495
2.95_187.1324m/z	187.132418	2.96	pos	Epomediol	71823	Unclassified	Unclassified	Unclassified			37.2	0	M+H	C10H18O3	2.412536937	233.2816706	280.4596985	292.0882812	257.4769399	324.5147516	279.6648444	344.0855657	240.0789213	
3.22_338.0609n	339.0682064	3.215533333	pos	2-O-Acetyl-trans-coutaric acid	90084	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives			37.2	0.616	M+H, M+Na	C15H14O9	-8.436359296	34847.59612	34097.24206	38292.73692	2385.254998	2092.340043	2133.235816	23206.27072	23202.4041	21134.99196
3.24_271.0409m/z	271.0409438	3.238016667	pos	D-Camphorsulfonic acid	2955	Unclassified	Unclassified	Unclassified			37.2	0	M+K	C10H16O4S	3.687212461	4452.489336	5200.75166	4594.454235	7095.691967	7802.59607	6967.419515	5089.234168	5196.059239	4800.551662
3.40_187.1324m/z	187.1323573	3.396566667	pos	(5R)-6-Hydroxy-5-isopropenyl-2-methylhexanoate	64072	Unclassified	Unclassified	Unclassified			37.2	0	M+H	C10H18O3	-2.759498893	790.3591489	716.587439	624.8080976	769.251646	707.9877632	801.4416983	891.3369683	591.3820228	677.8022652
3.45_211.1327m/z	211.1326995	3.446883333	pos	3-Ethenyl-2,5-dimethyl-4-oxohex-5-en-2-yl acetate	HMDB0041573	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds			37.2	0	M+K	C12H18O3	-0.815384294	690.8493142	501.6818326	545.6352633	508.0099387	500.6839045	471.9599442	716.5382309	436.8613201	574.070795
3.51_211.0575m/z	211.0574513	3.552233333	pos	S-(4-Allylthio)-L-cysteine	93326	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			37.2	0	M+NH4	C6H11NO2S2	2.617092385	1056.866023	1595.866923	1580.09331	984.5452992	1595.831122	2044.459477	1308.120724	1455.572045	1401.009611
3.58_225.1093m/z	225.1092887	3.582033333	pos	Dimethyl suberate	71908	Unclassified	Unclassified	Unclassified			37.2	0	M+Na	C10H18O4	-2.182237095	1290.437747	1452.478487	1075.485074	976.910575	1020.852108	1094.868663	1221.866955	1275.433159	1262.285851
3.60_205.0861m/z	205.0860766	3.604716667	pos	Apiole	HMDB0033776	Organoheterocyclic compounds	Benzodioxoles	Unclassified		C10429	37.2	0	M+H+2O	C12H14O4	0.702029498	586.4724992	722.4350169	432.5833005	642.0432816	544.418957	630.8905925	710.2157715	756.678216	605.345092
3.63_228.1227m/z	228.1226721	3.626683333	pos	Sinapyl alcohol	44805	Benzenoids	Phenols	Methoxyphenols	**	C02325	37.2	0	M+NH4	C11H14O4	-1.724969124	131.1506168	106.1805254	133.6332188	78.06924027	0.001403199	60.85896746	151.1518995	65.30431843	90.81550996
3.65_242.0655m/z	242.0654974	3.648783333	pos	2,4-Dihydroxy-7,8-dimethoxy-2H-1,4-benzoxazin-3(4H)-one	HMDB0037549	Organoheterocyclic compounds	Benzoxazines	Benzoxazinones			37.2	0	M+K	C10H11NO6	-1.726143069	137.0151733	188.6853116	122.3670672	164.7748833	122.4951279	101.1302335	42.7127413	105.2410698	76.81339773
3.65_247.0162m/z	247.0161894	3.648783333	pos	ANTHRAQUINONE	43813	Unclassified	Unclassified	Unclassified			37.2	0	M+K	C14H8O2	2.892779029	1105.024646	1266.797945	1360.270908	382.116487	351.5789935	324.5178916	712.3900339	752.8051016	685.0097033
3.67_180.0519m/z	180.0518699	3.677116667	pos	Creatinine O-Phosphate	73577	Unclassified	Unclassified	Unclassified			37.2	0	M+H+2O	C4H12N3O4P	-7.024942575	80.5218104	33.23685181	32.27191581	123.8329382	190.9116004	82.10407746	19.16553137	124.5615533	80.36376323
3.69_179.1175m/z	179.1174954	3.6941	pos	Glycine xylidide	1001	Benzenoids	Benzene and substituted derivatives	Xylenes	**	C16569	37.2	0	M+H	C10H14N2O	-2.212651393	248.8673644	243.9757754	178.9426968	135.8615163	153.5152991	70.29423416	124.1284533	145.7468672	92.926028
3.91_191.1065m/z	191.1064763	3.911966667	pos	3-(2-Methylpropylidene)-3alpha,4-dihydro-1(3H)-isobenzofuranone	HMDB0032027	Organoheterocyclic compounds	Isobenzofurans	Unclassified	*		37.2	0	M+H	C12H14O2	-0.945748757	157.6899133	189.9688592	193.9081472	231.2100255	239.8744243	182.1009594	186.1580628	192.9852219	148.0083473
3.93_376.1710m/z	376.171004	3.9343	pos	2-Phenylaminoadenosine	5981	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	*		37.2	0	M+NH4	C16H18N6O4	-4.955018614	2029.287308	1582.102136	2203.243015	1723.665301	2273.308222	2132.54671	1892.924209	1992.403997	1856.579173
4.11_227.1387m/z	227.1386883	4.114783333	pos	Tyr-Oet	65601	Unclassified	Unclassified	Unclassified			37.2	0	M+NH4	C11H15NO3	-1.580842493	556.5702935	429.3014919	517.822624	178.9930636	272.7264563	375.2896627	310.7518548	368.5090338	296.5198142
4.14_175.0753m/z	175.0752527	4.136716667	pos	UAR/ECR ACID	44089	Unclassified	Unclassified	Unclassified			37.2	0	M+H	C11H10O2	-0.593318906	243.2165492	278.675854	271.2963574	189.0622254	237.6226434	176.7697754	66.51858415	170.9975232	66.51858415
4.20_168.1020m/z	168.101976	4.204866667	pos	p-Hydroxynorpseudoephedrine	2017	Unclassified	Unclassified	Unclassified			37.2	0	M+H	C9H13NO2	0.424379501	788.5561767	642.5692106	696.4172257	562.6487327	766.1584854	741.0808498	761.8192215	700.6649727	748.8030881
4.20_205.0969m/z	205.0968589	4.204866667	pos	L-Tryptophan	HMDB0000929	Organoheterocyclic compounds	Indoles and derivatives	Indolyl carboxylic acids and derivatives	***	C00078	37.2	0	M+H	C11H12N2O2	-1.446472227	290.4487312	96.39528523	342.7081699	135.2831367	155.305757	99.9371054	117.3735648	150.6604736	137.9030044
4.32_207.1018m/z	207.101794	4.317083333	pos	p-Methoxycinnamic acid ethyl ester	68349	Unclassified	Unclassified	Unclassified			37.2	0	M+H	C12H14O3	1.083153709	596.8390948	517.446262	517.2299058	766.0170189	653.7729424	740.6014051	642.9622783	641.0684974	744.2102659
4.41_309.1302m/z	309.1302171	4.4062	pos	14-Dihydroxycornestin	67011	Unclassified	Unclassified	Unclassified			37.2	0	M+K	C16H20O6	-9.891080953	2025.835098	2188.672639	2544.679691	2310.907601	1914.27581	1917.334468	1469.106452	2722.970854	1858.339741
4.43_221.0212m/z	221.0212373	4.4315	pos	Methyl-Cysteine	85600	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		37.2	0	M+K	C6H11NO2S	6.33121846	5503.415957	6367.83144	3191.690864	2899.072772	2798.455382	4822.314268	3604.42249		
4.57_451.2144m/z	451.2143745	4.565116667	pos	6β-Hydroxytriamcinolone acetonide	2905	Unclassified	Unclassified	Unclassified			37.2	0	M+H	C24H31FO7	3.812717156	0.001403199	723.241953	576.8913958	219.5322681	826.4207524	164.0640381	476.4890943	528.2749323	447.9681141
4.72_173.1324m/z	173.1323843	4.723666667	pos	3,5,8-Megastigmatrien-7-one	91646	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		37.2	0	M+H+2O	C13H18O	-0.487272974	360.0385907	210.3517121	193.0146204	186.1796764	107.3189476	69.19279251	221.8275336	152.0344646	142.6447994
4.72_330.1438n	331.1510859	4.723666667	pos	Gibberellin A108	87404	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	*		37.2	0	M+H, M+Na	C19H22O5	-8.827530021	837.8826107	693.0840724	4592.68795	731.5301149	654.7289504	817.1790464	584.7055784	561.6850783	1193.546617
4.75_315.1412m/z	315.1412024	4.7456	pos	3'-O-Methylguanosine	HMDB0006038	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	*		37.2	0	M+NH4	C11H15N5O5	0.196129071	827.4987391	1141.034678	1082.408041	1348.281585	1099.76724	1109.446393	1229.584154	1414.803999	1296.615622
4.79_312.0426m/z	312.0426489	4.7912	pos	6-Nitrochrysene	72989	Unclassified	Unclassified	Unclassified			37.2	0	M+K	C18H11NO2	1.875839023	2301.466532	2359.341389	2589.551212	4379.292612	3436.989088	3674.522563	1731.161539	2213.027502	1801.538753
4.81_332.1526m/z	332.1526478	4.814066667	pos	Nimitaz	HMDB0248337	Unclassified	Unclassified	Unclassified			37.2	0	M+Na	C19H23N3	0.995062654	128.1459274	202.6933081	248.2979964	262.1264757	278.1507196	266.2158161	359.3776977	295.9616273	304.4207591
4.84_173.1326m/z	173.1325787	4.836966667	pos	xi-3-(4-Isopropylphenyl)-2-methylpropanal	92581	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		37.2	0	M+H+2O	C13H18O	0.535033973	505.3368425	360.7546125	576.4498453	362.6434973	242.1291133	273.3917232	325.3225547	255.2838932	411.2049897
5.08_187.0752m/z	187.0751704	5.081	pos	2-Naphthylacetic acid	HMDB0246987	Unclassified	Unclassified	Unclassified			37.2	0	M+H	C12H10O2	-0.997209983	293.1427101	266.3208201	369.3634668	165.7794747	97.38621512	180.1854557	0.001403199	211.7856524	193.1856712
5.15_358.2220m/z	358.2219708	5.148116667	pos	11-dehydro-2,3-dinor Thromboxane B2	45640	Unclassified	Unclassified	Unclassified			37.2	0	M+NH4	C18H28O6	-1.303119684	678.2624264	1580.984967	612.8255054	763.0063903	1228.228827	1278.051409	626.4337616	555.5261955	482.9007537
5.17_491.1658m/z	491.1658367	5.1709	pos	6,9-difluoro-11-hydroxy-16-methyl-3-oxo-17-(1-oxopropoxy)-, (6β,11β,16α,17α)-	2938	Unclassified	Unclassified	Unclassified			37.2	0	M+K	C24H30F2O6	3.612346143	1208.611195	844.2921272	956.6027231	1354.901701	1484.664754	1428.812251	1071.778651	1087.86187	1305.637037
5.28_221.1159m/z	221.1159021	5.284233333	pos	2-ISOPROPYL-3-METHOXYCINNAMIC ACID	43708	Unclassified	Unclassified	Unclassified			37.2	0	M+H	C13H16O3	-7.808446681	505.3014039	329.6927235	605.7362372	568.1312298	422.3291316	451.8940544	374.9957725	352.5464645	410.1774256
5.40_361.2192m/z	361.2192298	5.396716667	pos	21-Fluoro-11beta,17-dihydroxy-6alpha-methylpregn-4-ene-3,20-dione	70793	Unclassified	Unclassified	Unclassified			37.2	0	M+H+2O	C22H31FO4	4.971649772	2869.320623	5929.968094	6094.566295	17155.56652	299.4805814	1094.277692	1615.160429	3364.996259	1323.048514
5.50_316.1939m/z	316.1938629	5.49815	pos	Hydroxytrebenazine	2803	Unclassified	Unclassified	Unclassified			37.2	0	M+H+2O	C19H27NO4	9.432458811	1410.409409	1565.931759	1712.721439	2266.479584	1882.710014	1978.414199	1635.918804	1560.478526	1556.850826
5.54_226.1436m/z	226.1436077	5.543066667	pos	N-Methylmescaline	3364	Unclassified	Unclassified	Unclassified			37.2	0	M+H+2O	C12H19NO3	-0.720528825	1308.682988	1301.548978	916.9587307	923.7453277	965.490372	897.8543036	1349.537232	1132.582672	795.219603
5.66_567.2771m/z	567.2770672	5.656316667	pos	alpha-Antiarin	67223	Unclassified	Unclassified	Unclassified			37.2	0	M+NH4	C29H42O11	-5.158940989	7016.488173	7298.32126	7406.696945	9622.377172	10991.79304	9722.914713	7261.261527	6190.932891	7334.455358
6.03_529.2043m/z	529.2043485	6.03205	pos	Limonoate	65618	Unclassified	Unclassified	Unclassified			37.2	0	M+Na	C26H34O10	-0.137137729	2649.75329	2878.10211	2130.283161	647.9826402	609.4593586	487.2696654	1931.495769	2165.149916	1739.31022
6.05_177.1272m/z	177.1271634	6.0535	pos	Carvyl acetate	92818	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		37.2	0	M+H+2O	C12H18O2	-1.175227633	1350.63187	1199.742105	1220.702317	826.8407967	1284.643763	1176.49046	1034.478237	1034.478237	1034.47089
6.14_195.0876m/z	195.0875753	6.140733333	pos	4-O-Methy

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13.23_325.2708m/z	325.2708044	13.23251667	pos	MEDICA 16	62960	Unclassified	Unclassified	Unclassified			37	0	M+H-H2O	C20H38O4	-8.522606645	57555.66521	57036.05377	57678.22095	57603.61293	58033.49315	61127.61357	61507.82239	61729.90385	60824.46055
13.33_316.2245m/z	316.2245285	13.33273333	pos	Stearidonoyl glycine	62992	Unclassified	Unclassified	Unclassified			37	0	M+H-H2O	C20H31NO3	-7.733767455	2950.958408	2394.653604	2235.889609	2315.877526	2152.609221	2107.902477	2306.413861	2774.727035	2294.855382
14.08_425.2138m/z	425.2138279	14.07666167	pos	Dihydrovaltrate	89971	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		37	0	M+H	C22H32O8	-7.464609394	31710.441	28514.584	27885.90465	26831.00601	30436.04407	30441.32041	31102.26813	29745.09253	30774.24657
14.49_341.2657m/z	341.2656817	14.48943333	pos	15(S)-HpEDE	35361	Unclassified	Unclassified	Unclassified			37	0	M+H	C20H36O4	-8.682591845	1592.296463	2091.174273	2567.029221	2542.881656	2323.518184	2642.439099	2643.870989	2502.218156	2554.956883
14.62_341.2657m/z	341.2656912	14.61855	pos	13,14-dihydro Prostaglandin F1α	45617	Unclassified	Unclassified	Unclassified			37	0	M+H-H2O	C20H38O5	-8.219711631	1488.727703	1835.34959	1820.724626	1864.811582	1484.462104	2416.416167	2568.706678	2021.008487	2265.269674
14.70_264.0896m/z	264.0896308	14.70206667	pos	ortho-Aminoacetoluene	72917	Unclassified	Unclassified	Unclassified			37	0	M+K	C14H15N3	-0.554256495	9003.800423	464.1645876	498.1750647	304.9267852	252.2264042	307.9255048	361.9010715	291.1693032	254.1224732
15.50_135.1163m/z	135.1165578	15.50080333	pos	2-(trans-2-Pentenyl)cyclopentanone	HMDB0032536	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		37	0	M+H-H2O	C10H16O	-3.628257646	178.6216679	143.8581661	3.973364531	204.8425014	385.6154823	401.0558148	705.34731	5.274258852	12.33902683
2.05_325.0525m/z	325.0525076	2.048466667	pos	Ethofumesate	72594	Unclassified	Unclassified	Unclassified			37	0	M+K	C13H18O5S	6.483497393	16267.58431	15367.55472	18410.42176	638.2850482	492.3857867	518.8737497	14626.5687	16081.02373	15490.88604
2.07_229.0680m/z	229.0680345	2.069933333	pos	Phosphocreatine	326	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C02305	37	0	M+NH4	C4H10N3O5P	-7.572823558	621.3222859	205.1540355	344.4227326	118.3177171	99.4890598	369.9621011	95.94692037	339.95191	395.0587626
2.09_145.0685m/z	145.0684821	2.0913	pos	Ethyl 4-(methylthio)butyrate	92462	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		37	0	M+H-H2O	C7H14O2S	1.972444242	27.12599181	27.5974396	0.001403199	0.001403199	17.62295508	23.83463841	0.001403199	24.30545713	41.6365456
2.22_140.9821m/z	140.9820624	2.220616667	pos	Liquid thiophthene	HMDB0029716	Organoheterocyclic compounds	Thienothiophenes	Unclassified			37	0	M+H	C6H4S2	-4.688014133	230.6832025	60.39433891	105.10875	210.7518237	247.2363806	252.3083556	213.9682326	233.2698654	161.2022168
3.09_223.1074m/z	223.1074188	3.093516667	pos	Cinnamoylglycine	34534	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		37	0	M+NH4	C11H11NO3	-1.463625261	3202.545281	3448.183287	3889.376739	4449.565468	5110.01063	4410.749221	3387.515495	3528.503073	4307.511303
3.16_104.0708m/z	104.0708361	3.159083333	pos	2-Aminoisobutyric acid	HMDB0001906	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C03665	37	0	M+H	C4H9NO2	2.242628935	1066.997362	1057.660591	872.3336359	989.3438095	1044.654223	899.4266437	1084.996324	884.4930601	1024.427255
3.45_371.1008m/z	371.1007579	3.446883333	pos	5-Hydroxy-6-methoxycoumarin 7-glucoside	94324	Phenylpropanoids and polyketides	Coumarins and derivatives	Coumarin glycosides			37	0	M+H	C16H18O10	9.415786339	1378.880795	994.4623827	797.5649097	1316.858857	1097.24108	790.0790355	995.2797143	762.870458	1085.149478
3.74_207.1377m/z	207.1376841	3.73775	pos	3-Phenylpropyl 2-methylpropanoate	HMDB0034472	Benzenoids	Benzene and substituted derivatives	Unclassified		C02008	37	0	M+H	C13H18O2	-1.320032614	866.3560257	707.4259178	633.1209072	704.6052008	692.1067128	522.9020496	690.4372465	611.3218291	664.9719264
4.07_300.1554m/z	300.1553812	4.069116667	pos	Hydroxy-lacosamide	HMDB0061146	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		37	0	M+NH4	C13H18N2O5	-0.056827121	877.0069519	720.8233735	1079.578686	873.3356015	1018.696248	864.3154987	742.4939201	888.3949678	1011.46855
4.11_214.0870m/z	214.0869931	4.114783333	pos	Trihomomethionine	64500	Unclassified	Unclassified	Unclassified			37	0	M+Na	C8H17NO2S	-1.1899259	1424.28865	1223.492104	1416.234827	1384.255545	1626.084728	1551.933978	1450.788021	1660.036904	1816.707069
4.18_381.1870m/z	381.187026	4.182316667	pos	Farnesyl Thiosalicylic Acid	45270	Unclassified	Unclassified	Unclassified			37	0	M+Na	C22H30O2S	3.221997033	4678.259679	4906.003327	5373.174428	6266.276919	6169.527134	5975.475995	4703.148221	4722.291661	4443.826454
4.27_372.2587m/z	372.2586776	4.272416667	pos	Sannamycin A	71872	Unclassified	Unclassified	Unclassified			37	0	M+H-H2O	C17H35N5O5	-4.761179946	1876.197403	2075.942998	2027.645947	2331.13528	2158.348349	2154.005676	1658.129975	2001.044701	2307.235862
4.34_306.0293m/z	306.029342	4.33965	pos	Sulfisoxazole	43339	Benzenoids	Benzene and substituted derivatives	Benzenesulfonamides		C07318	37	0	M+K	C11H13N3O3S	-5.91013132	1133.63097	1299.488164	1600.371545	1355.584192	1340.506262	1331.363319	1459.501768	1619.135297	1198.091426
4.38_220.0964m/z	220.0964322	4.384366667	pos	2-Napthyloxyacetic acid	72523	Unclassified	Unclassified	Unclassified			37	0	M+NH4	C12H10O3	-1.917841722	316.9391224	616.2727272	594.5063215	329.4733224	471.7799595	337.7828358	398.330827	757.6001971	657.3580866
4.43_180.0588m/z	180.0588092	4.42815	pos	4-phenyl-1,2,3-Thiadiazole	96416	Unclassified	Unclassified	Unclassified			37	0	M+NH4	C8H6N2S	-1.144982549	115.1923573	0.001403199	56.32653832	21.66159076	14.98666489	11.57024017	0.001403199	46.83519554	14.42867834
4.43_288.1521m/z	288.1521846	4.42815	pos	Pivalylcarnitine	HMDB0041993	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	***		37	0	M+Na	C12H23NO4	1.042862868	1208.38794	1915.351161	1995.066966	1264.625212	1580.038092	1477.645883	1853.087819	1779.310059	1523.733144
4.43_423.1234m/z	423.1234329	4.42815	pos	19-hydroxy-17-oxoandrost-5-en-3-β-yl sulfate	4096	Unclassified	Unclassified	Unclassified			37	0	M+K	C19H28O6S	-1.001659846	4376.886654	4975.134176	4549.260333	6504.356443	6391.631584	6328.686579	5474.184718	6524.128589	5433.764017
4.52_200.1068m/z	200.1067504	4.51925	pos	2-Hydroxyflurene	HMDB0013163	Benzenoids	Fluorenes	Unclassified	*	C14460	37	0	M+NH4	C13H10O	-1.318622714	482.3768504	435.7766843	460.942465	277.1460592	287.6840625	304.5042037	152.6098434	115.8264561	120.8435561
4.57_211.1690m/z	211.1690012	4.565116667	pos	2-Propenyl cyclohexanebutanoate	93015	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		37	0	M+H	C13H22O2	-1.214201668	1015.053004	834.6242127	788.0157408	769.5789953	933.0184556	706.263757	1061.443209	832.0366039	814.1465243
4.66_176.1279m/z	176.1279319	4.656183333	pos	2-Methylpropyl 3-oxobutanoate	HMDB0036395	Organic acids and derivatives	Keto acids and derivatives	Beta-keto acids and derivatives			37	0	M+NH4	C8H14O3	-1.188903301	3409.914416	3219.623168	3312.398243	3369.419503	3553.939612	3311.408332	3778.404842	3012.702203	3348.944119
4.66_213.1847m/z	213.1846933	4.656183333	pos	3-[(5-Methyl-2-(1-methylethyl)cyclohexyl]oxy]-1,2-propanediol	91289	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		37	0	M+NH4	C13H26O3	-0.926160227	297.7357559	257.8671947	294.0686457	235.7570659	384.8245368	263.7462466	328.4938045	277.1635345	276.2106512
4.66_246.1697m/z	246.1696905	4.656183333	pos	Isovaleryl-L-carnitine	LMFA07070077	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters			37	0	M+H	C12H23NO4	-1.199919928	68.54577259	72.73252516	65.75268712	33.54899179	44.21628277	73.63734122	107.5058478	92.65901636	94.51051611
4.66_290.1417m/z	290.1417219	4.656183333	pos	LY364947	45543	Unclassified	Unclassified	Unclassified			37	0	M+NH4	C17H12N4	6.247282505	1310.688911	1260.231302	1537.745676	1477.562381	1724.095637	1638.613283	1040.771484	1087.719056	1040.291653
4.75_162.0673m/z	162.0673219	4.7456	pos	4-Acetylimidazo[4,5-c]pyridine	90276	Organoheterocyclic compounds	Imidazopyridines	Imidazo-[4,5-c]pyridines			37	0	M+H	C8H7N3O	7.038541601	1013.010569	1046.905345	945.6205218	893.1684302	811.5567924	860.6658683	818.1323133	908.2525673	790.8931795
4.75_312.1910m/z	312.1909776	4.7456	pos	Isoleucyl-Tyrosine	HMDB0028919	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		37	0	M+NH4	C15H22N2O4	-2.736952062	3669.161496	3420.527011	3349.62545	1637.487839	1151.308882	1339.359438	2568.034376	2476.32279	2190.730138
4.81_207.1012m/z	207.1011838	4.814066667	pos	Acoramone	HMDB0032663	Benzenoids	Benzene and substituted derivatives	Phenylpropanes	*		37	0	M+H-H2O	C12H16O4	-1.72655586	565.0367194	581.4153019	874.9954612	601.3904666	498.830994	568.337319	471.0935072	548.4019234	531.0441474
4.82_237.1481m/z	237.1481212	4.822333333	pos	Guanidinobutanal	HMDB0015301	Organic nitrogen compounds	Organonitrogen compounds	Guanidines		C07036	37	0	M+K	C10H22N4	2.605526349	1145.915565	1024.045881	1232.313917	1088.634186	923.2848413	1029.371659	1044.00157	924.2478236	1029.371659
4.88_427.1570m/z	427.157036	4.882333333	pos	6-(2-Carboxyethyl)-7-hydroxy-2,2-dimethyl-4-chromanone glucos	89669	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			37	0	M+H	C20H26O10	-6.658299802	18901.28007	19626.90087	20309.89235	22246.77591	19710.25069	20505.11865	19427.71888	21788.80419	20454.72716
4.93_336.1911m/z	336.1911042	4.927016667	pos	N-tridecanoyl-L-Homserine lactone	45458	Unclassified	Unclassified	Unclassified			37	0	M+K	C17H31NO3	-8.235123824	1460.289889	1802.039178	1834.082262	1995.210726	2365.609442	2222.986248	1302.225281	1469.676492	1346.357189
4.99_147.0716m/z	147.0716447	4.991816667	pos	S-Methylmethionine	HMDB0038670	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			37	0	M+H-H2O	C6H14NO2S+	2.488504249	76.64827215	49.40663523	103.3503738	67.67399007	162.6186856	53.56668083	80.37711238	133.93394	152.0201927
5.06_145.0682m/z	145.0681902	5.058233333	pos	S-(3-Methyl-2-butenyl) ethanethioate	87874	Organic acids and derivatives	Thiocarboxylic acids and derivatives	Thioesters	*		37	0	M+H	C7H12OS	0.192863603	0.001403199	0.001403199	0.001403199	0.001403199	586.5532657	527.6399064	531.1468835	0.001403199	0.001403199	0.001403199
5.09_221.1170m/z	221.1170235	5.081	pos	Pleocomine II	67355	Unclassified	Unclassified	Unclassified			37	0	M+H	C13H16O3	-0.896457356	2135.009606	2110.368489	1810.096575	2135.009606	2110.368489	2070.067597	1538.773794	1892.646998	1530.206005
5.13_181.0718m/z	181.0718062	5.125733333	pos	L-(+)-Gulose	64618	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C15923	37	0	M+H	C6H12O6	6.340475914	2881.744005	3302.230943	3427.829146	3984.299171	3851.64325	3873.919172	3956.977936	4012.774688	3942.844532
5.15_204.1381m/z	204.1380807	5.148116667	pos	Dioscorine	HMDB0030305	Organoheterocyclic compounds	Azaspirodecane derivatives	Unclassified	*	C10142	37	0	M+H-H2O	C13H19NO2	-0.949310936	701.3712689	573.3104334	488.3024733	516.4031254	594.5412064	552.6511273	665.2702089	498.691461	580.4937846
5.15_292.1936m/z	292.1936307	5.148116667	pos	Nadolol	1382	Benzenoids	Tetralins	Unclassified			37	0	M+H-H2O	C17H27NO4	9.941368667	1391.111918	1646.188262	1492.187307	2269.31301	2282.889634	2298.813194	1831.735085	1573.901773	1675.53543
5.26_347.2037m/z	347.2037489	5.26135	pos	6alpha-Fluoro-11beta,17-dihydroxypregn-4-ene-3,20-dione	70662	Unclassified	Unclassified	Unclassified			37	0	M+H-H2O	C21H29FO4	5.627337324	1660.894027	4341.255422	1479.971047	12988.27908	2108.603682	2131.905814	1027.549417	1933.617625	461.6213688
5.26_454.0893m/z	454.0893483	5.26135	pos	N6-(δ2-Isopentenyl)-adenosine 5'-monophosphate	64085	Unclassified	Unclassified	Unclassified			37	0	M+K	C15H22N5O7P	1.21787121	0.001403199	0.001403199	0.001403199	3183.988011	3127.363142	3108.834076	0.001403199	0.001403199	0.001403199
5.31_158.1304m/z	158.1303655	5.306555	pos	Heptyl acetate	HMDB0031480	Organic acids and derivatives	Carboxylic acids and derivatives	Carboxylic acid derivatives	*		37	0	M+H-H2O, M+Na	C9H18O2	-1.462204343	7776.163679	7822.93292	7588.699977	7278.459041	7417.918013	7492.882735	7168.229389	7483.540496	7131.502423
5.31_207.1377m/z	207.1376835	5.30655	pos	(E)-6-Methyl-6-(5-methyl-2-furanyl)-3-hepten-2-one	89069	Organoheterocyclic compounds	Heteroaromatic compounds	Unclassified			37	0	M+H	C13H18O2	-1.322997912	980.3909795	871.1806152	893.6014221	589.993119	743.8579928	680.1129753	836.2371641	800.4352868	709.4219331
5.33_299.1465m/z	299.1465358	5.329033333	pos	3'-O-Methyladenosine	HMDB0006023	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	*		37	0	M+NH4	C11H15N5O4	1.089514235	905.5244381	843.049196	1079.771617	572.691403	803.8562223	715.5461104	750.7213712	906.5155417	938.2337506
5.35_323.1448m/z	323.1448408	5.351683333	pos	Avenic acid A	86957	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		37	0	M+H	C12H22N2O8	-0.159277296	704.1138625	617.2181505	641.7397693	566.9539202	549.2103231	459.7133267	507.006301	679.9732275	709.757509
5.40_383.1160m/z	383.1159835	5.396716667	pos	Diphenylphosphine isopropyl ester	45301	Unclassified	Unclassified	Unclassified			37	0	M+NH4	C20H25O3P	-3.794513632	3812.353733	2874.302606	3617.441512	8349.503483	6715.11367	6709.575778	3921.42866	4311.170104	4223.275487
5.46_438.0946m/z	438.0946027	5.464983333	pos	Cephalosporin C	HMDB0060450	Organic nitrogen compounds	Organonitrogen compounds	Nitrogen mustard compounds	**	C00916	37	0	M+Na	C16H21N3O8S	1.075341121	0.001403199	0.001403199	2033.806619	2061.056306	1990.839812	0.001403199	0.001403199	0.001403199	0.001403199
5.56_229.1216m/z	229.1216361	5.56405	pos	Bisphenol A	69602	Benzenoids	Benzene and substituted derivatives	Diphenylmethanes	**	C13624	37	0	M+H	C15H16O2	-2.937577077	1277.289302	1036.708782	1436.556084	1111.892878	1139.599628	1279.911208	1707.329732	1184.456884	1513.483706
5.58_469.2040m/z	469.2040207	5.581883333	pos	15-Acetoxyscirpene-3,4-diol 4-O-a-D-glucopyranoside	90869	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		37	0	M+H-H2O	C23H34O11	-5.7648915	3892.025501	3459.606366	4611.831627	5593.800263	5804.005136	6101.355109	4783.334642	5089.734833	5185.045774
5.61_168.1098m/z	168.1097746	5.613933333	pos	L-Lysinamide	65680	Unclassified	Unclassified	Unclassified			37	0	M+Na	C6H15N3O	-6.602967599	167.9846704	205.7107962	188.4418334	254.9808828	233.9908055	299.1953045	218.2376368	198.367363	250.0194398
5.77_463.1569m/z	463.1568562	5.7661	pos	4,2'-Dihydroxy-4',6'-dimethoxychalcone 4-glucoside	52118	Unclassified	Unclassified	Unclassified			37	0	M+H	C23H26O10	-6.528665448	7383.174702	6927.503465	8030.912233	10612.95963	9691.735985	8399.261649	9692.961432	7850.901038	7827.052257
6.01_207.1377m/z	207.1377442	6.013115	pos	3-Methylbutyl phenylacetate	90368	Benzenoids	Benzene and substituted derivatives	Unclassified			37	0	M+H	C13H18O2	-1.028497094	1509.219644	1515.353396	1148.600232	1072.013211	1178.139365	1167.073238	1478.464841	1186.670471	1331.551802
6.09_181.0718m/z	181.0718342	6.093533333	pos	D-Tagatose	58151	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C00795	37	0	M+H	C6H12O6	6.495668436	830.6542977	961.7779002	1176.470481	1264.900619	1229.6226	1415.192499	1290.737446	1683.872767	1524.837481
6.26_328.2018m/z	328.2018061	6.262533333	pos	O-Desmethylquinidine	2223	Unclassified	Unclassified	Unclassified			37	0	M+NH4	C19H22N2O2	-0.475073339	4277.261823	4188.878889	3821.489996	4620.266904	4409.979945	5005.134111	4635.90128	4475.449658	4341.632256
6.28_237.1482m/z	237.1482459	6.276683333	pos	(-)-trans-C75	96552	Unclassified	Unclassified	Unclassified			37	0	M+H-H2O	C14H22O4	-1.082121401	6981.719747	7681.891811	7413.511545	7167.321751	6968.510981	6775.830779	6137.955761	5328.852382	6297.323324
6.28_354.1001m/z	354.1001168	6.276683333	pos	Tetracenomycin D1	63756	Unclassified	Unclassified	Unclassified			37	0	M+NH4	C19H12O6	8.638687987	10775.21775	10623.58704	11628.59548	17269.14743	18070.0157	17085.31602	18117.22029	20388.47905	19612.81959
6.34_197.1534m/z	197.1533809	6.339133333	pos	cis-3-Hexenyl trans-2-hexenoate	LMFA07010809	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		37	0	M+H	C12H20O2	-1.149325381	1662.218521	2193.806939	1823.974044	1459.750154	1757.651471	1745.618278	1382.29537	1346.306629	1406.353551
6.49_252.1567m/z	252.1566894	6.485983333	pos	N-Isovaleroylvaline	HMDB0013267	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		37	0	M+NH4	C12H24N2O3	-1.504826026	7611.967202	7025.615136	5391.740718	559.295596	733.2141406	475.1091948	765.2169645	608.2984512	604.2984512
6.63_207.1377m/z	207.1377247	6.627483333	pos	2-Phenylpropyl isobutyrate	89956	Benzenoids	Benzene and substituted derivatives	Unclassified			37	0	M+H	C13H18O2	-1.123107321	2572.694191	2118.338026	2083.900842	2084.657111	1912.666833	1963.366039	2205.60032	2208.159854	2056.206264
6.63_483.2194m/z	483.2194019	6.627483333	pos	3'-Hydroxy-T2 Toxin	91661	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		37	0	M+H	C24H34O10	-6.37028958	5096.340741	4367.996235	4343.964948	7863.101847	5996.429196	5477.397729	7210.739005	7348.789382	7067.240823
6.88_503.1725m/z	503.1724831	6.8774	pos	Acetylblasticidin S	65842	Unclassified	Unclassified	Unclassified			37	0	M+K	C19H28N8O6	-8.305807819	17545.66639	18247.74806	19188.20461	1483.183943	976.8785567	568.0313884	14981.54898	17594.77957	17264.22462
7.11_221.1170m/z	221.1170286	7.108583333	pos	Flossonol	68018	Unclassified	Unclassified	Unclassified			37	0	M+H	C13H16O3	-0.87337556	323.8224991	435.2478065	625.2028083	490.8245867	457.7741295	487.4055445	516.1084308	523.5611801	441.5282468
7.99_320.2249m/z	320.2249	7.987716667	pos	16-Hydroxyandrost-4-ene-3,17-dione	6990	Lipids and lipid-like molecules	Steroids and steroid derivatives	Androsterone and derivatives	**	C05290	37	0	M+H	C19H28O3	9.529794016	4467.852295	4777.987994	4988.440954	6904.61577	6040.037	5770.023904	4865.209369	5161.978118	4853.997209
8.28_535.2483m/z	535.2483033	8.280116667	pos	Absinthin	67576	Lipids and lipid-like molecules	Prenol lipids	Sesterterpenoids	*	C09286	37	0	M+K	C30H40O6	5.352300071	9186.255524	9691.881007	10171.79998	9289.451901	8044.081467	6752.208408	8375.946914	8520.530196	9497.31512
8.28_547.2041m/z	547.2041134	8.280116667	pos	Kanamycin A 3'-phosphate	65947	Unclassified	Unclassified	Unclassified			37	0	M+K	C18H37N4O14P	5.340556836	1740.289796	2411.189762	2698.078793	2101.506303	1213.597007	1707.699626	1809.944489	1476.271516	1896.096693
8.34_112.9878m/z	112.98782	8.3362	pos	2-Thiophenemethanethiol	HMDB0031853	Organoheterocyclic compounds	Heteroaromatic compounds	Unclassified	*		37	0	M+H-H2O	C5H6S2	0.123665237	10.29096094	45.04041852	0.001403199	13.22889408	22.45893556	21.03947397	0.001403199	0.001403199	27.61232572
9.05_200.2370m/z	200.2370309	9.0492	pos	6-Tridecene	LMFA11000480	Hydrocarbons	Unsaturated hydrocarbons	Unsaturated aliphatic hydrocarbons			37	0	M+NH4	C13H26	-1.347053174	3634.240287	3553.80278	2857.068967	2188.158611	3107.639188	3040.838093	3873.669974	2427.322293	3182.553554
9.44_605.5487m/z	605.5487171	9.444333333	pos	DG(22:0/14:1(9Z)/0:0)	59070	Lipids and lipid-like molecules	Glycerolipids	Diradylglycerols	*		37	0	M+H-H2O	C39H74O5	-2.602313014	3481.204276	4323.417544	4168.240888	3345.958512	1622.033777	3960.287988	3653.569531	3566.232775	3265.329747
9.77_306.0617m/z	306.0617301	9.7709	pos	(5'-Iodo-3,4'-bi-2-thien-1-yl)-[2,2'-thiophen]-5-yl]methyl acetate	LMFA12000356	Fatty Acyls	Lipids and lipid-like molecules	Fatty Acyls			37	0	M+NH4	C15H12O2S2	0.114228429	355.056912	297.0686413	1983.255518	0.001403199	116.8263026	0.001403199	0.001403199	0.001403199	828.8097746
10.54_207.1488m/z	207.1487868	0.535	pos	Monoethylglycinexylidide	HMDB0060656	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C16561	36.9	0	M+H	C12H18N2O	-1.954346368	0.001403199	153.8730327	171.8894127	0.001403199	20.48323447	207.3420959	128.1838887	153.3955902	213.2790161
0.64_274.9927m/z	274.9926551	0.63615	pos	Isosorbide dinitrate	857	Organoheterocyclic compounds	Furofurans	Isosorbides		C07456	36.9	0	M+K	C6H8N2O8	6.066330327	8801.456198	6213.388026	7437.439062	5765.442562	4368.114918	7272.68015	7152.691811	6991.239075	8276.356666
0.68_124.0958m/z	124.0958149	0.6788	pos	Diethylene glycol	70263	Unclassified	Unclassified	Unclassified			36.9	0	M+NH4	C4H10O3	-9.473398584	75.43174474	33.0145256	0.001403199	79.89182105	111.6430198	67.06456803	0.001403199	0.001403199	12.6989087
0.72_241.1288m/z	241.1288073	0.717716667	pos	4-(Methylnitrosamino)-1-(1-oxido-3-pyridinyl)-1-butanone	HMDB0062375	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C19602	36.9	0	M+NH4	C10H13N3O3	-3.18044945	1982.666138	2071.616634	2489.068953	2091.035701	2576.298193	2597.038366	2517.776666	2436.101895	2382.356512
0.72_642.8603m/z	642.8602527	0.717716667	pos	myo-Inositol hexakisphosphate	HMDB0003502	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols	**	C01204	36.9	0	M+H-H2O	C6H18O24P6	3.288189344	3579.09067	5922.30262	4609.805112	1490.974108	903.6053064	1686.228848	5409.498006	4322.924011	4453.56467
0.82_181.0080m/z	181.0080336	0.818116667	pos	2,5-Dimethyl-3-(methylthio)furan	94732	Organosulfur compounds	Aryl thioethers	Thioethers			36.9	0	M+K	C7H10OS	-2.53771377	2821.851922	4593.134558	4910.305343	1410.709203	1771.691003	1822.306712	3171.899325	3637.266099	3923.458253
0.82_220.1177m/z	220.1176549	0.818116667	pos	cis-Zeatin	64074	Unclassified	Unclassified	Unclassified			36.9	0	M+K	C10H13N5O	-7.446423148	4754.080009	4844.915452	4943.207006	5363.635624	5341.790166	5516.438351	3703.784407	3542.830719	3918.688574
0.82_251.0751m/z	251.0751368	0.818116667	pos	(α-D-Mannosyl)-D-glycerate	63171	Unclassified	Unclassified	Unclassified			36.9	0	M+H-H2O	C9H16O9	-3.756409873	0.001403199	354.0127497	113.1680074	0.001403199	0.001403199	244.8358081	0.001403199	0.001403199	312.7419315
0.86_213.1846m/z	213.1846213	0.859583333	pos	Rhodinyl propionate	HMDB0037187	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohol esters	*		36.9	0	M+H	C13H24O2	-1.343678507	233.3513605	72.87730023	208.7143864	187.2114441	125.3758488	103.3395895	286.1171348	73.39779619	72.98058597
1.07_132.9773m/z	132.9773182	1.072683333	pos	Asparagusate	65672	Unclassified	Unclassified	Dithiolanes	*	C01892	36.9	0	M+H-H2O	C4H6O2S2	-2.100302324	390.4523193	566.7343978	613.4474305	368.089069	464.1996312	466.2313685	360.4830355	637.0563943	492.9751387
1.16_405.0257m/z	405.025651	1.157483333	pos	Hesperetin 7-sulfate	HMDB0240525	Unclassified	Unclassified	Unclassified			36.9	0	M+Na	C16H14O9S	1.511221168	1874.738626	1438.852206	1574.657886	1090.715566	1057.885935	1043.756249	1082.559061	1088.894932	1077.407016
1.16_469.1050m/z	469.1050262	1.157483333	pos	5-(3''-Benzoyloxypropyl)-7-methoxy-2-(3',4'-methylenedioxypheny	265093	Unclassified	Unclassified	Unclassified			36.9	0	M+K	C26H22O

2.05_234.0709m/z	234.0709267	2.048466667	pos	2-Fluoroethcathinone	96623	Unclassified	Unclassified	Unclassified			36.9	0	M+K	C11H14FNO	9.36051518	9323.807987	9915.292482	10153.63953	6357.510928	6159.9249	5781.770514	8251.108794	9322.565622	9163.877623
2.70_181.0719m/z	181.0718871	2.699483333	pos	L-Galactose	4184	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C01825	36.9	0	M+K	C6H12O6	6.789566539	383.8465093	706.4118253	768.7877475	1245.585585	1502.270111	1135.196593	946.3092884	906.0269482	1124.128601
2.90_221.0004m/z	221.0003981	2.904316667	pos	Acenaphthenequinone	65841	Unclassified	Unclassified	Unclassified			36.9	0	M+K	C12H6O2	2.530365115	667.1641624	837.4552819	1008.165258	720.0228762	824.9320957	614.7544376	612.0302244	945.8884645	853.240545
3.15_197.0006m/z	197.0006183	3.14845	pos	1,2-Naphthoquinone	HMDB0244101	Unclassified	Unclassified	Unclassified			36.9	0	M+K	C10H6O2	4.3079188	636.7618103	698.577187	495.2353322	625.873714	545.1161453	426.9810697	633.7503142	570.0277617	579.6821299
3.54_486.2553m/z	486.2552543	3.5398	pos	PE(17:2(9Z,12Z)/0:0)	77682	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoethanolamines			36.9	0	M+Na	C22H42NO7P	-8.322704005	4315.945533	6515.256716	5934.240571	4699.307749	4696.895843	6292.225288	6007.754735	7965.998171	6847.381017
3.60_185.1243n	208.1134077	3.604716667	pos	cis- and trans-5-Ethyl-4-methyl-2-(2-butyl)-thiazoline	HMDB0032201	Organoheterocyclic compounds	Azolines	Thiazolines	*		36.9	0	M+H, M+Na	C10H19NS	2.391259318	27510.2865	29019.07587	31581.0099	35767.4407	29900.00408	30164.99993	26173.98459	34508.8022	28812.78839
3.83_200.1269m/z	200.1269331	3.825583333	pos	Dacarbazine	540	Organic acids and derivatives	Carboxylic acids and derivatives	Carboxylic acid derivatives			36.9	0	M+NH4	C6H10N6O	8.229774339	2587.008381	2939.598289	2515.820107	2678.926351	3322.170532	2435.437423	2968.226508	2151.472145	2316.295833
3.91_318.1657m/z	318.1656777	3.911966667	pos	Serratanidine	67995	Unclassified	Unclassified	Unclassified			36.9	0	M+Na	C16H25NO4	-6.441074327	3617.771608	3707.175659	4107.599673	4929.77545	4549.366081	4605.96907	2732.616905	3561.293956	3611.130066
4.02_325.0890m/z	325.0890082	4.024633333	pos	1-Caffeoyl-beta-D-glucose	68323	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	Monosaccharides		C10433	36.9	0	M+H-H2O	C15H18O9	-8.143150251	725.7650245	973.0853153	1042.254921	1455.293265	855.1136909	936.1361422	2495.516835	2806.811573	3051.342654
4.34_266.1005m/z	266.1004805	4.33965	pos	Glutamyl-Histidine	85735	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		36.9	0	M+H-H2O	C11H15N4O5-	-1.680710803	412.400747	398.7912324	468.9531261	435.7722973	307.0929448	368.4411946	313.7814529	471.6185704	310.9670486
4.34_325.1254m/z	325.1254439	4.33965	pos	S-Succinyldihydrolipoamide	6058	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*	C01169	36.9	0	M+NH4	C12H21NO4S2	1.362004614	4532.678177	4720.187226	4864.67801	5498.640422	4766.764044	5123.741578	4370.863198	4752.106839	4396.791617
4.41_302.0930m/z	303.1002675	4.4062	pos	Benzo[a]pyrene-7,8-dihydrodiol-9,10-oxide	HMDB0062470	Benzenoids	Pyrenes	Unclassified	**	C14853	36.9	0	M+H, M+Na	C20H14O3	-4.380381455	9025.826558	9955.122188	11041.20409	11132.57689	9803.008423	10436.01958	8350.320329	10160.02981	8853.136587
4.52_225.1482m/z	225.1481824	4.51925	pos	(+/-)-6-Hydroxy-3-oxo-alpha-ionol	66125	Unclassified	Unclassified	Unclassified			36.9	0	M+H	C13H20O3	-1.510305675	892.7295408	865.3414019	863.7357942	695.8131464	734.7977007	681.4131943	874.0624843	704.2398752	712.5321829
4.63_242.1748m/z	242.1747633	4.63335	pos	Octyl 2-furoate	92549	Organoheterocyclic compounds	Furans	Furoic acid and derivatives			36.9	0	M+NH4	C13H20O3	-1.368631528	455.4739993	209.3534884	123.4138801	544.3015177	483.1520878	395.5573739	324.884239	249.3459347	295.8580662
4.70_283.0737m/z	283.0736857	4.701116667	pos	1H-Indole-3-acetic acid, 5-[[(methylamino)sulfonyl]methyl]-	2613	Unclassified	Unclassified	Unclassified			36.9	0	M+H	C12H14N2O4S	-3.611270611	4079.454454	3879.871504	3817.730443	3608.941386	3853.682466	4135.373704	4293.250566	3673.608108	3841.980989
4.72_238.1070m/z	238.1069706	4.723666667	pos	Eugenitin	HMDB0029467	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans	*		36.9	0	M+NH4	C12H12O4	-1.88017344	490.1459736	195.9198816	163.6777828	500.6258757	190.5929212	389.0718517	433.9213044	193.9989344	94.18430636
4.75_150.0419m/z	150.0419064	4.7456	pos	Histamine	HMDB0000870	Organic nitrogen compounds	Organonitrogen compounds	Amines	***	C00388	36.9	0	M+K	C5H9N3	-8.09318445	47.03547487	46.00232685	51.5486044	17.92520889	42.48509972	39.63882676	71.37589136	45.99084805	44.40088036
4.75_368.0159m/z	368.0159203	4.7456	pos	Mecarbam	72447	Organic acids and derivatives	Organic dithiophosphoric acids and derivatives	Dithiophosphate O-esters	*	C18661	36.9	0	M+K	C10H20NO5PS2	2.160393709	663.4820202	1656.039844	2043.304312	891.2506024	1214.476695	1452.434636	1359.192906	1507.712006	1741.796116
4.77_209.0781m/z	209.0781131	4.768333333	pos	Isosorbide 5-mononitrate	860	Unclassified	Unclassified	Unclassified			36.9	0	M+NH4	C6H9NO6	6.807802048	3572.02897	3749.882797	4171.647692	3818.313175	4172.084789	3774.053893	3887.787483	3629.173793	3625.140542
4.95_414.2015m/z	414.2015102	4.948983333	pos	Benazeprilat	HMDB0060582	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		36.9	0	M+NH4	C22H24N2O5	-2.113335707	1481.825235	2102.078546	1731.394065	2134.34124	1608.916897	1729.969643	2042.673061	1955.967278	1738.206305
4.99_365.2406m/z	365.2405802	4.991816667	pos	R-4-benzyl-3-((R)-3-hydroxy-2,2-dimethyloctanoyl)oxazolidin-2-or	65462	Unclassified	Unclassified	Unclassified			36.9	0	M+NH4	C20H29NO4	-8.362973237	2791.338007	2103.816157	2436.010856	2393.073081	2725.634161	2915.111583	2879.060018	2294.153714	3017.757326
5.08_206.0891m/z	206.0890936	5.081	pos	N,N-dimethylhistidine	44783	Unclassified	Unclassified	Unclassified			36.9	0	M+Na	C8H13N3O2	-4.935545477	195.3126884	215.64646	159.7781877	0.001403199	0.43977566	0.001403199	30.19414885	0.001403199	0.001403199
5.33_538.1912m/z	538.1911995	5.329033333	pos	Chrysoeriol 6-malonylglucoside	68239	Unclassified	Unclassified	Unclassified			36.9	0	M+NH4	C25H28O12	-1.35026332	1695.175648	1392.313014	1789.867	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199
5.40_235.1328m/z	235.1327671	5.396716667	pos	(S)-Pterosin P	HMDB0036607	Benzenoids	Indanes	Indanones			36.9	0	M+H	C14H18O3	-0.443184391	1054.008736	1384.580176	999.8275056	1107.466386	1150.573083	1117.334043	853.2577845	1252.678724	1015.519233
5.42_425.1412m/z	425.1411993	5.419283333	pos	Ginkgolide M	71364	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*	C16816	36.9	0	M+H	C20H24O10	-7.1299542	2964.718406	2846.233387	3205.715995	3749.953622	3900.46522	4758.474362	2738.603696	3201.070946	3039.093391
5.52_365.1099m/z	365.1098818	5.5209	pos	Dictyoquinazol C	94945	Organoheterocyclic compounds	Diazanaphthalenes	Benzodiazines			36.9	0	M+Na	C18H18N2O5	-2.66153033	3287.389413	3711.91602	4509.244049	1094.983783	1217.565848	1224.910984	3337.079432	3512.015039	3367.04686
5.54_407.1305m/z	407.1304866	5.543066667	pos	Rutarin	67593	Phenylpropanoids and polyketides	Coumarins and derivatives	Coumarin glycosides	*		36.9	0	M+H-H2O	C20H24O10	-7.479007214	10330.85129	12054.54883	11979.32103	13237.81149	13074.16142	13103.4739	13216.86053	13325.99269	12887.70624
5.66_317.1931m/z	317.1931465	5.656316667	pos	2,6-Dimethyl-7-octene-1,6-diol 8-O-glucoside	89085	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		36.9	0	M+H-H2O	C16H30O7	-8.134536814	8754.252867	10983.04052	4464.293946	10740.5828	132.2334294	1919.372214	4262.697333	5034.13224	3388.267214
5.70_435.1984m/z	435.1984452	5.69755	pos	8-Butanoylneosolaniol	93231	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		36.9	0	M+H-H2O	C23H32O9	-6.411093697	6308.552087	6340.619066	6000.694644	3892.251606	5033.340725	3980.884357	6680.406615	6684.092693	6623.056851
5.78_195.0875m/z	195.0874974	5.778566667	pos	Mytilitol	89550	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols			36.9	0	M+H	C7H14O6	6.094260837	2184.52542	1708.639729	2257.833879	2007.110886	1855.431006	1900.547145	1942.935342	2294.91568	2235.590458
5.96_343.1359m/z	343.1358972	5.956833333	pos	Myzodendrone	95687	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			36.9	0	M+H	C16H22O8	-8.321152082	819.5208425	2567.366879	1093.67375	53.98655327	47.84469324	66.23569246	963.3154826	1321.342665	771.8310884
6.13_409.1464m/z	409.1463866	6.128133333	pos	Etiocholanolone sulfate	HMDB0013232	Lipids and lipid-like molecules	Steroids and steroid derivatives	Sulfated steroids	*		36.9	0	M+K	C19H30O5S	4.952852391	32405.52029	35401.2352	36912.99041	40014.97106	42466.90047	43692.51145	31110.54178	35512.91841	34333.52374
6.25_211.1689m/z	211.168929	6.2535	pos	Tsibulin 1	HMDB0037390	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds			36.9	0	M+H	C13H22O2	-1.557579617	526.4891384	548.0466993	466.3198748	560.3154128	523.0519414	530.4850405	713.9448832	516.3835034	535.9204139
6.26_208.0971m/z	208.0971368	6.262533333	pos	4-(2-Hydroxyethyl)-4-methylthiazole acetate	88884	Organoheterocyclic compounds	Azoles	Thiazoles			36.9	0	M+Na	C8H11NO2S	-6.125097255	7351.737398	7602.775026	6967.652431	6910.71031	7311.737738	7355.754741	7774.216089	7833.399167	7331.919122
6.71_439.1934m/z	439.1933554	6.709016667	pos	5alpha-Pregnan-3beta,20beta-diol 3-sulfate	HMDB0240579	Lipids and lipid-like molecules	Steroids and steroid derivatives	Sulfated steroids			36.9	0.294	M+K	C21H36O5S	4.627423509	25922.49806	27984.97914	26894.34124	27744.94803	26633.39054	27181.62171	21925.10916	26341.1415	25270.84481
6.90_450.2150m/z	450.2149908	6.8951	pos	(2S,4S,6S)-2-[2-(4-Hydroxy-3-meyhoxyphenyl)ethyl]tetrahydro-6-(	87022	Phenylpropanoids and polyketides	Diarylheptanoids	Diarylheptanols	*		36.9	0	M+NH4	C23H28O8	6.357042943	6191.986628	6378.984844	7044.113328	10734.80866	9726.4541	9661.221088	4854.95812	5703.635135	5917.179685
6.94_607.3079m/z	607.3079333	6.9443	pos	(24E)-3alpha,15alpha-Diacetoxy-23-oxo-7,9(11),24-lanostatrien-(	90684	Lipids and lipid-like molecules	Prenol lipids	Triterpenoids	*		36.9	0	M+K	C34H48O7	8.39530175	28524.87129	29436.98906	30081.09208	12500.91721	11269.28262	10724.47671	17554.87949	21185.30616	22656.07161
7.04_195.0874m/z	195.0874228	7.03765	pos	3-O-Methyl-myo-inositol	63284	Unclassified	Unclassified	Unclassified			36.9	0	M+H	C7H14O6	5.709890846	752.2517518	820.7755617	840.0913711	874.8606954	760.7585833	707.5465004	1051.929787	887.848388	897.2456713
7.07_211.1689m/z	211.168944	7.069916667	pos	Artemisinyl propionate	95936	Organic oxygen compounds	Carboxylic acids and derivatives	Carboxylic acid derivatives	*		36.9	0	M+H	C18H28O2	-1.486404363	1367.645121	1254.358137	1329.913417	1493.819787	1153.929683	1698.249727	1452.393132	1241.08249	
7.20_195.0875m/z	195.0874547	7.20385	pos	Methyl beta-D-glucopyranoside	86622	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		36.9	0	M+H	C7H14O6	5.87457516	959.4805444	1047.438737	912.9096798	749.0688684	962.7503858	969.0264815	1268.171131	1018.177968	1200.582288
7.23_217.1584m/z	217.1584348	7.230183333	pos	4,10-Longipinanedione	HMDB0032081	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		36.9	0	M+H-H2O	C15H22O2	-1.097021608	858.9337493	623.426849	701.8322389	504.6202901	490.2014213	492.1079606	609.6480815	559.849662	506.8885337
7.25_213.1846m/z	213.1845936	7.246116667	pos	Citronellyl propionate	HMDB0037226	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohol esters	*		36.9	0	M+H	C13H24O2	-1.474336748	924.5775815	736.5054202	845.8693262	748.8881269	703.7142464	722.6717235	792.1374044	713.0050538	732.4075215
7.27_439.1933m/z	439.1932512	7.274666667	pos	8-Propanoylneosolaniol	93233	Organoheterocyclic compounds	Isoquinolines and derivatives	Benzylisoquinolines	*		36.9	0	M+H	C22H30O9	-6.86420514	12306.06268	14210.80837	13767.91544	19940.2352	17049.8874	17572.14603	9970.594268	12571.3483	12376.53396
7.41_323.1828m/z	323.1828043	7.414583333	pos	13,14-dihydro-15-keto-tetranor PGF1α	2294	Unclassified	Unclassified	Unclassified			36.9	0	M+Na	C16H28O5	-0.301092595	1286.275373	1270.339919	1331.618753	1466.859604	1492.067176	1379.468247	981.5675738	1475.688892	1124.532365
7.49_245.1622m/z	245.1621647	7.4907	pos	Isoconitine	72852	Unclassified	Unclassified	Unclassified			36.9	0	M+H	C13H23NO5	-1.212138171	465.2746499	556.0267573	252.6348494	286.4298955	139.9143365	342.2223581	583.827497	390.1063435	
7.52_336.2503m/z	336.250251	7.5231	pos	Leukotriene A4	3449	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C00909	36.9	0	M+NH4	C20H30O3	-9.645445179	4412.707881	4088.738483	3686.674414	3514.423857	3489.965213	3767.039775	4082.266165	3256.802029	3638.098179
7.93_195.0875m/z	195.0874627	7.927683333	pos	D-Glucoside	6958	Unclassified	Unclassified	Unclassified			36.9	0	M+H	C7H14O6	5.915516196	472.6618062	542.7297914	611.8755816	521.7433021	651.8385616	666.872804	773.4397091	725.5451965	555.2512719
8.25_206.0666m/z	206.0665886	8.245133333	pos	Furfuryl propyl disulfide	HMDB0032289	Organoheterocyclic compounds	Heteroaromatic compounds	Unclassified	*		36.9	0	M+NH4	C8H12OS2	-1.031223601	1848.702617	1887.183182	1699.120304	1810.088432	2187.751796	2063.29672	1911.535029	1697.7853	1930.955071
8.50_334.2347m/z	334.2346676	8.497183333	pos	N-3-oxo-hexadec-11(Z)-enoyl-L-Homoserine lactone	45315	Unclassified	Unclassified	Unclassified			36.9	0	M+H-H2O	C20H33NO4	-8.548816659	61817.10501	59339.55629	59655.74751	64675.36009	67259.78406	64859.43791	67723.57595	59826.56989	67609.08499
9.56_228.1306m/z	228.1305702	9.56185	pos	Asparaginyl-Leucine	HMDB0028735	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		36.9	0	M+H-H2O	C10H19N3O4	-2.846031142	98.8972487115	36.98096786	39.30584193	42.49832647	37.33797403	76.16187457	41.1262357	30.01403199	
9.77_201.9755m/z	201.9754619	9.7709	pos	3-Methylsulfinylpropyl isothiocyanate	58356	Organic oxygen compounds	Organosulfur compounds	Sulfoxides	*		36.9	0	M+K	C5H9NOS2	-1.546307243	16291.00989	15463.20427	15119.74869	16351.71523	16616.73869	17622.20713	16487.35002	16585.32678	17136.68203
0.54_176.0947n	177.1019653	0.535	pos	N-Hydroxyl-tryptamine	63561	Unclassified	Unclassified	Unclassified			36.8	0	M+H, M+NH4	C10H12N2O	-1.556803612	564.5181422	976.2661304	914.1235457	308.416751	293.6356489	975.8732199	1220.202967	939.77242	1275.217773
0.54_541.3707m/z	541.3706665	0.535	pos	13-(beta-D-glucosyloxy)docosanoic acid	LMFA13010054	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides			36.8	0	M+Na	C28H54O8	-0.81573909	0.001403199	0.001403199	0.001403199	0.001403199	48.61243117	52.9658182	396.7148503	38.25986114	3354.852885
0.68_148.1159m/z	148.1158868	0.6788	pos	3-Methylcyclohexanethiol	HMDB0031537	Organosulfur compounds	Thiols	Alkylthiols	*		36.8	0	M+NH4	C7H14S	3.380832566	1418.213469	1671.930426	1695.346405	4903.329377	4852.514699	5611.803408	3216.615744	3134.556649	3585.572229
0.72_266.1592m/z	266.1592313	0.717716667	pos	Histidinyl-Lysine	85796	Benzenoids	Phenol ethers	Anisoles	*		36.8	0	M+H-H2O	C12H21N5O3	-6.780421494	3093.537423	3480.53361	4270.394797	3502.90715	2998.489355	3492.619232	2768.218518	3174.260941	3507.580482
0.78_231.1447m/z	231.144747	0.776916667	pos	Ammodendrine	68134	Unclassified	Unclassified	Unclassified			36.8	0	M+Na	C12H20N2O	-9.782157485	63619.65178	65398.74614	64256.17375	69344.82435	58347.76696	64327.98154	58388.77173	54635.0477	56624.77788
0.82_674.2370n	697.2258584	0.818116667	pos	(N-acetyineuraminosyl(a2-6)lactosamine)	HMDB0001081	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C04886	36.8	0	M+H, M+Na	C25H42N2O19	-1.74070408	20459.94857	20228.42664	20557.49181	24740.45115	25517.31503	21447.92547	17740.0719	20114.33438	20382.39594
0.86_261.1805m/z	261.1804588	0.859583333	pos	carisoprodol	3947	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		C07927	36.8	0	M+H	C12H24N2O4	-1.63295197	1807.565313	2265.99001	2663.327861	711.9673616	942.6792435	989.8739914	419.7131675	699.2515259	512.9820551
0.88_283.0411m/z	283.0411466	0.8802	pos	Suprofen	43341	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds		C07320	36.8	0	M+Na	C14H12O3S	4.655701694	10279.74458	10764.61635	10359.76931	12399.36092	10074.23795	9944.680159	9500.508996	11272.95223	10201.41325
0.90_287.1709m/z	287.1709195	0.898483333	pos	Tetracaine	2807	Unclassified	Unclassified	Unclassified			36.8	0	M+Na	C15H24N2O2	-7.870349828	7455.470689	6765.293429	7714.571241	9457.023815	11692.67108	9367.236441	9156.603557	9123.542153	8960.796783
0.96_167.0230m/z	168.030581	0.91985	pos	4-Nitrobenzoate	71157	Unclassified	Unclassified	Unclassified			36.8	0	M+H-H2O, M+H	C7H5NO4	6.543618324	1006.45171	1661.535611	1999.122152	1915.894089	2032.264733	1970.393295	1643.254138	1917.065655	
1.01_225.1846m/z	225.1846273	1.006283333	pos	L-Menthyl (R,S)-3-hydroxybutyrate	88397	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		36.8	0	M+H-H2O	C14H26O3	-1.152586771	620.9565506	544.4432214	442.8865476	487.1677451	372.5591353	524.5972265	236.3922387	570.9685167	276.4904384
1.16_231.1597m/z	231.1596841	1.157483333	pos	8-piperazin-1-yl-isoquinoline (hydrochloride)	45045	Unclassified	Unclassified	Unclassified			36.8	0	M+NH4	C13H15N3	-3.467031644	6099.547368	6251.419719	6123.550887	8163.752757	6622.015237	6721.790247	6155.737633	6535.208099	5851.50432
1.18_275.1232m/z	275.123206	1.178066667	pos	3,7,7,10-Tetramethyl-12-thiabicyclo[9.1.0]dodeca-3,7-diene	91595	Organoheterocyclic compounds	Thiiranes	Unclassified	*		36.8	0	M+K	C15H24S	0.745855426	6809.072905	7904.214765	7715.326003	8782.294117	8091.325652	9561.7239	5810.724822	7153.416572	6133.681348
1.20_267.0058m/z	267.0058334	1.199716667	pos	Euxanthone	68103	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans	*	C10061	36.8	0	M+K	C13H8O4	1.826721483	4615.909688	4325.656467	4665.147421	3643.411863	3481.633419	3387.52479	4367.581003	3969.67628	3803.559244
1.22_214.0925m/z	214.0925765	1.2075	pos	Galactonic acid	HMDB0000565	Organic acids and derivatives	Hydroxy acids and derivatives	Medium-chain hydroxy acids and derivatives	**	C00880	36.8	0	M+H	C6H12O7	2.286237157	1907.09324	1915.831699	1937.024606	640.6421538	462.8193586	486.5960379	341.5285339	0.001403199	0.001403199
1.29_306.1656m/z	306.1655942	1.285033333	pos	Amabiline	68206	Unclassified	Unclassified	Unclassified			36.8	0	M+Na	C15H25NO4	-7.00885833	1289.4707	1467.586108	1449.889588	5254.567496	4703.870574	4583.602968	1934.175805	2102.027508	2128.086054
1.63_131.0531m/z	131.0530788	1.633283333	pos	Propyl 2-mercaptopropionate	HMDB0032495	Organic acids and derivatives	Carboxylic acids and derivatives	Carboxylic acid derivatives	*		36.8	0	M+H-H2O	C6H12O2S	3.82572215	30.9345099	21.2828615	20.23381615	0.001403199	0.001403199	0.001403199	15.26232484	19.3298235	
1.79_228.2319m/z	228.2318695	1.7859	pos	8Z,10E-Tetradecadien-1-ol	LMFA05000186	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols			36.8	0	M+NH4	C14H26O	-1.529192052	1359.720682	1368.204458	1300.00704	1111.2063	1402.746745	1272.520149	1278.916069	1196.965691	1056.908469
10.14_244.2268m/z	244.2268225	10.14475	pos	5Z-Tetradecenoic acid	HMDB0000521	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		36.8	0	M+NH4	C14H26O2	-1.25174032	749.8588563	741.6401183	1899.506572	884.1354043	775.0160003	717.3210142	846.5952109	638.4707435	759.5065816
10.28_444.2558m/z	444.2558099	10.27931667	pos	N-nonadecanoyl taurine	LMFA08020248	Lipids and lipid-like molecules	Fatty Acyls	Fatty amides			36.8	0	M+NH4	C21H43NO4S	3.385147774	2715.979718	1883.081028	2817.394491	1609.260734	1381.264657	1392.517277	2969.493995	2422.667656	2044.64593
11.13_313.2346m/z	313.2344418	11.12978333	pos	9S,12S,13S-trihydroxy-10E-octadecenoic acid	36021	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C14833	36.8	0	M+H-H2O	C18H34O5	-8.835750363	1422.915629	16336.03099	13255.36274	14265.37851	14225.05056	16417.758	13634.08061	14401.18455	13158.58087
11.28_836.5403m/z	836.540299	11.28136667	pos	PS(18:3(6Z,9Z,12Z)/20:0)	HMDB0112454	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoserines	*		36.8	0	M+Na	C44H80NO10P	-1.113717547	14051.27452	10197.65928	8188.810539	5467.010953	5603.92799	4423.135207	6430.88014	4970.680641	5997.738784
12.37_771.5131m/z	771.5130535	12.37401667	pos	PG(18:0/16:1(9Z))	LMGP04010887	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols	*		36.8	0	M+Na	C40H77O10P	-2.140869944	17451.62028	13309.215	14549.65019	1902.386624	482.9071698	248.1515895	11886.15294	9434.909047	3847.727912
12.54_707.4904m/z	707.4904212	12.54226667	pos	PG(17:0/14:1(9Z))	3879	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols			36.8	0	M+H	C37H71O10P	6.595598651	32402.64399	30026.54265	30426.7096	30539.79811	29622.1931	31817.92977	33290.81361	33454.90824	29667.65789
12.59_484.2986m/z	484.2986164	12.58981667	pos	PS(O-16:0/0:0)	78863	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoserines			36.8	0	M+Na	C22H46NO8P	-9.857598024	10824.36215	10822.59146	9558.453285	9956.737068	10138.35491	11098.32763	10213.72368	10514.39056	10774.57589
12.72_316.2244m/z	316.2243737	12.72343333	pos	Norethynodrel	43279	Unclassified	Unclassified	Unclassified	*		36.8	0	M+NH4	C20H28O2	-9.161524548	8104.228591	5892.662903	7264.112431	6803.653738	6100.193854	5384.985394	6245.420185	6519.194177	5967.259423
13.09_742.5452n	765.5307519	13.08768333	pos	PA(17:0/22:2(13Z,16Z))	81410	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphates	*		36.8	0	M+NH4, M+Na	C42H79O8P	-8.177599421	30442.85109	29455.88184	28132.76469	28000.23709	26660.60389	24756.83798	28856.72005	24225.19577	28749.2635
13.69_349.1830m/z	349.1830314	13.68831667	pos	(1R*,2R*,4R*,8S*)-p-Menthane-1,2,8,9-tetrol 9-glucoside	94517	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		36.8	0	M+H-H2O	C16H30O9	-7.271789399	581.7348709	521.5394266	705.3304984	935.3974072	1115.681115	655.6455101	1133.575391	1039.783652	1042.727736
14.22_533.2793m/z	533.2792921	14.215	pos	adonitoxin	57789	Lipids and lipid-like molecules	Steroid Lipids	Sterols			36.8	0	M+H-H2O	C29H42O10	8.691676757	2950.570802	2793.742069	2913.348301	2090.328694	2726.032532	2683.528216	3503.760401	2724.159727	1962.732237
14.55_259.1148m/z	259.1148236	14.54965	pos	Fluenetil	72782	Unclassified	Unclassified	Unclassified			36.8	0	M+H	C16H15FO2	7.513203166	737.4751928	689.6535681	551.2512152	743.9986519	1030.322179	989.8476788	772.1228568	715.2451772	816.6486066
14.63_194.0921m/z	194.0921355	14.62908333	pos	N-Acetyl-3-methylhistidine	HMDB0240341	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			36.8	0	M+H-H2O	C9H13N3O3	-1.267617352	374.6753907	672.6638824	783.6316282	808.4431239	716.6109998	666.1389096	923.0086145	858.1349525	909.670123
15.02_134.0962m/z	134.0961948	15.02476667	pos	L-PHENYLALANINO

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7.20_489.2346m/z	489.2345736	7.20385	pos	Dabigatran	HMDB0250817	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols			36.7	0	M+NH4	C25H25N7O3	-2.41853584	1671.728778	2094.626272	1852.448692	1277.873579	892.6961013	1008.392184	668.6036003	761.2715721	771.3513805
7.48_217.1584m/z	217.1584281	7.480483333	pos	2-Hexyl-3-phenyl-2-propenal	87907	Phenylpropanoids and polyketides	Cinnamaldehydes	Unclassified	*		36.7	0	M+H	C15H20O	-1.219567325	817.4825565	622.8496232	525.9344409	375.8781148	472.5631686	406.6089566	556.8363994	450.1692587	441.1269299
7.51_227.1637m/z	227.1636824	7.50885	pos	6-methyl-dodecanedioic acid	74905	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			36.7	0	M+H-H2O	C13H24O4	-2.001001689	354.7340188	290.4870905	205.8352208	300.7460055	212.5513577	130.0989936	298.7371122	285.3705819	294.1491516
7.67_366.2246m/z	366.2246307	7.668366667	pos	Gibberellin A110	88115	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	*		36.7	0	M+NH4	C20H28O5	-8.239303885	3937.012432	3689.768118	3577.084253	4437.909972	4577.651861	2824.258116	3389.674647	3514.712554	3771.37559
7.85_344.1885m/z	344.1885029	7.8497	pos	Gossypurbilone	89127	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		36.7	0	M+H	C20H25NO4	8.357692438	2895.251644	2857.510742	3209.289852	4560.642526	4080.060096	4239.519643	2019.908346	2125.082279	2011.339791
8.07_487.2189m/z	487.2189165	8.074933333	pos	Granisetron metabolite 3 glucuronide	3149	Unclassified	Unclassified	Unclassified			36.7	0	M+H-H2O	C24H32N4O8	0.378240729	5200.680905	6100.340807	8269.527729	915.599242	511.4211738	730.6913596	2807.538823	3653.05981	3272.988313
8.59_201.1635m/z	201.1635136	8.593966667	pos	Patchoulenone	90999	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		36.7	0	M+H-H2O	C15H22O	-1.207898191	52.2449605	161.4699001	171.7913456	21.36999764	47.76565753	72.78366261	70.00835886	58.39770031	62.86463582
9.58_354.2401m/z	354.2400702	9.5843	pos	Acebutolol	405	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds		C06803	36.7	0	M+NH4	C18H28N2O4	3.977567884	1027.931428	1140.793805	847.8227534	1569.982523	919.7387111	1566.270126	1751.860391	1733.537028	933.6450709
9.85_332.2191m/z	332.2190959	9.848266667	pos	Yucalexin B5	90519	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	*		36.7	0	M+NH4	C20H26O3	-9.307676416	20557.02126	19247.62631	16873.79221	17351.87271	18802.94859	18121.5302	16097.01671	18879.45374	18635.9502
0.68_220.9343m/z	220.9343073	0.6788	pos	Succimer	HMDB0014706	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates		C07598	36.6	0	M+K	C4H6O4S2	2.190184295	4645.667864	4113.600732	3460.010335	2981.452376	3167.189266	2695.118541	3977.930765	3644.912671	3912.078868
0.74_138.0741m/z	138.0740721	0.73955	pos	7-Isothiocyanato-1-heptene	93125	Organosulfur compounds	Isothiocyanates	Unclassified			36.6	0	M+H-H2O	C8H13NS	3.159337491	2065.701419	1541.350385	1713.55365	4900.94052	3627.512695	3438.242318	2156.975387	1848.431313	1904.319081
0.74_320.1350m/z	320.1350619	0.739655	pos	4-O-alpha-D-Galactopyranosylcalystegine B2	92956	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			36.6	0	M+NH4	C13H23NO9	-1.45889893	784.2249824	401.2364506	812.0774215	756.1604587	593.5514787	451.5694873	260.2508958	454.7236633	513.2007089
0.78_136.0435m/z	136.0435337	0.776966667	pos	MECYSTEINE	43544	Unclassified	Unclassified	Unclassified			36.6	0	M+H	C4H9NO2S	6.351913319	0.001403199	43.71285674	153.4127029	104.4114701	123.0489134	203.521409	157.1672037	174.303833	160.4375032
0.80_139.0581m/z	139.0580983	0.796683333	pos	2,6-Dimethylbenzenethiol	HMDB0032019	Benzenoids	Thiophenols	Unclassified	*		36.6	0	M+H	C8H10S	3.6255866	15783.18582	15895.55704	16515.62658	11109.23323	11645.22173	8815.622796	8984.692456	8742.822116	
0.84_145.1051m/z	145.10505	0.8386	pos	(S1)-Methoxy-3-heptanethiol	HMDB0032380	Organic oxygen compounds	Organooxygen compounds	Ethers	*		36.6	0	M+H-H2O	C8H18OS	3.097104248	16172.53212	15946.70563	16407.00332	40511.75966	36608.72641	36447.42877	13591.34206	15509.90205	14820.54601
1.14_287.1709m/z	287.1708739	1.137683333	pos	13-Hydroxylupanine	64452	Unclassified	Unclassified	Unclassified			36.6	0	M+Na	C15H24N2O2	-8.042954814	8723.847561	5702.564797	6814.756587	12890.48875	6206.289143	6867.739402	10640.32654	11366.62913	7930.417777
1.16_246.1331m/z	246.1331285	1.157483333	pos	Neostigmine	HMDB0015472	Benzenoids	Benzene and substituted derivatives	Phenoxy compounds		C07258	36.6	0	M+Na	C12H19N2O2+	-3.338792504	763.0561908	1010.379224	1158.773589	1366.456648	1698.496245	1664.881992	835.6329175	1237.467682	1174.709654
1.26_245.1605m/z	245.1604911	1.264483333	pos	Noruron	72853	Unclassified	Unclassified	Unclassified			36.6	0	M+Na	C13H22N2O	-8.744952321	2690.138752	3198.389478	3365.389493	3416.923903	3499.550382	3717.815606	2801.863986	3466.304946	3372.639484
1.48_154.0690m/z	154.0689738	1.479433333	pos	Phenyl vinyl sulfide	87948	Organosulfur compounds	Thioethers	Aryl thioethers	*		36.6	0	M+NH4	C8H8S	3.506523003	3218.381684	3123.496726	3230.844916	10724.44773	10294.04678	10376.16785	3887.466066	4152.53639	4159.085556
1.52_204.0488m/z	204.0488484	1.52285	pos	3-maleylpyruvic acid	45909	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates	**	C02167	36.6	0	M+NH4	C7H6O6	-7.607336567	237.5000755	462.3111128	749.3457298	355.769125	646.1035348	827.228837	374.8036813	783.5784374	921.9058255
1.57_129.0739m/z	129.0738606	1.56695	pos	S-Methyl 4-methylpentanethioate	94040	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl thioesters	*		36.6	0	M+H-H2O	C7H14OS	4.194750805	74.33163458	32.10870148	78.89593769	51.71384061	63.34461777	107.2313397	73.43759688	31.47703542	20.53513746
10.00_336.2503m/z	336.2503466	10.00346667	pos	12-oxo-ETE	36285	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	**	C14807	36.6	0	M+NH4	C20H30O3	-9.344839859	60782.79879	61809.52139	54021.53643	57521.41414	62790.30747	60276.98241	59625.44568	58706.04332	57413.85637
10.02_233.1533m/z	233.1532898	10.08803333	pos	Isoalantolactone	HMDB0035934	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*	C09484	36.6	0	M+H	C15H20O2	-1.363440027	1477.312966	1011.59293	1554.637584	1029.402306	1417.551367	1434.73026	1311.341022	1023.217753	1215.012071
10.63_152.0465m/z	152.0465459	10.63171667	pos	Quinoline	HMDB0033731	Organoheterocyclic compounds	Quinolines and derivatives	Unclassified		C06413	36.6	0	M+Na	C9H7N	-4.060612342	27254.82469	25319.15353	25485.39063	24149.46219	23550.52445	24030.03082	26547.59846	24666.87903	24062.75328
11.81_219.1740m/z	219.1740394	11.81006667	pos	(4S)-Dihydrocurcumenone	88975	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		36.6	0	M+H-H2O	C15H24O2	-1.280423171	902.2345198	1100.828921	1087.00562	949.2645922	954.1823187	853.0177557	1001.91575	973.4435234	838.2385182
11.95_737.5009m/z	737.5009214	11.9467	pos	PS(15:0/16:1(9Z))	78580	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoserines	*		36.6	0	M+NH4	C37H70NO10P	-9.226498736	20893.4242	20450.36358	21807.11352	22770.15203	19875.5722	21241.51461	24954.61582	20070.48211	24095.25777
12.12_297.2397m/z	297.2397215	12.1244	pos	12,13-DiHOME	HMDB0004705	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	***	C14829	36.6	0	M+H-H2O	C18H34O4	-8.591482431	2239.12419	2444.685613	2871.480617	2183.637199	3852.036992	3285.54099	3064.862566	2997.757172	2685.476913
12.80_429.3181m/z	429.3180948	12.80346667	pos	Sorbitan oleate	86565	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		36.6	0	M+H	C24H44O6	-6.936057923	3665.070139	3649.518417	3455.965071	2613.386081	3624.815453	5045.259027	4062.105007	4790.227377	2797.924706
12.82_309.1304m/z	309.1304118	12.82411667	pos	8-Acetylgrayanotoxiside	92587	Organoheterocyclic compounds	Cycloheptafurans	Unclassified			36.6	0	M+H	C16H20O6	-9.259226989	2050.33333	1550.667917	2234.209765	1022.341169	2499.26388	2438.455636	1893.953056	1444.386641	2239.88626
13.07_469.3129m/z	469.3129218	13.07185	pos	Hovenine A	86791	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		36.6	0	M+H-H2O	C27H42N4O4	-9.03878388	5324.363778	5285.062887	4712.053047	5156.055407	5272.95315	4176.329847	4908.960295	4716.56752	3305.189821
13.14_369.2606m/z	369.260612	13.1354	pos	Glycerol trihexanoate	87428	Lipids and lipid-like molecules	Glycerolipids	Triradylglycerols	*		36.6	0	M+NH4	C21H38O6	-7.608028186	1276.756435	1228.86971	1850.301027	1856.705312	1375.549156	1703.200285	1547.981698	1678.103331	1697.269816
13.19_704.5664m/z	704.5663895	13.18723333	pos	SM(d18:2/15:0)	83738	Lipids and lipid-like molecules	Sphingolipids	Phosphosphingolipids			36.6	0	M+NH4	C38H75N2O6P	-5.405110185	897.1354521	1578.804403	1243.111536	1997.607036	2459.460567	2668.486646	1518.520207	1664.187584	2714.568605
14.27_341.2658m/z	341.2658232	14.26986667	pos	11-deoxy-PGF1α	36139	Unclassified	Unclassified	Unclassified			36.6	0	M+H	C20H36O4	-8.266642558	1679.349455	2313.57247	2279.948849	1577.574199	2385.540571	2374.961223	2447.263322	2360.397078	1828.465892
14.58_858.7525m/z	858.752517	14.59043333	pos	TG(17:0/18:2(9Z,12Z)/18:2(9Z,12Z))	HMDB0011711	Lipids and lipid-like molecules	Glycerolipids	Triradylglycerols	*		36.6	0	M+NH4	C54H96O6	-2.378105429	3600.92739	16378.45127	21690.59758	22946.88905	31969.35985	24519.00577	59116.91799	35690.67022	21477.1188
15.52_123.0790m/z	123.07901	15.51933333	pos	Ethyl isopropyl ketone	58330	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		36.6	0	M+Na	C6H12O	9.734011835	84993.763	27795.40274	11715.63883	65369.84447	216801.8217	237440.7057	160486.0577	814.2529521	867.1537123
2.03_369.1549m/z	369.1549451	2.026633333	pos	Methyl (R)-9-hydroxy-10-undecene-5,7-diynoate glucoside	95348	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		36.6	0	M+H	C18H24O8	1.496534319	3104.300666	2950.097173	2947.756248	3421.965531	3157.027016	3270.209369	2862.453277	3198.623424	3104.571367
2.28_297.1077m/z	297.1076596	2.28185	pos	4-Nitrophenyl-3-ketovalidamine	66096	Unclassified	Unclassified	Unclassified			36.6	0	M+H	C13H16N2O6	-1.5301512	3179.192573	3513.906117	2417.632607	3022.012549	3168.85652	3893.849145	3521.230414	3529.356873	3647.148538
2.79_227.1386m/z	227.1385918	2.79025	pos	p-Lactophenetide	69921	Unclassified	Unclassified	Unclassified			36.6	0	M+H	C11H15NO3	-2.042203264	1463.738909	1522.062436	1537.150886	1258.819497	1284.659113	1533.199161	1974.525946	2051.355513	1971.692499
2.82_115.0502m/z	115.0502743	3.215533333	pos	Methylazoxymethanol acetate	72978	Unclassified	Unclassified	Unclassified			36.6	0	M+H-H2O	C4H8N2O3	0.523977123	868.1207	777.9799136	900.1845383	984.3529158	1051.932379	1098.07112887	1015.759526	882.8980239	
3.33_252.0723m/z	252.0722879	3.330366667	pos	Bacteriocin 28b	89961	Unclassified	Unclassified	Unclassified			36.6	0	M+Na	C12H11N3O2	-8.989804532	5037.903685	5807.462102	5687.719431	7074.472968	5842.743799	6515.917456	5350.138378	5313.62479	5397.874692
3.67_198.0701m/z	198.0700652	3.671416667	pos	N-benzoylthiourea	96310	Unclassified	Unclassified	Unclassified			36.6	0	M+Na	C8H8N2OS	2.809574968	5001.625149	5223.801688	5569.872629	7224.432199	6314.767296	5694.677137	4931.715658	5690.988811	5528.634019
3.72_218.1026m/z	218.102646	3.716333333	pos	3,6-Dihydro-4-(4-methyl-3-pentenyl)-1,2-dithiin	86660	Organoheterocyclic compounds	Dithiins	Unclassified	*		36.6	0	M+NH4	C10H16S2	-2.609260268	107.7335232	28.22159659	110.4657167	136.441106	109.825788	46.85526613	167.6986492	127.2184938	35.48357071
3.74_465.1434m/z	465.1433652	3.73775	pos	(Z)-Narceine imide	86929	Organoheterocyclic compounds	Isoindoles and derivatives	Isoindolines	*		36.6	0	M+K	C23H26N2O6	2.629215374	2978.730067	2978.063003	3050.994383	3409.730086	2797.205768	2940.796419	2213.970074	2847.862318	2158.616089
3.78_394.0739m/z	394.0738655	3.781933333	pos	Gonyautoxin 1	71387	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates		C16855	36.6	0	M+H-H2O	C10H17N7O9S	-8.982184897	4774.939485	5375.179713	5146.826338	442.9628838	301.6416355	615.0176809	810.4887609	883.7818363	897.3682966
3.80_271.0409m/z	271.0408834	3.80375	pos	Terbufos	HMDB0258828	Unclassified	Unclassified	Unclassified			36.6	0.947	M+H-H2O	C9H21O2PS3	0.146109549	9040.555483	9179.557206	9959.637683	9958.227581	9062.424714	8667.167357	10312.43107	11388.3579	
3.85_244.0107m/z	244.010725	3.845583333	pos	Methasulfocarb	72520	Unclassified	Unclassified	Unclassified			36.6	0	M+H-H2O	C9H11NO4S2	4.074034166	34309.6572	31386.26276	30178.6953	37742.97852	32794.58072	29845.73815	31444.84002	32176.83119	50934.34138
3.91_260.0727m/z	260.0726815	3.911966667	pos	Glycolyl-D-mannosamine	65993	Unclassified	Unclassified	Unclassified			36.6	0	M+Na	C8H15NO7	-5.867275264	102.8166763	139.1438449	117.308926	675.8146893	563.7290804	388.045484	517.6365109	701.3437028	712.0420488
3.93_145.1101n	168.1018745	3.9343	pos	3-Carboxypropyl trimethylammonium	34501	Unclassified	Unclassified	Unclassified			36.6	0	M+H, M+Na	C7H15NO2	-1.117767597	570.393347	601.4388621	558.8063725	541.9162952	546.1299715	522.5374974	547.5043823	533.8689858	608.3793403
3.96_167.1429m/z	167.1429451	3.956866667	pos	Prenyl caproate	HMDB0032489	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*	C13422	36.6	0	M+H-H2O	C11H20O2	-0.524420407	433.9083561	314.4375466	309.8618735	306.1077724	386.4151004	351.6346156	384.2211706	306.7857942	352.2516761
4.11_297.1346m/z	297.1334379	4.114783333	pos	Cyclocoprinin A	94359	Organoheterocyclic compounds	Furopyrans	Unclassified	*		36.6	0	M+H	C19H20O6	0.584579482	365.4733	436.9854392	557.1387919	508.3277153	356.6263259	430.2709193	387.1762807	641.0719549	
4.20_336.1386m/z	336.138645	4.204866667	pos	Methionyl-Tryptophan	85886	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		36.6	0	M+H	C16H21N3O3S	3.001894148	939.3678703	792.1024031	870.1357946	1464.238364	1465.80713	1352.360626	1509.275053	1370.528844	1390.232746
4.25_214.0869m/z	214.0868665	4.249833333	pos	XANTHONE	HMDB0259922	Unclassified	Unclassified	Unclassified			36.6	0	M+NH4	C13H8O2	3.119136539	1071.010497	1109.270141	1094.020227	396.8562237	362.7502724	457.8555587	665.5857585	860.0679283	867.5181262
4.32_223.0939m/z	223.0939133	4.317083333	pos	2E-Decenedioic acid	LMFA01170032	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			36.6	0	M+Na	C10H16O4	-0.831205721	4657.712449	4264.26675	4347.913959	4079.338559	4027.435726	4310.504138	4293.691672	4246.332452	4123.333254
4.34_229.0638m/z	229.0637824	4.33965	pos	CAY10565	45277	Unclassified	Unclassified	Unclassified			36.6	0	M+NH4	C9H9NO3S	-1.693042029	54.42648238	402.2691262	465.69522	411.6009658	331.7182737	109.3553831	394.3772931	381.9910995	280.9867749
4.36_307.0660m/z	307.065974	4.3623	pos	Isoprothiolane sulfoxide	68853	Unclassified	Unclassified	Unclassified			36.6	0	M+H	C12H18O5S2	-2.836548996	2309.884297	2106.322789	2489.256671	2799.267194	2494.552662	2543.570474	2932.06987	2801.786065	3339.262509
4.38_181.0371m/z	181.0370765	4.384333667	pos	Nifurazone	43276	Organoheterocyclic compounds	Furans	Nitrofurans		C08042	36.6	0	M+NH4	C6H6N4O4	7.372788299	1930.841009	1334.522921	1298.142423	1102.692209	1025.648182	960.039419	1500.338332	1430.434928	1692.178739
4.47_346.1970m/z	346.1970022	4.473983333	pos	N-Jasmonoylisoleucine	86237	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C18699	36.6	0	M+Na	C18H29NO4	-5.806910973	827.6904154	1133.92296	1134.699977	1645.928147	1549.946871	1331.087828	845.401161	982.4633126	877.5187429
4.54_188.0717m/z	188.0717178	4.542216667	pos	Gentianamine	68048	Unclassified	Unclassified	Unclassified			36.6	0	M+H-H2O	C11H11NO3	5.42662131	709.1766157	830.0742077	793.0700517	739.8503332	703.8010722	666.1819849	762.5990257	862.7762706	757.2550542
4.66_245.1282m/z	245.1282246	4.656183333	pos	α-Aminodiphenylacetic acid	1858	Unclassified	Unclassified	Unclassified			36.6	0	M+NH4	C14H13NO2	-1.010868299	586.6946884	1044.672748	1102.233555	674.7391374	890.4952102	553.4156225	687.337051	958.937211	878.6142477
4.77_329.0602m/z	329.0602475	4.768333333	pos	4-[(2-Hydroxy-1-naphthalenyl)azo]benzenesulfonic acid	92644	Benzenoids	Naphthalenes	Naphthols and derivatives			36.6	0	M+H	C16H12N2O4S	3.637367877	2790.05249	2696.411157	2436.591249	2184.412764	2369.431097	2323.488448	2502.911742	2895.639563	2743.254022
4.99_291.0972m/z	291.0972178	4.991816667	pos	N-Acetyl-D-tryptophan	65974	Unclassified	Unclassified	Unclassified			36.6	0	M+H	C14H14N2O3	-1.138377701	951.9651611	1158.77526	1127	236.0657297	441.6721424	327.7868751	626.8116985	613.1225585	674.0924588
4.99_467.1210m/z	467.120966	4.991816667	pos	Halobetasol	HMDB0253038	Lipids and lipid-like molecules	Steroids and steroid derivatives	Pregnane steroids			36.6	0	M+K	C22H27ClF2O4	2.836347214	0.001403199	0.001403199	0.001403199	8534.267133	8317.644366	7790.416713	0.001403199	0.001403199	0.001403199
5.01_143.0483m/z	143.0482649	5.013433333	pos	2-Formyl-1-indanone	66723	Unclassified	Unclassified	Unclassified			36.6	0	M+H-H2O	C10H8O2	-5.475337373	281.20729	338.5517961	255.3090612	350.6067951	289.5133517	274.7330373	365.7107214	238.2887214	362.3013434
5.04_322.1984m/z	322.1984297	5.035783333	pos	2-METHYLENE-5-(2,5-DIOXOTETRAHYDROFURAN-3-YL)-6-O	44604	Unclassified	Unclassified	Unclassified			36.6	0	M+NH4	C18H24O4	-9.386600939	11218.54596	12975.97496	12330.72914	6794.219878	5798.802252	6353.886337	11083.63013	11969.57561	11402.35551
5.04_341.0603m/z	341.0603361	5.035783333	pos	5,7,2',5'-Tetrahydroxy-6-methoxyflavanone	53077	Unclassified	Unclassified	Unclassified			36.6	0	M+H	C16H14O7	-8.920580986	2368.187573	2559.648872	2714.402525	201.3068833	240.2416199	292.7076669	2595.045825	2768.620361	2614.831138
5.28_292.1991m/z	292.1990136	5.284233333	pos	4-Dehydronobiletin	91727	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*		36.6	0	M+NH4	C20H26O5	8.532726984	2911.009067	3276.896191	4533.32797	3955.849267	3799.49721	2089.848474	3377.974377		
5.35_257.1357m/z	257.1356783	5.351683333	pos	N-Glucosyl ethanolamine	88337	Organic nitrogen compounds	Organonitrogen compounds	Amines	*		36.6	0	M+NH4	C8H17NO7	5.64999382	1479.526912	1447.302465	1173.144674	968.3418232	1680.125128	1223.685995	1163.1944	1405.050252	1087.729174
5.42_155.0595m/z	155.0594819	5.419283333	pos	3-Acetyl-2,7-naphthyridine	92245	Organoheterocyclic compounds	Diazanaphthalenes	Naphthyridines			36.6	0	M+H-H2O	C10H8N2O	-5.188124315	1173.891375	958.0318053	1066.865722	772.9309581	692.969761	759.6431632	830.2808242	761.6012617	837.300102
5.42_320.0821m/z	320.0820918	5.419283333	pos	L-Menthone 1,2-glycerol ketal	88395	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		36.6	0	M+Na	C16H15N3OS	-2.396588417	588.2617069	1078.20325	350.4039022	694.8631068	650.2907738	408.1692952	367.8716462	699.3073533	380.0974191
5.50_452.1908m/z	452.1908381	5.49815	pos	6'-Hydroxy-2,3,4,5,2',3',4'-heptamethoxychalcone	52154	Unclassified	Unclassified	Unclassified			36.6	0	M+NH4	C22H26O9	-1.542855065	2643.164949	2112.597966	3061.776274	1193.474767	418.6527689	887.9216337	2036.411423	2556.553201	2654.24949
5.70_432.1990m/z	455.1882011	5.69755	pos	S-Furanopetasitin	91287	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		36.6	0	M+NH4, M+Na, M+H-H2O	C24H32O5S	4.464615753	82446.05389	79668.29895	82572.84638	84409.46819	85853.82978	80312.48913	93137.69914	90609.23225	92071.0009
5.74_312.2070m/z	312.2070303	5.790983333	pos	Cichoriine	3422	Unclassified	Unclassified	Unclassified			36.6	0	M+NH4	C19H22O9	0.020957406	4609.987151	3728.641669	5439.486169	9489.493543	7835.756686	8523.928407	4850.822207	6380.150433	5917.695591
5.93_201.1635m/z	201.1634858	5.933983333	pos	Furanoeremophilane	HMDB0035835	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*	C09685	36.6	0	M+H-H2O	C15H22O	-1.335232565	327.3803505	431.9813965	535.6504215	96.42305249	104.7892822	150.3258311	336.0438308	376.4993479	357.0518185
6.00_290.1781m/z	290.1780765	5.995733333	pos	ibopamine	96171	Benzenoids	Benzene and substituted derivatives	Phenol esters			36.6	0	M+H-H2O	C17H25NO4	9.787476972	7683.722743	8264.085451	8560.370984	10991.94293	11513.7621	11935.55863	5724.504271	6074.050766	5985.934283
6.22_307.1624m/z	307.1623976	6.216316667	pos	Citalopram	1781	Benzenoids	Benzene and substituted derivatives	Phenylbutylamines	**	C07572	36.6	0	M+H-H2O	C20H21FN2O	5.843827026	9056.944239	9516.365305	8834.577702	13149.21453	12986.41197	13615.80695	7475.380337	9113.20359	8564.639016
6.32_529.2614m/z	529.2614431	6.323133333	pos	Verruculogen	73523	Unclassified	Unclassified	Unclassified			36.6	0	M+NH4	C27H33N3O7	-8.279778253	8942.679487	11855.48294	12508.17169	8308.739266	8110.025173	7538.2163	10300.5913	11915.66117	12666.58211
6.36_431.1884m/z	431.1884046	6.355166667	pos	Tiospirium	85343	Benzenoids	Benzene and substituted derivatives	Diphenylmethanes			36.6	0	M+K	C25H30NO3+	6.826861778	5803.03796	7159.182214	7661.483141	8839.099484	8552.829295	7088.262039	5960.220035	8385.563149	7437.224785
6.38_459.1778m/z	459.1778105	6.3814	pos	2'-O-Methylcajanone	HMDB0033806	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavans	*		36.6	0	M+Na	C26H28O6	0.002813407	5096.985898	4146.085907	5285.485524	5717.177517	5774.611163	5085.379465	3018.746077	4481.640659	3388.441035
6.47_457.2037m/z	457.2036869	6.466083333	pos	Sildenafil	HMDB0005039	Benzenoids	Benzene and substituted derivatives	Benzenesulfonamides		C07259	36.6	0	M+H-H2O	C22H30N6O4S	4.324408486	23235.6995	25661.24644	20376.86212	21963.52491	21904.7182	24311.03194	40396.62896	42636.00256	31696.82373
6.64_347.2302m/z	347.2301643	6.638433333	pos	13-(2-Methylcrotonoyl)oxylupanine	64459	Unclassified	Unclassified	Unclassified			36.6	0	M+H	C20H30N2O3	-7.957099786	2763.728263	3978.890508	676.6253628	1401.275593	5947.115179	3033.912177	1511.271765	1508.170184	2398.040282
6.69_457.2038m/z	457.2037716	6.690566667	pos	Delavirdine	HMDB0014843	Organoheterocyclic compounds	Tetrapyrroles and derivatives	Porphyrins		C06941	36.6	0	M+H	C22H28N6O3S	4.680882493	6682.308793	6951.962104	6754.103453	7164.393233	6702.649854	7875.224761	9161.348512	11148.58259	10094.50262
7.10_485.2351m/z	485.2350616	7.1021	pos	3-Oxo-alpha-ionol 9-[apiosyl-(1->6)-glucoside]	95150	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		36.6	0	M+NH4	C24H38O11	-6.097109058	5593.22715	8154.548866	8240.072801	8408.983806	8231.449964	7416.911483	7933.906862	8740.546576	7659.470636
7.70_320.1888m/z	320.1888741	7.699383333	pos	3,6-Didehydroyohimban-7-ol	86189	Alkaloids and derivatives	Alkaloids and derivatives	Tropane alkaloids	*		36.6	0	M+H	C18H21NO3	9.60710284	1902.127572	1133.970433	1361.000149	2090.72037	1563.640731	2069.630122	969.6243789	1394.694053	1395.342266
8.03_217.1584m/z	217.1583724	8.031733333	pos	7-Hydroxycostal	HMDB0035202	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		36.6	0	M+H-H2O	C15H22O2	-1.363611874	651.2525544	430.6347832	369.3288904	316.8069355	397.1977751	339.6036746	473.1490803	369.9596376	421.6564776
8.45_266.1722

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5.74_587.2434m/z	587.2433551	5.743266667	pos	6-Hydroxysandoricin	92413	Organic acids and derivatives	Carboxylic acids and derivatives	Tetracarboxylic acids and derivatives	*		36.4	0	M+H-H2O	C31H40O12	-8.826351596	8219.496765	7995.228482	8554.92037	10481.37248	9950.913592	9212.732864	10040.99717	7561.691443	7553.200019
5.84_437.1777m/z	437.1777001	5.843716667	pos	Allopregnanolone sulfate	HMDB0240591	Lipids and lipid-like molecules	Steroids and steroid derivatives	Sulfated steroids			36.4	0	M+K	C21H34O5S	4.637708007	3893.423065	3704.721131	3861.21927	4330.303698	4194.403304	4028.106048	2604.266157	3853.971168	3841.984606
6.04_358.2583m/z	358.2582741	6.041083333	pos	p-Menth-3-ene-3-thiol	92928	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*		36.4	0	M+NH4	C20H36S2	-4.098850196	107737.877	112631.4039	108569.6869	131646.5667	135511.4512	135775.9206	102332.1306	114922.2592	113924.1457
6.23_176.0705m/z	176.0704601	6.22895	pos	3-Methylhippuric acid	34510	Organic acids and derivatives	Carboxylic acids and derivatives		*		36.4	0	M+H	C10H11NO3	-0.750272996	541.2073848	580.4650886	614.0822272	568.272036	613.6671444	738.8663659	622.7495321	643.7350391	649.3776656
6.29_201.0731m/z	201.0730516	6.287516667	pos	1,8-Octanedithiol	94862	Organosulfur compounds	Thiols	Alkylthiols			36.4	0	M+Na	C8H18S2	-6.522873313	594.5909084	818.3986449	649.4791959	876.7194779	941.1875689	941.9302197	965.6100359	516.1967211	968.4730371
6.47_293.1968m/z	293.1968101	6.466083333	pos	5-Hydroxyprimaquine	HMDB0246810	Unclassified	Unclassified	Unclassified			36.4	0	M+NH4	C15H21N3O2	-1.142961354	76.9539996	182.2820022	161.3070565	268.3324426	92.46918041	111.262849	92.35638817	136.6302282	58.23413041
6.52_269.1743m/z	269.1743952	6.523916667	pos	Coray PG-Lactone Diol	63037	Unclassified	Unclassified	Unclassified			36.4	0	M+H	C15H24O4	-1.590225283	332.5433631	398.2250653	316.4900661	254.2348923	347.0184275	310.3985701	376.0629905	319.8145359	213.408013
6.58_321.1674m/z	321.1674303	6.584266667	pos	Pipemidic acid	HMDB0041989	Organoheterocyclic compounds	Diazinanes	Piperazines			36.4	0	M+NH4	C14H17N5O3	1.534957116	603.0013227	563.6850185	666.2641559	993.5482672	991.0387301	858.5067014	506.3902258	525.2491258	591.2693866
6.81_257.1530m/z	257.1529563	6.810883333	pos	2-Polyprenyl-6-methoxy-1,4-benzoquinone	HMDB0060354	Lipids and lipid-like molecules	Prenol lipids	Quinone and hydroquinone lipids	**	C17560	36.4	0.965	M+H-H2O	C17H22O3	-2.371103756	1827.497006	1885.207375	2184.424294	3414.650197	3429.166265	2559.171894	1800.613369	1770.508999	2133.354879
6.90_157.0280m/z	157.0279943	6.8951	pos	4-Fluorocyclohexadiene-cis,cis-1,2-diol-1-carboxylate	71221	Unclassified	Unclassified	Unclassified			36.4	0	M+H-H2O	C7H7FO4	-8.931502597	506.3237346	323.1507313	471.4391266	598.8865398	543.3895204	540.1148088	554.9465397	611.9062989	466.0590823
6.91_373.2458m	356.2425423	6.909216667	pos	Curacin A	69157	Unclassified	Unclassified	Unclassified			36.4	0	M+H-H2O, M+K	C23H35NOS	5.076708685	31548.40144	34064.37919	36075.35434	71291.17275	60930.75018	61303.96894	24944.2288	30452.73196	30981.01271
6.92_505.2029m/z	505.2029056	6.919716667	pos	Quassimarin	67195	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*	C08777	36.4	0	M+NH4	C26H34O11	-7.502746996	2730.023905	2805.793196	1989.463442	3098.60873	1772.168448	1885.441882	1987.850109	3558.513044	3108.324428
7.11_321.1779m/z	321.1778595	7.108583333	pos	Scopolamine	3433	Organic acids and derivatives	Hydroxy acids and derivatives	Beta hydroxy acids and derivatives	**	C01851	36.4	0	M+NH4	C17H21NO4	-9.975929241	447.724237	1019.529111	956.9516272	2607.223919	2642.044083	2845.705866	1022.067127	1123.307218	1175.194938
7.55_602.3526m/z	602.3525941	7.553266667	pos	Caracurine V	67427	Unclassified	Unclassified	Unclassified			36.4	0	M+NH4	C38H40N4O2	6.232941766	6669.422955	6358.070716	6209.258251	469.0465515	366.9685342	574.1495342	1725.68705	1998.56654	2121.710689
9.16_403.2319m/z	403.231913	9.158516667	pos	AL 8810	45689	Unclassified	Unclassified	Unclassified			36.4	0	M+H	C24H31FO4	9.941909898	6565.142072	6051.111478	7103.365807	6940.49096	6450.859697	8872.750494	7567.921751	6152.403427	6268.5345
9.39_563.3757m/z	563.3756525	9.386383333	pos	PA(12:0/14:1(9Z))	81210	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphates			36.4	0	M+H	C29H55O8P	8.750048648	135.6949917	0.001403199	23325.51108	0.001403199	0.001403199	0.001403199	645.6880341	0.001403199	
9.68_211.0099m/z	211.0098528	9.680983333	pos	Dimethipin	72495	Unclassified	Unclassified	Unclassified			36.4	0	M+H	C6H10O4S2	2.502895925	2156.833215	1804.22452	2623.583154	2033.303286	2855.181621	2515.031872	2845.174305	2219.794558	2816.411623
9.85_250.1773m/z	250.1773405	9.848266667	pos	Piperazine adipate	69714	Unclassified	Unclassified	Unclassified			36.4	0	M+NH4	C10H20N2O4	5.202964807	1382.303968	940.5761334	1174.243613	1200.0057	1418.962457	1250.161375	1380.889777	1116.717068	1053.932146
9.93_494.1434m	517.1357427	9.9276	pos	4'-O-methyl-(-)-epicatechin-3'-O-beta-glucuronide	HMDB0029180	Phenylpropanoids and polyketides	Flavonoids		*		36.4	0	M+H, M+Na	C23H26O12	2.031737761	8490.018867	5325.942449	9756.61891	12454.1158	5993.143504	5277.312476	5675.703695	9647.158954	9844.341181
0.54_355.0692m/z	355.069227	0.535	pos	2-O-Caffeoylglucarate	65895	Unclassified	Unclassified	Unclassified			36.3	0	M+H-H2O	C15H16O11	8.745498913	6932.469148	461.455142	96.42145547	2887.107777	161.1137767	1399.974335	111.6440893	401.1699983	1130.642506
0.62_115.0588m/z	115.0587885	0.616683333	pos	4-Mercapto-4-methyl-2-pentanone	87734	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		36.3	0	M+H-H2O	C6H12OS	9.016988422	945.4741265	485.1557639	828.741407	1383.822111	858.9739999	935.1697939	1236.057266	1323.399133	816.2732131
0.64_123.0484m/z	123.0483746	0.63615	pos	THIODIGLYCOL	43814	Organosulfur compounds	Thioethers	Dialkylthioethers	*		36.3	0	M+H	C4H10O2S	7.76462834	7267.849365	8023.301223	6461.998258	3747.746838	3537.693615	3768.469642	7375.980657	4574.985652	8267.029749
0.66_202.9965m/z	202.9965053	0.657416667	pos	R-1-Propenyl 1-propanesulfinothioate	HMDB0032748	Unclassified	Organic acids and derivatives	Thiosulfinic acid esters			36.3	0	M+K	C6H10OS2	2.379078798	646.0292727	276.1764645	307.5538926	296.6832985	120.6142244	185.0334745	263.2149143	225.8206711	277.9265059
0.74_288.1185m/z	288.1185066	0.73955	pos	N(alpha)-Benzyloxycarbonyl-L-leucine	66165	Unclassified	Unclassified	Unclassified			36.4	0	M+NH4	C14H19NO4	-8.004191075	3132.537678	3179.843926	3525.418362	4379.472536	4373.820663	4397.303495	3789.03178	3707.029943	2772.182528
0.86_119.0161m/z	119.0161242	0.859583333	pos	3-Hydroxysulfolane	653	Unclassified	Unclassified	Unclassified			36.3	0	M+H-H2O	C4H8O3S	-0.01932933	179.8546254	365.2015372	363.0818194	331.5217146	530.2561189	410.4716653	370.8194367	365.0608591	518.496054
0.90_269.2107m/z	269.2107159	0.898483333	pos	9-hydroxy-16-oxo-hexadecanoic acid	74929	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			36.3	0	M+H-H2O	C16H30O4	-1.415894615	1156.047133	1179.89702	1304.84944	1093.547747	1174.84746	980.7773331	1417.673887	1120.94664	1076.153425
0.94_168.9823m/z	168.9822745	0.941583333	pos	3-Methyl-2-thiohydantoin	1188	Unclassified	Unclassified	Unclassified			36.3	0	M+K	C4H6N2OS	-7.440059408	252.7648009	328.6210389	328.5787709	345.9612928	316.7410955	315.8634325	298.9732369	271.6897945	428.7650202
0.98_174.9685m/z	174.9684711	0.98445	pos	3-Sulfinylpyruvic acid	6222	Organic acids and derivatives	Keto acids and derivatives	Alpha-keto acids and derivatives	**	C05527	36.3	0	M+Na	C3H4O5S	8.594474172	135.3359813	120.5833707	196.784788	176.8880544	0.001403199	0.001403199	120.8325706	122.7487301	112.1462245	182.3392334
1.22_241.2156m/z	241.2156099	1.22075	pos	9-Pentadecenoic acid	HMDB0029765	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		36.3	0	M+H	C15H28O2	-2.483977665	1074.887005	868.965768	512.3280818	719.621674	654.584803	814.2502346	962.9428136	688.5176935	1041.349956
1.92_217.0948n	240.0838296	1.916533333	pos	1-Isothiocyanato-8-(methylthio)octane	HMDB0038447	Organosulfur compounds	Isothiocyanates	Unclassified			36.3	0	M+H-H2O, M+Na, M+H	C10H19NS2	-4.800609034	18460.90841	19261.45855	19357.60532	20999.91575	19286.56398	20019.22635	17367.90621	19229.89676	18412.83271
10.00_288.2529m/z	288.2529276	10.00346667	pos	8-keto palmitic acid	35749	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		36.3	0	M+NH4	C16H30O3	-1.453585047	1009.590165	71.05386825	276.8849799	293.1557548	127.3633341	137.4999302	365.4722922	424.5069695	62.62910509
10.06_307.2245m/z	307.2245401	10.06391667	pos	Muricatacin	93340	Lipids and lipid-like molecules	Fatty Acyls	Fatty alcohols	*		36.3	0	M+Na	C17H32O3	0.614139368	249.1518193	360.6567614	70.51313705	314.2710373	154.4640324	372.4988294	133.9746396	262.2860851	66.15039316
11.17_284.2581m/z	284.2581461	11.17076667	pos	Methyl 2E,4Z-hexadecadienoate	HMDB0031050	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		36.3	0	M+NH4	C17H30O2	-0.975259616	889.3924025	1079.024439	761.4629125	804.9100283	732.1575759	624.6845145	883.8040691	864.0537643	784.7899087
11.78_786.5977m/z	786.5977052	11.49356667	pos	PC(18:1(9Z)/18:1(9Z))	HMDB0000593	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	*		36.3	0	M+H	C44H84NO8P	-3.737945258	7992.061509	5835.091998	5779.252839	3750.981534	3389.782485	5795.263495	5772.99938	5180.661798	5205.263565
11.72_762.5985m/z	762.5985109	11.71891667	pos	PA(24:1(15Z)/15:0)	HMDB0115457	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphates			36.3	0	M+NH4	C42H81O8P	-2.98264401	57720.88632	39281.37906	24556.00369	6525.155477	5624.408842	4166.668642	18422.00467	13182.79581	9822.423187
11.96_322.0773m/z	322.0773047	11.96068333	pos	Thymidine 3,5-cyclic monophosphate	6330	Unclassified	Unclassified	Unclassified			36.3	0	M+NH4	C10H13N2O7P	-8.413922032	50092.19856	719.2942551	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199
12.79_838.5555m/z	838.5555317	12.78523333	pos	PS(16:0/22:2(13Z,16Z))	LMGP03010200	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoserines	*		36.3	0	M+Na	C44H82NO10P	-1.622743001	6038.29199	5044.362404	4201.432868	2136.892928	1466.77538	795.8804981	3824.970939	2085.545589	1723.804872
14.91_457.3493m/z	457.3493282	14.9076	pos	Citranaxanthin	91883	Lipids and lipid-like molecules	Prenol lipids	Triterpenoids	*		36.3	0	M+H	C33H44O	6.214093555	7793.696908	6863.898941	5929.962513	7557.544376	5291.572934	6810.048981	8332.497066	7171.517893	6508.381186
14.95_845.7572m/z	845.7572571	14.95311667	pos	PE(15:0/18:2(9Z,12Z))	HMDB0011703	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoethanolamines	*		36.3	0	M+H	C41H76O10P	-2.379659906	61974.44901	25235.33925	27766.102	9805.059106	8534.847058	15513.24931	19627.15048	43622.84877	
2.79_128.0192m/z	128.0191981	2.79025	pos	S-Methyl methanesulfinothioate	88666	Organic acids and derivatives	Thiosulfinic acid esters	Thiosulfinic acid esters			36.3	0	M+NH4	C2H6OS2	-5.766609724	152.7962459	202.709304	153.574203	284.7741929	169.9213073	232.8302226	266.9943668	199.0831594	220.368233
3.11_255.0423m/z	255.0422537	3.112683333	pos	(Z)-6-(2-Methoxyvinyl)-7-methyl-2H-1-benzopyran-2-one	88597	Phenylpropanoids and polyketides	Coumarins and derivatives	Unclassified	*		36.3	0	M+K	C13H12O3	2.088826186	1530.332211	1788.222511	1642.670429	2323.992063	2431.17973	2276.757359	1521.493372	2083.085258	1575.443519
3.14_130.1225m/z	130.1225206	3.139516667	pos	5-Methyl-3-hexen-2-one	87758	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		36.3	0	M+NH4	C7H12O	-1.069964558	168.1382593	159.6168211	85.02333308	115.48937	143.3247615	120.1456372	142.2911129	108.2245575	144.5099584
3.48_175.1115m/z	175.1115342	3.48465	pos	11,12,13-Trinor-1(10)-spirovetivene-2,7-dione	HMDB0036734	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		36.3	0	M+H	C12H16O2	-1.079080218	578.3312701	850.424865	701.0684427	490.9957195	416.6677368	532.0453732	638.0367395	621.5528885	621.93259
3.69_181.0859m/z	181.085917	3.6941	pos	Benzaldehyde glyceryl acetal	88243	Organoheterocyclic compounds	Dioxanes	1,3-dioxanes	*		36.3	0	M+H	C10H12O3	-0.020423286	682.3700989	452.9129361	658.000647	712.3784503	615.2958403	578.3718631	530.2333041	447.2343242	419.6661681
3.85_246.0778m/z	246.0077815	3.845583333	pos	Benzthiamine	72806	Unclassified	Unclassified	Unclassified			36.3	0	M+NH4	C9H9N3OS	-9.705760427	10782.5688	9839.186901	9437.357783	11531.18726	9543.453863	10072.85207	9932.319179	15133.77877	
3.89_257.1358m/z	257.1358356	3.889633333	pos	Glutamyl-Lysine	85738	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		36.3	0	M+H-H2O	C11H20N3O5-	-4.274794526	459.5042622	472.5410047	449.8951652	506.5735463	270.482075	254.1990829	405.5437315	473.5604113	373.7850471
3.91_342.0862m/z	342.08623	3.911966667	pos	Ibandronate	85416	Organic acids and derivatives	Organic phosphonic acids and derivatives	Bisphosphonates			36.3	0	M+Na	C9H23NO7P2	6.374191627	1348.979153	1000.50153	1602.53223	1956.745602	2358.922262	2411.836057	1839.881634	1853.586693	1916.640894
3.96_303.0947m/z	303.0947246	3.956866667	pos	Prothoate	72765	Unclassified	Unclassified	Unclassified			36.3	0	M+NH4	C9H20NO3PS2	-4.641166456	905.9365604	1691.715692	1330.435052	2017.944606	1565.652565	1712.407683	1100.744135	1339.197848	991.8474836
4.00_193.0836m/z	193.0835934	4.002016667	pos	2-amino-3-oxo-hexanedioic acid	35946	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		C05520	36.3	0	M+NH4	C6H9NO5	9.685528503	187.5553315	197.9375434	164.9236116	148.0057686	194.5708467	137.1754035	218.2936659	171.780028	104.6342478
4.05_246.1593m/z	246.1593559	4.046633333	pos	Metyrapone	HMDB0060605	Organoheterocyclic compounds	Pyridines and derivatives	Unclassified	*		36.3	0	M+NH4	C14H16N2O	-3.21228218	352.7735262	230.581445	347.6097311	481.0883833	589.5102082	641.5103497	429.7114925	439.7416299	388.1981392
4.20_264.1260m/z	264.1260293	4.204866667	pos	7-Mercaptoheptanoylthreonine	71251	Unclassified	Unclassified	Unclassified			36.3	0	M+H	C11H21NO4S	-1.430225161	799.8401652	335.1675725	735.0760558	912.8898679	801.2713075	325.3140306	569.7243136	661.3845367	504.8608132
4.63_351.1519m/z	351.1519325	4.63335	pos	N-Desmethyleletriptan	85306	Organoheterocyclic compounds	Indoles and derivatives	Indoles	*		36.3	0	M+H-H2O	C21H24N2O2S	-1.706567586	453.6374189	702.9273756	1002.410115	2164.994485	2496.342376	2324.195819	1360.531515	1145.531266	1081.158355
4.66_260.1368n	261.1440291	4.656183333	pos	Leucyl-Glutamate	HMDB0028928	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		36.3	0	M+H, M+Na	C11H20N2O5	-1.803356024	4323.458415	4657.83748	4658.920522	607.441408	637.0532679	814.9226226	837.8482769	981.3197394	1073.649713
4.84_209.0575m/z	209.0574653	4.836966667	pos	Isorhamnetin	HMDB0002655	Phenylpropanoids and polyketides	Flavonoids	Flavones	***	C10084	36.3	0	M+H-H2O	C16H12O7	7.754426893	135.2759565	396.2688749	425.3512448	733.9744328	1094.232104	781.4913391	205.0780121	454.8144732	371.767931
5.04_306.1161m/z	306.1160869	5.035783333	pos	Histidinyl-Glutamine	85789	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		36.3	0	M+Na	C11H17N5O4	-4.195455111	191.0901937	83.25379539	112.6138237	175.2048244	150.7247114	196.2190371	61.96349894	134.5922563	73.8949888
5.42_288.1259m/z	288.1258976	5.419283333	pos	Lycorine	43822	Unclassified	Unclassified	Unclassified	*		36.3	0	M+NH4	C16H17NO4	9.972168081	2879.97914	3215.34334	3737.882567	3375.10043	3284.415817	3104.505207	2194.720978	2628.282863	2644.603678
5.52_482.3110m/z	482.3109784	5.5209	pos	HEPC	44943	Unclassified	Unclassified	Unclassified			36.3	0	M+H	C23H48NO5PS	9.600438374	3087.227592	3707.620181	3040.74497	681.8305006	802.7579195	673.3864969	1999.966442	1633.211989	1728.70646
6.00_249.1845m/z	249.1844776	5.995733333	pos	5-Pentyl-2-furanheptanoic acid	HMDB0112092	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates			36.3	0	M+H-H2O	C16H26O3	-1.610929333	574.0824841	587.545311	579.8457397	455.0892832	599.1803029	560.5067941	514.2277115	517.913035	581.1529097
7.06_284.2216m/z	284.2215933	7.060866667	pos	Juvabione	67888	Unclassified	Unclassified	Unclassified			36.3	0	M+NH4	C16H26O3	-1.603863247	80.03523842	130.9319537	189.1816919	97.46940207	156.3818239	123.5533115	223.4566997	232.4400825	149.6038743
7.20_547.2671m/z	547.2670987	7.20385	pos	PKHdiA-PA	LMGP20070012	Lipids and lipid-like molecules	Glycerophospholipids	Oxidized glycerophospholipids			36.3	0	M+H-H2O	C26H45O11P	0.776372793	2526.351421	2501.592767	2819.155178	1330.705523	1066.320299	1422.691944	985.7605616	636.8730888	1583.400891
7.46_462.1959m/z	462.1959376	7.414583333	pos	Rutilocarpine	66746	Unclassified	Unclassified	Unclassified	*		36.3	0	M+H	C28H27NO4	8.758308841	4219.146095	3009.663238	3853.617989	2129.146095	3009.663238	3853.617989	2129.146095	1413.702716	2223.914118
7.82_335.1932m/z	335.193209	7.817466667	pos	Fortimicin KL1	71969	Unclassified	Unclassified	Unclassified			36.3	0	M+H-H2O	C13H28N4O7	1.981701649	1049.099438	874.5871416	895.4880792	716.4544308	1128.574926	1114.281327	808.4670779	790.6683937	859.6105044
7.92_533.2333m/z	533.2332938	7.915266667	pos	2',4',6',3,4-Pentahydroxy-3'-geranyl-5-prenyldihydrochalcone	52334	Unclassified	Unclassified	Unclassified			36.3	0	M+K	C30H38O6	6.669986987	1841.872972	1930.047626	2027.380194	2284.512801	2485.830188	2214.497424	1594.520977	1951.840626	1207.338712
7.93_511.2501m/z	511.2501044	7.927683333	pos	Coccinin	93219	Unclassified	Unclassified	Unclassified			36.3	0	M+H-H2O	C26H40O11	-6.946341188	21201.16142	20539.66618	20735.03604	27829.06058	23090.80286	23608.95151	18740.86963	23232.42678	19061.40898
7.97_269.2471m/z	269.2470636	7.9736	pos	10Z-Heptadecenoic acid	HMDB0060038	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	***		36.3	0	M+H	C17H32O2	-1.651744576	551.5388047	401.7266537	387.8212357	438.0205032	401.2704491	307.7367887	559.7170212	525.1253157	325.1575565
8.41_157.0279m/z	157.0279148	8.405166667	pos	4-Fluorocyclohexadiene-cis,cis-1,2-diol-1-carboxylate	71222	Unclassified	Unclassified	Unclassified	*		36.3	0	M+H-H2O	C7H7FO4	-9.388331107	2091.484208	2219.146095	222.0570140	125.4140708	208.5482288	194.434545	229.9984464	165.7654832	220.2232314
8.60_535.2481m/z	535.2481413	8.602816667	pos	Anabsinthin	91552	Lipids and lipid-like molecules	Prenol lipids	Sesterterpenoids	*		36.3	0	M+K	C30H40O6	5.0258807	6125.884835	6721.59339	8915.838222	8781.27585	9681.430942	8614.772072	7569.479662	7814.149482	7932.515853
9.73_195.0197m/z	195.0196673	9.72875	pos	1-Naphthaldehyde	2757	Benzenoids	Naphthalenes			C14090	36.3	0	M+K	C11H8O	-6.444019988	2096.000615	2530.15396	1906.593367	1845.886582	2138.103752	1307.148847	1582.521405	2016.795752	2083.676835
0.51_214.1584m/z	214.1583955	0.51135	pos	Lactarazulene	HMDB0038162	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		36.2	0	M+NH4	C15H16	-3.214899668	428.3663153	314.4732565	412.6218294	493.5024687	361.0685429	550.8459793	387.7305676	555.172544	503.7833788
0.56_153.0107m/z	153.0106766	0.555633333	pos	Thiourocaic acid	63494	Unclassified	Unclassified	Unclassified			36.2	0	M+H-H2O	C6H6N2O2S	-6.079224359	12841.492	12789.20128	11946.96882	12063.9845	9063.748581	12032.85474	10417.1888	11604.95621	10698.99402
0.62_164.0665m/z	164.0665451	0.616683333	pos	3-Oxo-3-ureidopropanoate	63408	Unclassified	Unclassified	Unclassified			36.2	0	M+NH4	C4H6N2O4	-0.254269272	189711.5593	186409.1968	188956.4032	237649.4366	236723.9919	231167.1445	246728.72	254798.22	260629.4367
0.64_209.0515m/z	209.0515407	0.63615	pos	AMPA	69625	Unclassified	Unclassified	Unclassified			36.2	0	M+Na	C7H10N3O4	-9.334354616	3160.371111	1532.370399	2457.937759	2935.979129	2611.800609	2813.047309	2978.472263	2319.003201	
0.78_306.0613m/z	306.0612856	0.776966667	pos	3-Hydroxy-7-aminonitrazepam	1562	Unclassified	Unclassified	Unclassified			36.2	0	M+K	C15H13N3O2	-9.918149859	2612.571304	5695.397082	10750.40903	2486.403014	2537.210103	2182.236335	5909.083447	7128.857155	5754.790888
0.82_134.1174m/z	134.1173682	0.818116667	pos	Methyl pentanoate	87495	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		36.2	0	M+NH4	C6H12O2	-1.610800786	541.4286288	324.8578402	445.9346676	686.9524096	601.5662333	646.98846	610.9826209	455.7130631	450.7023391
0.84_223.1052n	224.1125247	0.8386	pos	Tiletamine	43352	Unclassified	Unclassified	Unclassified			36.2	5.4	M+H, M+Na, M+H-H2O	C12H17NOS	9.695462738	18905.29071	20511.31522	20419.81548	26466.28837	24979.43638	25184.25063	19826.7438	20685.85252	19160.21432
1.16_346.1239m/z	346.1239114	1.157483333	pos	GSK264220A	45429	Unclassified	Unclassified	Unclassified			36.2	0	M+H-H2O	C17H21N3O4S	5.294392219	26401.93214	22832.41497	23056.94442	25760.68662	21399.14067	22173.09171	21927.69075	24826.32915	20941.38688
1.24_188.0540m/z	188.0540417	1.243033333	pos	2-(Acetamidomethylene)succinate	63871	Unclassified	Unclassified	Unclassified			36.2	0	M+K	C7H9NO5	6.987901991	5062.440645	6037.776145	5055.832266	5304.487389	4937.991834	5355.509548	5291.963746	5728.661165	6051.897701
1.37_270.0946m/z	270.0945524	1.372666667	pos	Glycyl-Arginine	85748	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		36.2	0	M+K	C8H17N5O3	-7.550413799	915.2185359	1486.277474	1435.170422	840.2810041	655.0875428	733.4520066	403.5596593	574.8197133	834.0035731
1.52_275.1097m/z	275.1096763	1.52285	pos	Gamma-glutamyl-Glutamate	86040	Unclassified	Unclassified	Unclassified			36.2	0	M+H	C10H16N3O6-	-5.510273639	1683.32113	1585.288252	1779.794607	1375.503932	1215.814365	1203.727375	1091.189221	1195.326549	1301.68651
1.57_190.0448m/z	190.0448073	1.56695	pos	Tricyclazole	72298	Organoheterocyclic compounds	Benzothiazoles	Triazolobenzothiazoles	*	C18492	36.2	1.62	M+H	C9H7N3S	7.737372319	3957.0146	4387.89705	4577.634085	4084.52101	3963.769641	3948.554834	4316.063214	4719.004817	3968.245111
10.14_195.0197m/z	195.0196618	10.14475	pos	2-Naphthaldehyde	69794	Benzenoids	Naphthalenes			C14099	36.2	0	M+K	C11H8O	-6.479153853	32340.00303	29388.41634	28980.42438	28641.69292	31088.98884	30044.87173	30227.21345	29781.15825	30412.15669
10.33_332.2191m/z	332.2190643	10.32878333	pos	Kathweol	90878	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*	C09893	36.2	0	M+NH4	C20H26O3	-9.408100445	10605.15969	10583.17335	10090.6894	11327.40839	10611.79126	11826.21421	12185.00984	11645.31288	12479.73926
10.84_285.2421m/z	285.2421251	10.8369	pos	MG(0:0/14:1(9Z):0/0:0)	62314	Lipids and lipid-like molecules	Glycerolipids	Monoradylglycerols	*		36.2	0	M+H	C17H34O4	-9.980068927	411.3276015	1.403705	15.82401515	19.30358288	13.90550773	437.9509714	321.330978	324.4213122	315.6117259
11.00_760.5838m/z	760.583823	11.00186667	pos	PC(16:0/18:1(11Z))	LMGP01010576	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	*		36.2	0	M+H	C42H82NO8P	-1.657059667	19884.66005	17510.32019	12820.8552	12659.39586	10579.17468	7244.052802	15223.42371	13385.80366	10528.5554
11.49_269.2

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5.33_157.0759m/z	157.0758574	5.329033333	pos	WR 1065	66703	Unclassified	Unclassified	Unclassified			36	0	M+Na	C5H14N2S	-8.44737869	1181.530292	951.4484023	915.8151509	577.7449858	671.2241944	599.0726435	808.0719784	710.4341431	722.863263
5.40_455.1882m/z	455.1881933	5.396716667	pos	Nalbuphine-6-sulfate	1405	Unclassified	Unclassified	Unclassified			36	0	M+NH4	C21H27NO7S	8.108357261	35430.47038	37835.81419	41446.21748	37746.48755	34574.3429	36918.78928	32616.58668	34312.22075	34437.72714
5.52_271.1531m/z	271.1530757	5.5209	pos	Asparaginyl-Arginine	85640	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		36	0	M+H-H2O	C10H20N6O4	6.110773919	355.6349233	512.2724665	408.6635796	297.3915363	279.5347164	278.0127043	338.1014451	421.124892	380.1240377
5.77_303.0633m/z	303.0633189	5.7661	pos	3-methylflavone-8-carboxylic acid	LMPK12113395	Lipids and lipid-like molecules	Polyketides	Flavonoids			36	0	M+Na	C17H12O4	1.925875154	213.1040312	235.764933	283.4428623	72.86856895	37.47597633	163.0301389	238.9607684	169.0949869	303.2303152
5.91_420.1858m/z	420.1857581	5.9112	pos	PYRVINIUM	44259	Organoheterocyclic compounds	Pyrroles	Substituted pyrroles		C07412	36	0	M+K	C26H27N3	5.514111286	3760.005752	4133.243062	4410.475615	1242.964639	1292.466656	1456.199222	2198.115603	2636.102506	2710.400707
6.20_353.1001m/z	353.1000967	6.1979	pos	beta-nicotinamide D-ribonucleotide	96248	Nucleosides, nucleotides, and analogues	Pyridine nucleotides	Nicotinamide nucleotides	**	C00455	36	0	M+NH4	C11H16N2O8P+	5.503669894	314.7639371	411.395143	443.206745	622.4322968	466.3278699	543.656237	371.3437287	326.6800747	290.0078435
6.23_411.1621m/z	411.162063	6.22895	pos	Trifluadom	69227	Unclassified	Unclassified	Unclassified			36	0	M+NH4	C22H20FN3O5	-7.310528616	12259.24722	13078.37679	12587.35079	14645.46974	13926.45253	15010.64239	8983.451107	11232.28581	11229.41366
6.47_452.2484m/z	452.248436	6.466083333	pos	DEXAMETHASONE ACETATE	44164	Lipids and lipid-like molecules	Steroids and steroid derivatives	Hydroxysteroids		C15643	36	0	M+NH4	C24H31FO6	9.542684639	3008.810813	3452.515243	2797.415378	2785.426337	2745.612752	3289.890374	6279.715917	6183.29761	4750.471162
6.71_389.2504m/z	389.2504405	6.709016667	pos	Nandrolone phenpropionate	66836	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid esters		C08155	36	0	M+H-H2O	C27H34O3	7.221673136	2216.997876	2463.384686	28196.76279	1712.076438	393.5013869	714.4597803	380.2966415	2396.746499	674.6770029
6.81_203.1429m/z	203.1428566	6.810883333	pos	Dictagymnin	HMDB0039274	Benzenoids	Phenol ethers	Unclassified			36	0	M+H	C14H18O	-0.915126442	2006.629121	2000.784482	1953.855926	1802.308912	1867.157016	1684.757142	2058.818527	1742.328698	2161.402845
6.90_389.2186m/z	389.2186352	6.8951	pos	methyl 9,12,13,15-bisepidioxy-16-hydroperoxy-10-octadecenoate	74483	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			36	0	M+H	C19H32O8	4.226553858	3730.656044	628.4504433	12788.63898	1154.877913	1191.590157	822.7988653	758.2171774	1072.060025	2136.887958
6.96_366.2245m/z	366.2244626	6.959933333	pos	Gibberellin A112	88116	Lipids and lipid-like molecules	Prenol lipids	Diterpenoids	*		36	0	M+NH4	C20H28O5	-8.721867693	2626.213104	2295.321928	2728.324626	2502.961283	2458.495245	2801.651596	2466.95458	2874.848792	3173.302973
7.00_163.0643m/z	163.0643374	7.0043	pos	1,10-Phenanthroline	65523	Unclassified	Unclassified	Unclassified			36	0	M+H-H2O	C12H8N2	-6.234460801	307.84082	109.1085983	96.80086201	76.56075784	51.76329835	15.45774993	44.30258749	32.65506458	107.2679975
7.29_214.1798m/z	214.179822	7.294266667	pos	Allyl 3-cyclohexylpropionate	LMFA07010775	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*	C12306	36	0	M+NH4	C12H20O2	-1.699632568	401.0626152	661.9394861	327.002897	534.8754603	256.1046135	498.1978121	464.4159394	494.424221	507.8327326
7.96_210.1616n	228.1955381	7.9616	pos	Octahydro-2,5,5,8a-tetramethyl-7H-1-benzopyran-7-one	94763	Organoheterocyclic compounds	Benzopyrans	Unclassified			36	0	M+H, M+NH4	C13H22O2	-1.607721924	6760.60804	5279.815753	5534.144235	5958.71385	5919.964176	5596.985323	6971.346957	5968.222833	5694.396257
0.51_106.0530n	124.0867105	0.51135	pos													9771.813385	36300.1073	14260.10611	21461.25213	7325.280995	27942.54072	38849.09713	14922.37728	19407.82987
0.51_111.0665m/z	111.0665015	0.51135	pos													5.301236603	55.4235364	32.41218006	10.88040751	12.2590216	48.10093304	17.4904727	45.92335922	86.69263948
0.51_120.9589m/z	121.9660464	0.51135	pos													5457.367623	4193.472859	4511.782962	3141.264745	2576.606789	2804.283718	4454.318893	4060.885555	4075.927251
0.51_122.9571n	123.9642452	0.51135	pos													2613.384527	2044.108341	2185.631363	1468.097509	1251.697564	1254.36163	2150.474658	1972.35331	2018.868014
0.51_125.0900m/z	125.0900393	0.51135	pos													613.2448331	2562.34749	920.6085503	1467.550215	472.9065485	1888.589671	2764.703808	909.4333222	1287.375493
0.51_126.1276m/z	126.1276471	0.51135	pos													157.6237829	441.2355864	276.1487632	259.0254349	188.9331032	451.4161035	552.7708391	433.4554963	737.6824217
0.51_134.0709m/z	134.0708775	0.51135	pos													80.15746868	488.985179	93.93797747	183.4328321	82.32360929	486.7596218	663.1806148	205.0212004	571.5330982
0.51_135.0793n	136.0865586	0.51135	pos													597.8647138	2177.516488	278.3846534	1171.277695	443.3781245	1811.578961	3812.949575	877.1434148	1691.28494
0.51_137.0587n	138.0657662	0.51135	pos													126.5718613	539.6128801	218.5211863	287.1292063	86.82214355	547.2378184	694.8935891	363.0172986	556.0761611
0.51_141.1382m/z	141.1381984	0.51135	pos													297.8058917	321.6541531	258.4123565	343.5050869	254.0550016	450.972961	352.5235725	377.8292653	516.925062
0.51_144.9771m/z	144.9771232	0.51135	pos													43.50552349	30.26880833	43.79722831	0.001403199	3.357245188	7.416261871	47.32690907	0.001403199	0.001403199
0.51_144.9819m/z	144.9818566	0.51135	pos													60931.25171	59309.10108	58807.26133	47124.41797	37732.1012	41276.76763	64774.48465	51845.4943	64375.26973
0.51_146.9800m/z	146.9799651	0.51135	pos													27592.27962	26549.1854	26315.78772	21455.39526	16873.04429	18853.70867	30282.22513	23097.49979	29727.41146
0.51_147.9770m/z	147.9770415	0.51135	pos													145.1769733	106.0525055	113.9541624	103.5686214	105.2249802	75.28875357	166.2251503	94.45582839	187.6328947
0.51_148.0897m/z	148.0897335	0.51135	pos													75.69843765	46.17341087	128.8973086	49.40465483	115.8595943	109.8054863	99.75431852	101.1688796	74.99334335
0.51_149.0739m/z	149.0739199	0.51135	pos													181.2580795	177.7407262	141.2160998	178.8901296	149.0922541	163.9440538	199.5120282	180.56607	155.0978018
0.51_149.0949n	150.1021434	0.51135	pos													1130.757467	4767.408148	1010.470948	2522.979539	857.1503266	3602.01021	7496.389964	2001.357285	3140.602412
0.51_151.1053m/z	151.1052508	0.51135	pos													30.3528966	127.8747119	31.42518721	69.63095016	12.84143872	87.44661086	204.1720141	48.81927681	79.73126281
0.51_152.0815m/z	152.0814671	0.51135	pos													87.4151861	214.3738741	188.8898956	176.9095742	93.98941744	374.5136253	315.113916	241.0703603	171.0844605
0.51_154.1334m/z	154.133436	0.51135	pos													130.3100871	356.6184515	39.18095875	173.6563787	90.5126736	306.5675027	683.9672475	136.7888754	216.7560552
0.51_155.1538m/z	155.1538291	0.51135	pos													1536.39357	1169.045548	1663.835687	1773.568722	939.8716389	1871.554044	1432.710373	1962.745454	1511.28147
0.51_163.1105n	164.117757	0.51135	pos													421.3370531	2148.645352	292.3135878	982.831631	356.431719	1510.151008	2941.60686	673.594391	1296.872003
0.51_165.0766m/z	165.0766311	0.51135	pos													67.46234949	220.5832817	141.593058	149.2315874	42.49085368	259.0341609	338.627594	217.3951464	139.1918791
0.51_175.1104n	193.1442782	0.51135	pos													323.0259882	1293.241767	310.6718512	672.1331797	285.8896896	985.7076555	2452.919326	618.2384357	1089.082042
0.51_176.1908n	199.1800248	0.51135	pos													2376.626992	2128.553211	2067.248617	2454.72009	1789.527097	2330.65106	2177.199031	2151.595517	2489.669304
0.51_177.1129m/z	177.1128863	0.51135	pos													406.244978	1514.974381	193.6617867	786.5457951	279.6248072	1031.502275	2355.367252	574.7487187	1004.210778
0.51_179.1165n	202.1080733	0.51135	pos													547.0579743	2542.921423	517.319865	1432.900857	420.0852261	1746.768665	3384.825065	1040.917976	1502.635036
0.51_179.1285m/z	179.1285284	0.51135	pos													231.6745342	838.780664	67.48455254	440.1057161	199.4234113	650.3328674	1669.308814	262.5438154	506.2706813
0.51_180.1006n	163.097313	0.51135	pos													615.2632159	3355.300559	543.4955829	1732.881414	317.7913231	2234.33946	4256.061344	1362.393833	1956.176484
0.51_185.1280m/z	185.1280143	0.51135	pos													147.7285448	274.2706739	280.261052	222.7089651	214.8833453	265.7457959	282.6857657	329.1469017	330.340709
0.51_187.1438m/z	187.1437806	0.51135	pos													89.1649653	177.0962451	104.478715	88.23773684	90.27584422	107.5987754	161.8213165	109.2153617	326.5809751
0.51_190.1002m/z	190.1001562	0.51135	pos													107.0349839	143.0417638	244.1170664	125.9749634	158.8293453	254.6804815	184.1281225	185.4230336	157.4801652
0.51_190.1213n	191.1285039	0.51135	pos													348.4014704	932.1781201	243.9118352	534.5466554	409.5941336	758.5028549	1624.824586	477.5166088	852.0653295
0.51_191.0844m/z	191.0844371	0.51135	pos													287.6517128	298.8186449	288.6488997	273.611683	188.8507772	332.7133696	365.7582165	368.2632476	271.7288601
0.51_196.0955n	179.0922205	0.51135	pos													682.5835434	3929.989445	863.4816439	2175.244391	642.664513	2641.051802	5746.708995	1557.047359	2177.176073
0.51_200.1833m/z	200.1833003	0.51135	pos													174.0497275	157.4267212	153.4773558	180.699331	104.6026623	154.0898955	123.505805	130.1791152	163.5562363
0.51_206.1394m/z	206.1394429	0.51135	pos													332.0485431	1266.08543	117.9084519	493.0353954	205.4407332	744.4996244	2108.339096	332.4237692	591.3974058
0.51_210.1484m/z	210.1483556	0.51135	pos													17.74101407	46.97526293	74.07266162	42.67997787	34.12581811	66.91061817	63.10876228	58.72558468	48.87175275
0.51_214.1080m/z	214.1080318	0.51135	pos													71.39944756	320.5452007	20.67827934	168.5677517	90.48162353	273.1183629	517.4848582	145.823488	275.9855078
0.51_220.1550m/z	220.1549793	0.51135	pos													201.2110491	860.283167	90.51591183	385.4214941	142.6115171	562.1146004	1370.467857	225.4636293	491.528766
0.51_224.1387m/z	224.1387345	0.51135	pos													103.2897326	203.0727535	154.5197747	173.5385795	101.5405438	198.8485873	272.2283451	138.5132486	152.7778578
0.51_232.1187m/z	232.118669	0.51135	pos													98.445686	193.0233606	29.98260392	141.5874902	68.90849462	128.031634	215.4893979	68.22431603	115.5547086
0.51_234.1707m/z	234.1706713	0.51135	pos													127.2912828	522.6532041	68.40126353	259.8870593	105.6303121	410.6259618	1030.213708	196.716865	308.6819353
0.51_236.0271m/z	236.0270949	0.51135	pos													2179.330301	1534.117928	1205.365371	1481.806729	1190.716189	689.5560481	1728.825235	1045.661778	1524.424535
0.51_242.1896m/z	242.1895831	0.51135	pos													125.0682279	77.06407109	115.5367206	133.1406662	102.2146088	143.7913175	93.78058925	117.5327918	133.495492
0.51_276.0376m/z	276.0375802	0.51135	pos													918.8249978	620.295965	415.9606378	437.8853	163.0582547	203.6796153	562.268047	402.9750605	530.1826842
0.51_965.2927m/z	965.2926589	0.51135	pos													0.001403199	0.001403199	117.958738	13.4895781	121.7687417	2365.065204	187.7237754	4188.72409	0.001403199
0.52_205.1443m/z	205.1442525	0.518183333	pos													0.001403199	0.001403199	13.16972184	0.001403199	0.001403199	9.52892189	414.5496565	79.54780647	116.8933068
0.52_448.1174m/z	448.1173906	0.518183333	pos													405.2837831	0.001403199	0.001403199	199.4794541	21.19188685	119.6752471	0.001403199	32.93731054	24.52887584
0.52_505.0859m/z	505.0859086	0.518183333	pos													1120.996634	357.7637671	46.64817412	12.84002756	0.001403199	0.001403199	39.42695473	0.001403199	21.40609263
0.53_1001.7173m/z	1001.717259	0.529666667	pos													0.001403199	0.001403199	498.6919262	0.001403199	854.2462468	629.7081234	1001.58002	515.1933378	710.2003997
0.53_1024.7348m/z	1024.734771	0.529666667	pos													0.001403199	0.001403199	891.8290913	0.001403199	737.8344634	1054.269837	1877.22218	919.8041487	0.001403199
0.53_1067.2492n	1068.256456	0.529666667	pos													0.001403199	0.001403199	3819.083453	0.001403199	2713.111055	2155.571232	3517.480365	2447.159116	0.001403199
0.53_1077.2622m/z	1077.262182	0.529666667	pos													277.1703543	0.001403199	6949.641159	0.001403199	517.2858253	662.18329	6513.205348	1624.825212	0.001403199
0.53_1089.7685n	1090.775821	0.529666667	pos													0.001403199	0.001403199	1064.895503	0.001403199	1324.404852	1603.269399	1722.60311	1784.001935	0.001403199
0.53_1118.1022m/z	1118.102179	0.529666667	pos													0.001403199	0.001403199	651.6849039	0.001403199	797.9579178	650.0309869	518.5290596	921.9454117	0.001403199
0.53_113.1074m/z	113.1074346	0.529666667	pos													82.12471303	286.8073044	65.50901928	132.5960525	101.4731005	250.7045419	394.9740964	116.9938394	413.6305116
0.53_1137.4527m/z	1137.45268	0.529666667	pos													0.001403199	0.001403199	1245.731693	0.001403199	1957.936905	1251.898049	678.3000838	2635.041252	0.001403199
0.53_1137.7865m/z	1137.786459	0.529666667	pos													0.001403199	153.2004769	1236.801289	0.001403199	1536.025757	1604.465693	832.0416649	1254.223694	0.001403199
0.53_1138.1214m/z	1138.121406	0.529666667	pos													0.001403199	0.001403199	543.9083072	64.2426854	945.9800287	2011.640267	883.1693613	813.1216736	0.001403199
0.53_1156.4655m/z	1156.465494	0.529666667	pos													0.001403199	0.001403199	598.0178648	0.001403199	249.1364727	652.4102246	0.001403199	511.7751881	0.001403199
0.53_1156.8035m/z	1156.803516	0.529666667	pos													0.001403199	0.001403199	1185.292183	103.3336114	1035.359343	1881.087893	467.240969	1549.335149	0.001403199
0.53_1157.1350m/z	1157.134986	0.529666667	pos													0.001403199	0.001403199	737.0633114	89.04090578	730.6917772	567.2724363	599.3145264	1609.465642	105.179478
0.53_1171.3146n	1194.336103	0.529666667	pos													0.001403199	0.001403199	1057.020141	2162.64153	2000.431543	1720.315876	3884.329551	1407.639692	3768.455116
0.53_136.0214m/z	136.0213797	0.529666667	pos													454.8127416	303.6191196	338.4554257	360.656204	807.4319544	650.7777351	773.3847585	334.0913365	407.0683705
0.53_532.3566m/z	532.3566161	0.529666667	pos													0.001403199	0.001403199	188.1762808	0.001403199	230.4709293	328.3281396	644.7449576	309.33853	0.001403199
0.53_719.5016m/z	719.501599	0.529666667	pos													0.001403199	0.001403199	412.3637905	0.001403199	485.0327338	431.3979811	1364.509222	229.5856575	2372.509778
0.53_734.5093m/z	734.5093375	0.529666667	pos													0.001403199	1125.490693	530.0179516	0.001403199	856.6278739	326.9459681	1252.796441	751.051734	1979.949062
0.53_764.1869m/z	764.1868767	0.529666667	pos													0.001403199	0.001403199	275.7725356	0.001403199	947.7003639	382.9713199	660.5036559	272.4393463	0.001403199
0.53_834.6164m/z	834.616432	0.529666667	pos													0.001403199	1655.831599	535.2072892	0.001403199	1217.517456	2211.811533	1297.273949	1303.564408	2039.180812
0.53_844.0750m/z	844.0749816	0.529666667	pos													0.001403199	0.001403199	1000.494264	0.001403199	704.5260021	928.3541934	1549.764681	1069.921631	1087.895245
0.53_844.3253m/z	844.3252894	0.529666667	pos													0.001403199	0.001403199	1183.026672	0.001403199	884.7971814	1134.115292	2325.287415	2074.748295	0.001403199
0.53_844.8263m/z	844.8262533	0.529666667	pos													0.001403199	0.001403199	1971.776929	0.001403199	0.001403199	710.624153	919.4994325	1567.840491	1164.482259
0.53_858.8350m/z	858.8349828	0.529666667	pos													0.001403199	0.001403199	2458.413468	0.001403199	2224.219196	3392.37525	3923.882087	2875.70831	3143.881942
0.53_859.0866m/z	859.0865783	0.529666667	pos													0.001403199	0.001403199	2284.267742	0.001403199	2119.725156	3170.165429	3700.529441	2413.132922	1536.111381
0.53_859.3371m/z	859.3371237	0.529666667	pos													0.001403199	0.001403199	1376.51965	0.001403199	1221.831099	2279.707271	2584.303101	2239.596964	1889.055138
0.53_873.0957m/z	873.0956701	0.529666667	pos													0.001403199	0.001403199	1675.51711	0.001403199	1874.467098	2485.791322	2810.713941	2400.381469	0.001403199
0.53_873.3461m/z	873.346133	0.529666667	pos													0.001403199	1551.246606	1969.462704	0.001403199	2431.92086	4914.817426	3648.545004	2973.894348	2705.562034
0.53_875.5872n	858.5838989	0.529666667	pos													0.001403199	0.001403199	5786.350321	2955.647375	2226.896877	5000.454413	5440.137914	2976.603927	3516.572357
0.53_980.2050m/z	980.2049945	0.529666667	pos													0.001403199	3077.945455	1187.91725	2020.22058	1323.804478	2519.399762	2729.32833	1327.966395	4066.537371
0.54_100.0113m/z	100.01128	0.535	pos													250.6314658	295.4141213	266.1909874	310.0643502	136.3152128	396.5621433	177.6980599	274.1809174	148.1421645
0.54_1002.7196m/z	1002.719574	0.535	pos													0.001403199	1695.922488	2781.907701	0.001403199	584.5573483	3201.683357	897.1256381	745.2332459	0.001403199
0.54_1009.7135n	1010.720784	0.535	pos													4530.278139	2750.81226	10418.27627	110.5682308	2184.151252	709.6304901	4066.548609	10750.33066	13914.41238
0.54_1032.2286n	1033.235918	0.535	pos													3375.770645	4509.102207	6231.95354	0.001403199	753.2427502	602.1262235	15292.92962	19978.62122	9893.175442
0.54_1033.7362m/z	1033.736164	0.535	pos													1141.82799	2028.742778	592.4563866	0.001403199	390.0085488	253.9539276	2452.989653	5430.889568	5127.462725
0.54_107.0737n	125.1071207	0.535	pos													276.2553132	795.5487481	763.5537627	632.7187304	194.4150612	1109.813939	714.571526	921.5087825	1527.437046
0.54_1077.7639m/z	1077.763948	0.535	pos													86.79866384	0.001403199	4196.439191	0.001403199	248.1082011	278.5827116	2405.313532	486.6295166	0.001403199
0.54_108.5145n	109.5217279	0.535	pos													37612.05601	21078.72186	19873.13741	33844.4306	10311.74737	18729.47012	10882.76726	19145.34609	12817.03993
0.54_109.0448n	132.0349599	0.535	pos													4183.331627	4138.10613	4679.815028	4473.743881	1438.652333	3819.840694	2041.729623	4191.192923	3439.066823
0.54_109.9878m/z	109.9878201	0.535	pos													767.8668394	641.4272888	733.1455462	698.6887965	436.0662695	911.0965826	446.5226353	579.8869166	465.9839613
0.54_110.0169m/z	110.01695	0.535	pos													0.001403199	0.001403199	308.6344327	0.001403199	35.19618132	36.46069874	46.72876509	0.001403199	34.31587405
0.54_110.0201m/z	110.0201085	0.535	pos													676219.8688	690571.4704	669682.904	676710.6342	438509.631	689497.4117	459275.5738	642760.4222	581456.8837

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0.64_167.0086n	168.0158452	0.63615	pos
0.64_173.0299m/z	173.0298961	0.63615	pos
0.64_180.0441m/z	180.0440981	0.63615	pos
0.64_182.4923m/z	182.4923442	0.63615	pos
0.64_184.0027m/z	184.002669	0.63615	pos
0.64_184.0158n	167.0125136	0.63615	pos
0.64_192.9760m/z	192.9759708	0.63615	pos
0.64_194.9995n	217.9887476	0.63615	pos
0.64_203.9757m/z	203.9757211	0.63615	pos
0.64_215.9427n	216.9504144	0.63615	pos
0.64_218.9691m/z	218.9691132	0.63615	pos
0.64_227.9437m/z	227.943741	0.63615	pos
0.64_230.9539n	269.9205094	0.63615	pos
0.64_231.9204n	214.9170682	0.63615	pos
0.64_247.8927n	248.9003137	0.63615	pos
0.64_249.9385m/z	249.9384786	0.63615	pos
0.64_256.9694n	239.9660972	0.63615	pos
0.64_261.9614m/z	261.9614418	0.63615	pos
0.64_277.9272n	260.9239104	0.63615	pos
0.64_288.9192n	271.915944	0.63615	pos
0.64_314.9749m/z	314.9749145	0.63615	pos
0.64_330.9570n	369.9238347	0.63615	pos
0.64_385.8958m/z	385.8957554	0.63615	pos
0.66_102.0312m/z	102.0312479	0.6574666	pos
0.66_111.9684m/z	111.9684133	0.6574666	pos
0.66_113.9637m/z	113.9637191	0.6574666	pos
0.66_114.9670m/z	114.9669787	0.6574666	pos
0.66_116.9719m/z	116.9719195	0.6574666	pos
0.66_119.0253m/z	119.0252966	0.6574666	pos
0.66_119.5229m/z	119.5228717	0.6574666	pos
0.66_131.9741m/z	131.9740714	0.6574666	pos
0.66_139.9630m/z	139.963008	0.6574666	pos
0.66_141.9584m/z	141.9583741	0.6574666	pos
0.66_144.9658m/z	144.9657972	0.6574666	pos
0.66_147.0111n	130.0078126	0.6574666	pos
0.66_154.9848m/z	154.9847991	0.6574666	pos
0.66_157.9736m/z	157.973562	0.6574666	pos
0.66_158.9611m/z	158.9610613	0.6574666	pos
0.66_159.9689m/z	159.968862	0.6574666	pos
0.66_160.0947m/z	160.0947085	0.6574666	pos
0.66_163.9644n	146.9610912	0.6574666	pos
0.66_172.9769m/z	172.9768771	0.6574666	pos
0.66_183.9817m/z	183.981699	0.6574666	pos
0.66_186.0182m/z	186.0182217	0.6574666	pos
0.66_189.1786m/z	189.1785804	0.6574666	pos
0.66_202.9508m/z	202.9507707	0.6574666	pos
0.66_209.1532m/z	209.1532497	0.6574666	pos
0.66_243.9215m/z	243.9215305	0.6574666	pos
0.66_276.8962m/z	276.8962107	0.6574666	pos
0.66_284.8857n	302.9135644	0.6574666	pos
0.66_287.8882m/z	287.8882259	0.6574666	pos
0.66_289.2521m/z	289.2520742	0.6574666	pos
0.66_314.1033m/z	314.1033243	0.6574666	pos
0.66_314.6050m/z	314.6050234	0.6574666	pos
0.66_341.5641m/z	341.5641194	0.6574666	pos
0.66_91.9833n	114.9715195	0.6574666	pos
0.68_111.0747m/z	111.0747111	0.6788	pos
0.68_112.5552m/z	112.5551809	0.6788	pos
0.68_114.0606m/z	114.0605902	0.6788	pos
0.68_123.5942m/z	123.5941506	0.6788	pos
0.68_148.0341m/z	148.0341132	0.6788	pos
0.68_163.0836m/z	163.0835638	0.6788	pos
0.68_182.0563m/z	182.0562814	0.6788	pos
0.68_191.1386m/z	191.1386	0.6788	pos
0.68_204.9564m/z	204.9564472	0.6788	pos
0.68_209.9456m/z	209.9456064	0.6788	pos
0.68_212.1026m/z	212.1026434	0.6788	pos
0.68_223.0439n	224.0512002	0.6788	pos
0.68_239.0213n	277.9829288	0.6788	pos
0.68_256.0010m/z	256.0009873	0.6788	pos
0.68_271.5713m/z	271.5713177	0.6788	pos
0.68_291.5828m/z	291.5827597	0.6788	pos
0.68_345.9702m/z	345.9701696	0.6788	pos
0.68_368.1273m/z	368.1272972	0.6788	pos
0.68_398.1479m/z	398.1478687	0.6788	pos
0.68_455.0338m/z	455.0338163	0.6788	pos
0.68_481.9452m/z	481.94523	0.6788	pos
0.68_531.1765m/z	531.176511	0.6788	pos
0.70_1031.8605m/z	1031.860517	0.6981333	pos
0.70_108.9486m/z	108.9486335	0.6981333	pos
0.70_168.0870n	191.076259	0.6981333	pos
0.70_176.1471m/z	176.1471248	0.6981333	pos
0.70_177.0510n	200.0402366	0.6981333	pos
0.70_178.0544n	201.043588	0.6981333	pos
0.70_182.1028n	205.091984	0.6981333	pos
0.70_185.1144m/z	185.1144254	0.6981333	pos
0.70_190.1627m/z	190.1626963	0.6981333	pos
0.70_196.1183n	197.1256862	0.6981333	pos
0.70_236.9064m/z	236.9064165	0.6981333	pos
0.70_238.9067m/z	238.9067434	0.6981333	pos
0.70_245.0383n	268.0274997	0.6981333	pos
0.70_259.0635m/z	259.0635123	0.6981333	pos
0.70_272.9426m/z	272.9425688	0.6981333	pos
0.70_281.9044n	304.8936697	0.6981333	pos
0.70_288.9213m/z	288.9212541	0.6981333	pos
0.70_304.0616n	327.0508285	0.6981333	pos
0.70_313.0255n	336.0147154	0.6981333	pos
0.70_340.9312m/z	340.9312493	0.6981333	pos
0.70_349.8918n	372.8810613	0.6981333	pos
0.70_367.9625m/z	367.9624877	0.6981333	pos
0.70_377.0913m/z	377.091297	0.6981333	pos
0.70_396.9867n	419.9759184	0.6981333	pos
0.70_404.0020m/z	404.0020209	0.6981333	pos
0.70_408.9185m/z	408.9184713	0.6981333	pos
0.70_413.2653m/z	413.2652947	0.6981333	pos
0.70_413.9574m/z	413.9574116	0.6981333	pos
0.70_417.8791n	440.8683478	0.6981333	pos

23652.96512	29344.90766	21485.92297	22047.82046	20949.14723	24259.72938	28969.75175	24824.66072	32259.36541	
13215.73908	8232.105227	11309.20644	10630.48205	7620.721485	14167.36821	11157.31474	9577.057909	9825.267933	
4855.30166	6363.892579	4282.537022	4494.076717	4558.358547	4272.40387	5798.803116	5336.837866	6890.809011	
3811.980326	4244.233526	4024.59228	2919.451595	2712.06885	2761.623202	3397.751781	3050.636588	3614.543195	
8187.104266	7982.131415	6905.830589	6647.343605	5476.049758	7150.038667	8152.470351	6763.235931	8300.616913	
303805.4047	446652.7149	308659.6222	321362.203	306322.1679	320232.903	426796.7224	386494.6935	467346.9606	
4339.963703	4042.753356	3561.804182	2727.241772	3334.141962	2358.332774	3152.706937	3229.565754	2537.740499	
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1159.108196	1606.815132	2080.443049	1701.181959	1151.222072	1837.488308	1932.127149	1260.30294	2313.972969	
10015.07802	17163.43582	11732.2581	13957.24096	15164.33566	16627.89776	20142.50276	21721.80841	24650.34875	
974.8905817	2546.294662	2075.076403	1403.96148	1540.415463	1027.460545	1938.441869	1593.862732	1971.495483	
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33183.61369	41008.90127	36167.06733	35313.20331	30679.55766	33003.70205	34944.78756	37982.06774	38596.17517	
71826.27174	104281.5736	77361.2808	80182.52234	85080.08255	80739.83064	96522.20633	84239.80908	99811.78839	
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7359.758555	6597.001059	7131.916414	8265.998752	6103.897053	7189.257181	6370.298464	6589.091186	6389.112614	
93322.60973	96607.89488	98034.80788	103900.159	97420.91559	109481.9639	101807.6537	93816.11482	99075.42393	
61.02007952	49.94391414	85.62451347	69.23621315	0.001403199	0.001403199	0.001403199	0.001403199	102.1832546	
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71517.505	63418.72189	60976.52363	70183.15619	64767.0765	71727.33856	66480.06533	57999.61337	60547.49362	
33799.55742	34828.94934	34028.12937	36272.21995	37094.10605	41178.87882	38177.81564	33322.14585	33624.07327	
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25298.58096	25479.50391	29205.76711	29937.31531	29497.56981	29582.31867	29079.95443	27412.27224	28265.33452	
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286.1127912	277.7150331	336.876754	285.3124832	442.8689606	382.68784	331.3742452	457.4514513	278.3781943	
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1133.415954	1089.715179	1149.773323	1339.45069	1444.989406	1455.219843	1095.029404	1421.181753	1304.865227	
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103.8619288	373.570829	161.5034919	137.0515497	110.4083461	231.5809543	203.3031443	395.3791483	508.0809469	
361.7013859	609.3670118	808.0750389	889.4718102	532.6110295	760.7409641	256.1870562	479.3735776	563.9481078	
976.908758	912.8335925	1109.777373	1144.399478	930.525994	796.8828774	1575.827516	1688.674164	1188.630337	
3176.137354	3858.840539	3828.353795	3818.478772	3966.224199	2444.359353	3543.263865	3407.667806	3352.632655	
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1989.379907	1380.023454	1546.516525	3839.591621	2658.88428	2796.766043	2544.703376	3567.759994	2919.709272	
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58766.87802	50957.1645	53672.79448	45025.57872	45161.99836	42430.29341	53076.61583	48051.31557	49038.09488	
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0.98_275.9344m/z	275.9343626	0.98445	pos																		
0.98_277.9739m/z	277.9739028	0.98445	pos																		
0.98_344.9205m/z	344.9205488	0.98445	pos																		
0.98_384.9390m/z	384.9390155	0.98445	pos																		
0.98_414.7724m/z	414.7724359	0.98445	pos																		
0.98_486.8506m/z	486.8505938	0.98445	pos																		
1.01_183.1014m/z	183.101449	1.006283333	pos																		
1.01_189.9801n	172.976803	1.006283333	pos																		
1.01_197.9844m/z	197.9844349	1.006283333	pos																		
1.01_202.4902m/z	202.4902074	1.006283333	pos																		
1.01_221.9567m/z	221.9567047	1.006283333	pos																		
1.01_224.9386m/z	224.938561	1.006283333	pos																		
1.01_354.8958m/z	354.8957947	1.006283333	pos																		
1.03_110.0171m/z	110.0170872	1.028516667	pos																		
1.03_111.9845m/z	111.9845057	1.028516667	pos																		
1.03_119.0254m/z	119.0253616	1.028516667	pos																		
1.03_120.0556m/z	120.0556461	1.028516667	pos																		
1.03_142.9664m/z	142.9664437	1.028516667	pos																		
1.03_154.0438m/z	154.0438437	1.028516667	pos																		
1.03_157.9736m/z	157.9736322	1.028516667	pos																		
1.03_181.9771m/z	181.9771249	1.028516667	pos																		
1.03_209.0005m/z	209.0005403	1.028516667	pos																		
1.03_221.1534m/z	221.153412	1.028516667	pos																		
1.03_233.9395n	234.9467586	1.028516667	pos																		
1.03_252.9572m/z	252.9572423	1.028516667	pos																		
1.03_275.9733m/z	275.9732538	1.028516667	pos																		
1.03_313.8694m/z	313.8693524	1.028516667	pos																		
1.03_413.2654m/z	413.2654063	1.028516667	pos																		
1.05_107.5175m/z	107.517549	1.0504	pos																		
1.05_111.0393m/z	111.0392803	1.0504	pos																		
1.05_120.0444m/z	120.0443977	1.0504	pos																		
1.05_121.9661m/z	121.966102	1.0504	pos																		
1.05_134.4768m/z	134.4768299	1.0504	pos																		
1.05_138.9951m/z	138.9951157	1.0504	pos																		
1.05_145.9540n	128.9506812	1.0504	pos																		
1.05_183.4603m/z	183.4602869	1.0504	pos																		
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1.05_232.9050m/z	232.9049521	1.0504	pos																		
1.05_232.9514m/z	232.9514213	1.0504	pos																		
1.05_335.8513m/z	335.8512735	1.0504	pos																		
1.05_386.8328m/z	386.8327645	1.0504	pos																		
1.05_391.7836m/z	391.7836373	1.0504	pos																		
1.05_392.7917m/z	392.7916564	1.0504	pos																		
1.07_113.9604m/z	113.96042	1.072683333	pos																		
1.07_121.9661m/z	121.9661181	1.072683333	pos																		
1.07_125.9861m/z	125.9861426	1.072683333	pos																		
1.07_144.9426m/z	144.9425724	1.072683333	pos																		
1.07_151.0963m/z	151.0962941	1.072683333	pos																		
1.07_156.9939m/z	156.9939282	1.072683333	pos																		
1.07_166.0579m/z	166.0578677	1.072683333	pos																		
1.07_174.4552m/z	174.4551508	1.072683333	pos																		
1.07_185.9631m/z	185.9630993	1.072683333	pos																		
1.07_194.9685m/z	194.9684805	1.072683333	pos																		
1.07_195.4660m/z	195.4659663	1.072683333	pos																		
1.07_206.4764m/z	206.4763672	1.072683333	pos																		
1.07_211.9308m/z	211.9307894	1.072683333	pos																		
1.07_213.0079m/z	213.0078563	1.072683333	pos																		
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1.07_248.9013m/z	248.9012653	1.072683333	pos																		
1.07_261.9076m/z	261.9075632	1.072683333	pos																		
1.07_310.8501m/z	310.8501184	1.072683333	pos																		
1.07_427.8594m/z	427.8594383	1.072683333	pos																		
1.09_132.9746m/z	132.9746038	1.09455	pos																		
1.09_149.0344m/z	149.0343556	1.09455	pos																		
1.09_155.0700m/z	155.0700306	1.09455	pos																		
1.09_164.9480m/z	164.9479587	1.09455	pos																		
1.09_170.5147m/z	170.514672	1.09455	pos																		
1.09_173.4574m/z	173.4574467	1.09455	pos																		
1.09_175.4743m/z	175.4742572	1.09455	pos																		
1.09_179.5200m/z	179.5200208	1.09455	pos																		
1.09_179.9714m/z	179.9713631	1.09455	pos																		
1.09_180.0214m/z	180.0214274	1.09455	pos																		
1.09_191.0279m/z	191.0279239	1.09455	pos																		
1.09_191.5297m/z	191.5296752	1.09455	pos																		
1.09_242.8630m/z	242.863035	1.09455	pos																		
1.09_254.9490m/z	254.9489978	1.09455	pos																		
1.09_262.4812m/z	262.4811665	1.09455	pos																		
1.09_262.9833m/z	262.9833493	1.09455	pos																		
1.09_266.9711m/z	266.9711183	1.09455	pos																		
1.09_269.0630m/z	269.0629775	1.09455	pos																		
1.09_306.0434n	345.0011598	1.09455	pos																		
1.09_334.8713m/z	334.8712662	1.09455	pos																		
1.09_340.0223m/z	340.0222846	1.09455	pos																		
1.09_396.9628m/z	396.9627678	1.09455	pos																		
1.12_115.9678m/z	115.9678394	1.115783333	pos																		
1.12_154.9848m/z	154.9848456	1.115783333	pos																		
1.12_159.9619m/z	159.9618954	1.115783333	pos																		
1.12_169.9653m/z	169.965306	1.115783333	pos																		
1.12_169.9973m/z	169.9973076	1.115783333	pos																		
1.12_184.4851m/z	184.4850977	1.115783333	pos																		
1.12_200.9954m/z	200.9954056	1.115783333	pos																		
1.12_202.9872m/z	202.9872248	1.115783333	pos																		
1.12_276.8964m/z	276.8964068	1.115783333	pos																		
1.12_287.8884m/z	287.8884031	1.115783333	pos																		
1.12_331.8784m/z	331.8783655	1.115783333	pos																		
1.12_351.0310m/z	351.0310242	1.115783333	pos																		
1.14_111.5369m/z	111.5368724	1.137683333	pos																		
1.14_115.0633m/z	115.0632662	1.137683333	pos																		
1.14_116.9720m/z	116.9720012	1.137683333	pos																		
1.14_151.0013n	169.0353413	1.137683333	pos																		
1.14_156.5229m/z	156.5228827	1.137683333	pos																		
1.14_157.0737n	175.1074701	1.137683333	pos																		
1.14_167.5693m/z	167.5693227	1.137683333	pos																		
1.14_169.9895m/z	169.9895424	1.137683333	pos																		
1.14_176.0826m/z	176.0826066	1.137683333	pos																		
1.14_197.0896m/z	197.0895632	1.137683333	pos																		
1.14_199.0784n	200.0856411	1.137683333	pos																		

1190.666237	1803.489531	1736.367963	1839.283599	1773.874247	1709.670406	1571.786394	1766.844175	1893.151481													
3452.854485	2456.833229	2783.940933	3599.731728	3416.004963	3512.675295	3709.764157	3371.146044	3242.767093													
7332.351316	8560.775441	9664.731284	14902.17787	12017.24912	12640.45222	9339.867761	11187.03295	9894.907067													
1545.101892	2238.433324	2119.532812	2767.698741	2989.459762	2833.64573	1885.53839	2574.604031	2687.975911													
2986.902434	3510.342945	3329.070664	4495.022893	4491.129718	4812.920172	3544.380008	4271.058105	4156.137315													
2936.90765	4277.016794	5325.89923	6061.123277	6629.239497	6432.641498	4573.3273	6297.350159	6787.391761													
1274.534712	1295.103335	1207.778413	1070.270899	988.4755694	1127.040508	1159.120059	1084.517814	1090.541972													
53004.35472	45581.71511	43656.89646	39367.4651	43569.43119	43329.54649	48888.77984	40913.8299	43804.21257													
2601.247431	2897.595986	3081.820645	3008.717612	3180.844138	3009.389199	3041.603496	3181.882129	3068.042856													
84.00299841	37.48473905	58.43728512	37.00843412	0.001403199	0.001403199	41.62991596	35.96764755	0.001403199													
1457.257195	1656.66539	1733.483152	1644.968543	1726.105265	1972.343344	1378.120714	1599.950947	1702.013269													
5478.059838	4611.387994	4530.234959	5638.619701	5777.591758	5381.597613	5579.293741	5439.548853	5746.733935													
8477.474912	8689.815898	7926.535377	11303.36703	11360.7249	11290.17787	10081.90407	10478.8975	10026.15532													
32.02605127	0.001403199	19.68088681	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199													
1692.665748	1690.330613	1679.632093	1450.92511	1656.510997	1690.165214	1771.582663	1629.215073	1725.488482													
2610.142903	2237.564959	2081.898424	1844.157878	2185.816174	2389.422666	2464.654988	1921.565447	2346.637229													
198.3477821	236.5879438	188.690679	226.9317324	233.9420783	220.0062383	224.112814	197.6919045	218.6775134													
532.86342	515.9366005	437.8371345	421.3570919	438.4886916	454.4002697	431.3762234	468.5476269	472.9085684													
0.001403199	47.04558683	30.51015373	31.31031764	31.49996825	39.02308174	0.55019371	0.001403199	85.76343199													
4376.691101	4139.264366	4097.080054	3963.76645	4107.756093	4043.648835	4165.904499	4374.133222	3877.256205													
2630.355331	2615.272563	2646.592443	2221.43923	2033.579593	2343.327906	2629.305166	2478.693729	2743.189331													
917.4039632	1451.698223	1581.103905	916.8852622	917.3934651	980.5756686	1391.395329	1213.788322	1235.191505													
1513.332207	1307.858589	1157.58458	1142.394657	1125.806438	1143.577217	1255.851551	1116.332915	987.0478039													
200397.1387	202583.103	194813.5497	221840.3307	236111.7283	232880.5442	225066.1771	214187.3499	221159.0915													
6800.867318	7280.089169	7694.540094	8789.670809	9551.791424	9780.479089	7634.42124	8553.972578	8775.473029													
15764.69745	14281.61291	14398.24951	15487.9249	17335.33828	15767.56592	16724.39999	15877.11635	15504.08531													
24516.84629	26727.72923	27897.87843	34205.69442	37224.72494	35893.17868	31249.20458	32158.20505	32362.60257													
1672.1511	961.0110431	1126.935131	966.8083008	1157.177595	1134.883432	1341.881593	955.6894913	1039.296759													
649.1789478	684.4953571	670.8890637	643.4705305	642.6134982	652.4803975	585.3054005	726.224543	640.3782295													
868.1764462	634.1029701	618.689414	545.0982842	555.3822836	671.5529316	855.265993	615.2905375	755.1543028													
143.1107173	213.9220683	231.376988	188.2177136	135.831817	153.5256954	192.5766615	212.7103229	195.6778936													
234.6526239	233.6131204	200.2914235	231.3272693	273.5167139	258.4393461	181.4523294	226.4310713	212.8331016													
468.0586022	383.9175649	409.9863243	375.573947	439.5471459	337.8436623	356.1728039	362.9045223	417.8553486													
5829.079219	5225.714748	5337.289574	4713.372026	5103.162844	5157.047801	5815.259858	4890.407948	4982.138084													
56730.65596	48044.94352	47006.04467	45816.45351	48411.3459	49042.9139	53509.09	46226.29681	47243.84486													
768.8178662	625.8991362	973.1389232	665.5524911	1093.764986	1005.584893	747.8694768	942.6249801	894.0028861													
584.9893605	935.2142823	937.3964569	913.1447724	1092.254664	796.5727152	780.2807031	1004.714355	995.5726604													
5568.233881	5275.665647	4997.821495	5144.718962	6079.959375	5519.586515	5391.595715	5450.789216	5829.314921													
6719.281342	5895.895193	5790.383983	6687.450903	7010.653312	6829.248115	6723.812552	6317.041594	6784.716352													
6612.115292	7544.444637	6481.504276	8199.984701	9280.905309	8940.791138	8305.586695	8755.853957	8878.742378													
10026.48904	9213.604609	9702.500084	11811.27226	13887.20307	13808.03999	11936.43138	12475.46156	12923.02436													
0.001403199	451.9027424	335.1789512	390.64981	380.520984	632.4145286	474.3923136	805.2824371	108.4745215													
1661.934331	2212.209422	2765.347042	3159.148799	3300.004212	3043.050492	2207.129677	2915.479164	2989.533357													
10.87127151	18.43796178	0.001403199	48.28410581	85.57675844	0.001403199	21.40266494	36.41913891	16.17796325													
64.47808747	136.1696886	84.08536891	142.6073477	108.0078125	116.4026294	142.9472204	185.2046347	231.8910135													
3506.377431	3126.825803	2697.260455	2892.805357	2926.785561	3269.511818	3232.669037	2927.569321	2930.92185													
39.26034987	100.3641362	23.63947364	72.45666611	29.98509352	91.18367624	0.001403199	52.10619831	24.43578696													
1867.483446	1779.363002	1912.486586	1723.49366	1657.441439	1777.562281	1898.690754	1842.318588	1707.829765													
76.45282961	127.8295121	44.97292342	107.2978498	0.001403199	195.9035261	146.8311947	0.001403199	64.06059957													
981.9547777	367.9194667	464.1894768	1426.278698	1031.577174	996.8921424	1247.891502	553.9267159	604.6050537													
2023.225094	2464.048516	2204.468586	1799.502842	2134.230634	2213.128253	1755.918227	2089.670701	2366.241479													
11180.76694	11101.34362	9503.496394	9806.918046	11169.10688	11022.47636	11576.46516	10092.18212	11403.61524													
1368.378531	1573.042937	1219.452183	1670.097856	1581.172297	1581.29232	1708.218912	1674.733391	1724.317281													
887.4553154	870.6354518	959.3773229	1271.174876	1234.843774	1273.776077	1072.947891	1053.316402	1089.832044													
1710.820111	2092.451576	1469.808956	1673.024299	1562.69652	1689.991559	1749.441948	2015.86167	1798.847602													
13188.96909	12360.75656	12168.29818	16322.39751	17885.55725	17547.40184	14332.23455	14361.63137	13978.14087													
48.18191505	154.4631572	0.001403199	0.001403199	91.00585095	86.13417335	83.00001058	47.72899246	36.70639796													
8437.98787	9336.528381	9640.418858	8974.326494	9988.037212	9651.246671	9677.761276	10030.51086	10616.06742													
810.9124251	666.7662677	654.1490442	653.9116171	655.4889873	664.08855	727.3558436	572.5197494	539.4487687													
13763.33034	14471.70121	12444.09232	12121.8394	14183.76644	14368.04104	13922.81517	13668.28656	14390.75048													
3698.209867	4184.822255	3616.809134	2847.085283	3431.450979	3200.030167	3734.311108	3708.756226	3587.73171													
1911.040651	3224.924777	2676.572238	2897.634241	3505.885782	2689.370661	2998.171176	3889.179994	3501.785251													
2337.038452	2032.524345	2108.328885	1777.380441	2114.131007	1996.776352	2328.418124	2050.214578	2180.757799													
96.37008195	94.79847683	143.6959003	84.07179292	93.81319381	70.37166351	55.47847221	94.12794488	121.5876822													
759.7259344	851.6160691	866.5213373	647.6408787	770.2679463	663.2968122	857.0116621	807.8429079	833.8108819													
307.3650061	323.0899785	329.7229031	338.8381177	387.0026381	472.8994056	378.2195361	346.3418401	369.0810507													
3991.679959	4267.52493	4479.275628	3344.484536	3278.641925	3728.152521	2958.070021	3421.745781	3045.767347													
156.1239808	132.5727717	207.3558055	155.8585191	82.53718148	96.71363284	244.327085	187.9021122	163.880558													
125.8164166	117.1015989	222.3569191	192.9305537	235.3277219	170.8712905	227.2586043	185.2586503	195.9308973													
1723.979318	1669.409155	1888.652464	1414.013719	1508.64003	1758.084729	1027.288514	1856.541615	1460.42733													
169.9848277	111.7776476	0.001403199	91.34444856	135.799487	103.2877549	124.9503507	66.99711497	129.3824132													
193.4766784	186.1930662	320.4328727	90.88963964	314.2539268	270.3514323	243.2571166	309.2281502	129.45433													
8188.039715	7498.199268	6981.368621	5839.402971	6716.867674	6456.536605	6577.253614	6627.466949	6443.482598													
818.1318929	754.1760504	590.518322	484.3222471	422.7775354	456.576983	491.2374468	595.0004334	677.6055569													
2816.494667	3525.438371	3276.505171	2610.88146	3075.970536	3052.826413	2937.822624	2886.208344	3405.799192													
64.87935065	287.8814862	274.1101695	224.3468303	270.6604541	57.08314568	56.3976239	335.9322648	205.3890674													
476.9348503	605.1920214	850.2706329	135.2042729	253.7289876	461.7849175	201.5090583	336.7226778	358.5968506													
278.7124975	481.2977125	493.0892051	139.1270366	135.5413741	219.4307309	235.6830043	193.0743757	240.3413264													
748.4694942	748.3564025	706.3603738	478.6246067	485.2260778	612.0823157	237.9977946	658.8888028	425.1681966													
85.46706078	269.578163	249.1203208	330.9135676	211.6291332	246.562731	138.2527756	193.8913574	117.5636865													
6720.744025	7536.417694	7618.238951	5084.809856	5493.403291	5281.41908	3645.695329	7282.694149	5209.956697													
16265.81251	15586.09218	15796.45391	12815.67208	15293.76292	15517.47629	16904.57807	16294.97384	16821.46211													
1897.45828	1979.970842	2071.650681	1194.803882	1315.588115	1708.509494	768.2722749	1978.589115	1163.317282													
4508.018331	5368.209044	5968.59099	4838.67603	5572.413522	6537.015736	3107.540944	5834.709999	5247.602216													
297.1463657	222.0464266	191.1893155	184.1128902	253.8075749	271.5074545	196.8724092	244.2711107	253.3737995													
302.2151067	344.7698927	284.8067257	95.63725275	29.54141361	233.157783	185.721008	167.5471325	90.35548871													
99.25616075	217.9810903	0.001403199	0.001403199	92.51124578	0.001403199	0.001403199	101.1079636	97.53829919													
2128.375622	2192.150868	2090.074198	1466.774	1893.063464	1924.439202	1844.112058	2019.072097	2149.76802													
1554.429212	1848.614204	1763.39456	1351.098928	1534.559666	1418.208546	1549.694039	1594.044006	1785.539385													
138.989147	0.001403199	79.02884079	76.50985349	79.02000961	68.69712607	66.36444056	0.001403199	37.29818415													
16037.09318	15086.08917	13353.09429	12580.66615	12697.09204	12130.53592	14852.14789	12988.15249	14116.84018													
1926.153399	1927.87135	1620.374878	1462.983689	1942.555964	1579.707384	1847.717151	1261.165757	1670.883744													
4290.689982	4997.665928	4753.98138	3047.068947	4226.640169	4066.188039	4156.690159	4232.519409	4414.967771													
2125.241872	2567.410235	2204.660228	1360.685338	1998.247571	1932.448959	1851.624856	1703.496109	2138.993841													
1736.553859	1489.83867	1518.517222	1082.299237	1874.582174	1511.79056	1186.639293	1473.075116	1470.475703													
2856.953752	3128.372308	3284.93803	2676.349838	2814.435958	2844.089531	2493.992338	2556.026371	2322.190685													
48.07125341	28.69448432	74.29689436	57.13186671	117.8539456	154.3251768	153.8276401	115.0866358	89.17578692													
322.4934302	328.1337967	345.1660147	290.3019533	275.5965225	326.6111514	322.2834459	369.9275898	400.2294732													
3099.924755	2844.413732	2809.535125	2871.642678	3336.179094	3088.064918	3180.22238	2769.204211	3179.899795													
462658.9231	384239.9078	393986.7315	531059.322	394148.2307	397359.5417	411471.9973	412164.9191	358226.0599													
2579.157257	2746.140166	3095.61075	2998.246871	3394.52883	3451.503259	2454.453371	3015.802199	3261.347042													
58835.5442	51554.90492	55517.78433	27961.64208	19204.46365	18946.20012	27167.67254	38255.64488	31933.21064													
853.9443514	821.7184076	845.996121	1187.450814	909.8308461	995.3511482	483.2589598	704.1218279	568.9335638													
5947.177948	6838.206047	6760.434291	8053.144486	8330.218434	7724.230812	5567.61368	6493.194449	6970.273518													
546.271246	398.678464	537.8621525	423.4497657	639.6743456	335.9588413	78.80155817	394.7230728	383.7804459													
1659.945832	2583.604496	1616.724897	1107.100576	894.5052053	884.5346213	899.8705075	1311.367526	1102.12343													
4319.917029	4423.91083	4797.877024	5583.281057	4893.038598	4963.170772	3928.67468	4751.910349	4460.106292													

1.14_212.9990m/z	212.9989514	1.137683333	pos							6074.836023	5517.813968	5715.947187	5387.70213	4554.35766	4534.774569	6873.820863	6040.929932	7077.434871	
1.14_215.9951m/z	215.9950726	1.137683333	pos							6046.182027	7215.920616	6881.057877	6993.99065	7968.841404	7512.800404	5532.876973	6093.349791	6850.194397	
1.14_272.9360m/z	272.9359893	1.137683333	pos							787.456548	1033.870508	1331.537949	1506.399517	1749.630624	1780.220317	708.5221201	1053.480468	1385.199444	
1.14_273.1077m/z	273.1076673	1.137683333	pos							3130.22388	2726.686299	2889.319961	6606.871161	5519.974825	4947.394388	3359.459848	4435.826878	4021.152816	
1.14_281.9916m/z	281.9916076	1.137683333	pos							5212.90009	4211.730361	4543.266176	5524.732148	3342.999178	3734.517749	5038.050869	4812.550208	4780.993012	
1.14_299.0068m/z	299.0067718	1.137683333	pos							4337.9533	4639.467683	4449.276563	5429.137314	4893.140108	4876.254126	3423.868258	5263.986257	4893.283147	
1.14_322.9795n	361.948142	1.137683333	pos							15237.9619	13028.16002	13697.98334	17536.56257	13697.35291	13124.90571	16275.99012	17420.61499	19265.2069	
1.14_347.0173m/z	347.0172599	1.137683333	pos							1312.454474	1668.029478	1552.032331	865.0767781	1224.992074	1436.487729	904.2566647	1414.79924	1386.294229	
1.14_350.9689m/z	350.968869	1.137683333	pos							1384.144585	1554.55453	1960.415832	1999.077151	2091.601489	2409.35648	1266.7882	1607.065483	2369.076347	
1.14_360.0000n	361.007028	1.137683333	pos							6344.222091	3559.822019	5772.1803	9760.462931	3721.668143	3470.80862	6015.832872	7018.51195	5128.737366	
1.14_365.9875m/z	365.9874598	1.137683333	pos							2434.490631	1609.893174	2271.444485	3735.828127	2593.209385	2182.880417	1813.709344	3009.936897	1980.16791	
1.16_110.0350m/z	110.0350042	1.157483333	pos							431.1781758	387.8312566	252.6350255	390.2227966	356.8774596	432.9712476	409.5723793	338.3515177	278.8921129	
1.16_111.0554n	150.0183263	1.157483333	pos							2550.47981	2576.420373	2815.59653	3281.731593	3229.185091	3364.802239	2863.638129	2637.957026	2801.06629	
1.16_112.0161n	130.049747	1.157483333	pos							43974.96722	49960.90982	48855.08543	43377.09619	42929.09005	44739.02585	39908.22414	44836.7676	41990.08374	
1.16_112.0394m/z	112.0394267	1.157483333	pos							4089.535712	4048.669735	3911.507096	4603.375293	4231.420714	4515.899118	4070.737334	3707.107781	3665.682048	
1.16_114.0551m/z	114.0550519	1.157483333	pos							15189.86541	15593.66248	15680.78939	18600.88634	17600.56121	17387.03469	15820.0222	16642.19489	15286.81427	
1.16_119.1312n	158.0922009	1.157483333	pos							47187.77926	48797.52204	46779.08023	7696.268999	7299.039927	8517.499051	11272.4443	10866.88602	9214.406003	
1.16_125.0961m/z	125.0960585	1.157483333	pos							1753.40983	1809.191183	1495.819363	1602.582389	1503.423369	1503.06608	1519.24376	1711.564022	1548.857656	
1.16_126.0549m/z	126.0548511	1.157483333	pos							5860.293461	6106.995021	5826.133158	5312.235727	5427.011792	5187.726915	5694.873085	5537.038632	5551.293124	
1.16_138.0490m/z	138.0489835	1.157483333	pos							2360.632443	2861.177035	2389.516558	1940.248799	1979.11097	1997.840288	1237.84459	1347.570207	1049.801459	
1.16_139.0633n	122.0600251	1.157483333	pos							1718.29414	1828.382816	1589.286981	1211.780687	1265.126555	1308.076964	1382.785222	1397.556862	1454.608048	
1.16_167.0755m/z	167.0754723	1.157483333	pos							11111.8153	11606.89104	10817.25859	12248.96354	11780.43853	11657.552	11042.13482	11192.52614	11059.93807	
1.16_170.0386m/z	170.03864	1.157483333	pos							25642.7429	20403.03956	20725.83452	28794.75324	29048.52668	26606.98482	20757.58697	21648.88283	21948.53836	18812.54362
1.16_174.0638n	197.0529644	1.157483333	pos							6986.789638	6830.474014	7136.542877	10431.2563	9775.101951	9650.920167	8151.819862	8132.235325	8073.530997	
1.16_176.5842m/z	176.584182	1.157483333	pos							404.127692	0.001403199	393.4105042	276.2938766	261.8706801	544.5584512	552.5589579	271.4305687	248.8621159	
1.16_186.0759m/z	186.0758634	1.157483333	pos							3130.625209	3141.490477	2788.769395	3025.496635	3082.454547	2852.852467	2649.710877	3020.657075	2542.18687	
1.16_187.1079n	226.0681265	1.157483333	pos							6289.693416	5891.106807	4454.576512	6079.277579	5036.480851	5527.43604	5796.049328	6245.746875	5605.269587	
1.16_191.1631n	230.1244225	1.157483333	pos							17178.88289	14560.99585	19799.42413	18589.66394	16784.99529	14982.74679	17900.0899	20026.37178	16983.3068	
1.16_193.5696m/z	193.5695893	1.157483333	pos							0.001403199	171.8738715	0.001403199	0.001403199	0.001403199	0.001403199	118.4261492	250.5306794	185.0078172	
1.16_196.9772n	219.9661042	1.157483333	pos							13238.0171	12486.04591	12706.81486	13388.73594	13393.736	13476.81298	13294.28559	12314.19119	13822.70883	
1.16_198.1001n	199.1074199	1.157483333	pos							903.0874884	1916.347153	1668.380701	741.8881643	830.6158374	993.3219742	523.0394792	946.6324882	675.9604458	
1.16_201.0366m/z	201.0365529	1.157483333	pos							1177.558618	1621.710345	1484.578043	1091.567126	1321.081715	969.4997979	888.9201352	1390.047111	1344.83726	
1.16_203.1216m/z	203.1215608	1.157483333	pos							4119.243309	4495.742517	4794.984349	6735.701053	6721.701799	5284.673568	4712.080102	5248.370492	4339.771576	
1.16_213.1111n	231.1447344	1.157483333	pos							10232.28281	9614.172545	9674.927475	10868.19021	10723.93489	10213.55552	10211.05223	10167.29044	10543.74445	
1.16_214.0086n	215.0158521	1.157483333	pos							421142.9165	447353.3135	440852.5873	579653.7205	514327.7828	554891.5069	485347.3233	485159.9256	455315.2677	
1.16_218.1019m/z	218.101922	1.157483333	pos							799.203842	859.4658159	519.2713213	756.068929	627.8104647	741.1930107	725.7817053	1007.680252	731.9703537	
1.16_229.0947n	247.1283966	1.157483333	pos							6208.416933	5481.646614	6336.649033	7352.186695	6124.761981	6819.517299	4816.20891	5390.400853	4907.777555	
1.16_229.2516m/z	229.2516095	1.157483333	pos							488.0469644	543.6465603	0.001403199	750.765057	146.1912081	670.8453664	332.366448	554.7077789	72.96656974	
1.16_232.1056n	255.0947418	1.157483333	pos							9493.336368	9167.683725	7924.107241	10679.29233	9616.190995	10208.84483	9058.745278	8064.866175	7423.937253	
1.16_242.0510m/z	242.0509523	1.157483333	pos							1190.99608	2085.251053	1826.473691	1641.363379	1480.884815	1092.284083	1133.076529	2147.074937	2961.500079	
1.16_242.9821m/z	242.9821499	1.157483333	pos							69159.17015	70047.21731	70968.30027	71482.45536	72583.8321	71489.32393	71959.57038	68788.76447	73758.09811	
1.16_244.0926m/z	244.0925926	1.157483333	pos							2136.048967	2677.049401	2389.202502	2435.383923	2545.857958	2896.061214	1982.985708	2179.604224	2314.914971	
1.16_256.0302m/z	256.0302448	1.157483333	pos							3990.355944	4866.202463	4360.420761	4537.097059	3990.018487	4551.716745	6078.921401	6781.712666	5430.689926	
1.16_259.1282m/z	259.1281842	1.157483333	pos							3940.840943	4047.21063	3892.244473	4156.476659	3486.661209	3579.679246	2994.724705	3404.039591	3437.661501	
1.16_276.1076m/z	276.107611	1.157483333	pos							915.4959161	923.3283356	1540.791257	946.0588916	818.8124411	1444.135104	402.6265147	1299.211477	1360.616134	
1.16_290.0743n	313.0635388	1.157483333	pos							11472.90325	12395.38745	12293.77265	13332.40377	11965.90938	12228.95246	10264.92989	10306.5466	9274.516079	
1.16_291.0950n	314.0839551	1.157483333	pos							14266.08882	15245.90555	12193.23054	12028.03772	12010.36252	11688.30586	8172.389099	8794.175787	7283.759828	
1.16_302.0846m/z	302.0846331	1.157483333	pos							4549.204437	4433.607037	4303.970644	3919.086315	3190.858994	3153.177228	3695.149093	4492.935127	3320.042294	
1.16_303.1182m/z	303.1181957	1.157483333	pos							637.8448841	1267.04998	1354.933293	1251.126259	984.8220071	957.4968652	0.001403199	427.0648956	0.001403199	
1.16_306.1542m/z	306.1541502	1.157483333	pos							1701.624826	1848.188083	2177.016765	2825.271805	2590.267158	1876.645656	2101.842524	2195.006444	1781.185246	
1.16_306.9852m/z	306.9851985	1.157483333	pos							3096.896649	3808.064104	3969.22357	6974.624326	7019.325885	5806.29259	4366.814283	5670.101584	4266.404187	
1.16_307.9906m/z	307.9905872	1.157483333	pos							1884.621552	1236.801657	1644.983547	2016.518036	1492.340296	970.9808225	1568.8169	1521.162836	1427.868792	
1.16_309.9864m/z	309.9864264	1.157483333	pos							33286.23143	22266.38363	23939.11735	29973.90214	20565.58325	18119.89495	27838.70253	26733.95968	24906.14993	
1.16_310.9663m/z	310.9663059	1.157483333	pos							14162.58301	11768.09559	12080.1115	18310.86768	12152.84575	11706.51243	16560.14261	15814.31527	13686.96682	
1.16_333.9575n	334.9647825	1.157483333	pos							7473.638697	10037.48349	8529.943978	12277.29653	12284.26399	11131.08131	12091.67527	12242.76147	12870.26455	
1.16_337.0630m/z	337.06297	1.157483333	pos							3566.915199	4231.167558	2736.975968	4787.484254	3522.5056	5249.148829	2895.351663	3013.728927	1992.243565	
1.16_343.9133n	344.9205281	1.157483333	pos							12450.22975	12604.16437	13091.78556	20023.00842	15895.22605	15373.34804	17469.40705	16153.15067	15686.75007	
1.16_375.9956m/z	375.9955617	1.157483333	pos							13238.51354	13291.66866	12865.54572	13867.94739	11959.59505	12740.32089	11634.24424	11838.28226	11432.86717	
1.16_393.9822m/z	393.9821868	1.157483333	pos							3535.311215	4776.676506	4035.57395	5669.660079	5932.223159	6398.543587	3955.351371	4465.629669	3999.296075	
1.16_426.0627m/z	426.0627059	1.157483333	pos							16923.59705	15794.05774	14919.32781	19169.63855	14481.01932	16394.67346	11172.78298	12310.51071	11706.1681	
1.16_431.9843n	414.9810564	1.157483333	pos							67855.29873	62404.63159	64576.10616	91386.87087	78866.87087	81826.96156	67050.29739	71150.90028	56463.74163	
1.16_435.9766m/z	435.9765969	1.157483333	pos							934.2250744	2158.457671	1269.330675	1986.731338	2494.973091	1717.971504	730.0311008	84.99898058	1307.545176	
1.16_437.9725n	438.9797759	1.157483333	pos							45973.45664	56890.72031	54792.9218	75683.77831	75565.87593	75507.11071	56532.29677	62305.35377	57986.56086	
1.16_445.0282m/z	445.0281756	1.157483333	pos							4668.799277	3261.372063	4721.676574	6430.065195	3966.444513	4525.095818	4294.413011	6184.173126	4178.503465	
1.16_491.8913m/z	491.8913453	1.157483333	pos							2650.484376	1284.006323	1206.724784	2015.125303	2501.123954	1912.396438	2262.400944	2022.677152	1914.382998	
1.16_583.0093m/z	583.0092964	1.157483333	pos							5693.507221	7309.382106	5424.259681	8113.656851	7587.755396	11138.44522	6685.571904	6581.639832	4645.315761	
1.16_607.0076m/z	607.0076467	1.157483333	pos							10193.36637	16571.05544	16186.33599	23392.23069	25243.41045	28603.66829	12656.92281	16057.02618	14270.51288	
1.18_112.0506m/z	112.0506391	1.178066667	pos							2236.386165	3050.218973	3089.481836	2899.303617	2996.892917	3330.111148	2368.108131	3242.065022	2716.745468	
1.18_133.5146m/z	133.5145995	1.178066667	pos							2430.142525	2698.100889	2973.493472	2051.38558	2211.771983	1961.452826	2475.37239	2383.364846	2374.095085	
1.18_152.0316m/z	152.0315864	1.178066667	pos							463.8746382	571.3290421	568.4638216	490.1353064	393.7511122	585.5175351	341.3150775	482.3979925	574.5690247	
1.18_154.0721m/z	154.0720543	1.178066667	pos							301.0782831	526.6790582	566.3247793	353.826004	399.7561852	349.21122	394.1221982	629.1363759	468.1845853	
1.18_161.9608m/z	161.9608103	1.178066667	pos							204.1325045	248.9571515	264.2950356	142.9216857	152.5477582	213.082807	193.8952995	275.3844654	234.1827892	
1.18_195.0875m/z	195.0875277	1.178066667	pos							503.1790171	663.7300729	850.3181336	833.9724817	901.5140378	728.6952085	968.1485252	940.7780644	882.2895374	
1.18_204.0865m/z	204.0864935	1.178066667	pos							4289.469689	4723.772057	4620.141031	3897.336384	4060.516906	4179.446773	4305.606355	4525.098732	3969.50686	
1.18_228.0475m/z	228.0474686	1.178066667	pos							89.14550447	625.0977758	560.8219643	210.5167519	217.8103156	353.6882891	0.001403199	436.8490978	432.7002302	
1.18_229.9744m/z	229.9744048	1.178066667	pos							10105.92355	11799.87166	11251.46553	9391.583416	9709.029403	9058.12845	9839.094103	9722.884863	10925.00999	
1.18_245.9929m/z	245.9929122	1.178066667	pos							842.7158427	625.9259867	643.6588917	648.3800542	866.0628209	746.858996	607.4680239	351.7113342	789.9697545	
1.18_258.1080m/z	258.1080349	1.178066667	pos							25558.95886	28915.72782	28472.89485	29344.82989	30039.17361	30948.63372	23068.11427	31210.95435	27137.77581	
1.18_264.9639m/z	264.9639344	1.178066667	pos							427.1744892	865.5668284	742.4894508	344.1481898	598.4928674	757.639521	379.3981869	1023.309149	992.011404	
1.18_314.9403m/z	314.9402908	1.178066667	pos							1107.117617	1260.592182	933.0002009	1115.380375	1212.972001	1381.750839	1133.815379	1468.773433	1388.679431	
1.18_322.9625m/z	322.9625408	1.178066667	pos							3326.350974	4960.421186	3976.819608	4165.970218	4673.657859	4345.354019	4485.091523	4003.921642	4447.144776	
1.18_335.9409m/z	335.9408527	1.178066667	pos							1667.93152	3698.770241	3416.236365	2199.177801	2328.297643	2642.833434	2157.723326	3956.742668	3852.407677	
1.18_495.9445m/z	495.944527	1.178066667	pos							1239.207464	1904.220103	1304.050138	1731.797009	2217.49957	2518.397432	1079.787257	1307.266064	1740.506082	
1.20_107.0492m/z	107.049174	1.199716667	pos							380.5849237	375.0279776	356.4139762	507.868699	402.1660325	424.9370796	474.5307216	573.3709512	408.1104477	
1.20_112.9718m/z	112.9718238	1.199716667	pos							132.0069414	99.47726432	100.5687068	117.7148125	72.99040783	133.7448402	144.7881857	72.15457621	56.15549944	
1.20_116.0528m/z	116.0528408	1.199716667	pos							447.7551253	636.964204	756.5004274	327.7944792	385.69262	412.2864199	537.3878499	656.1413125	682.936129	
1.20_122.0681m/z	122.0681387	1.199716667	pos							32.91516509	61.34707664	54.16729806	43.74541378	102.023515	29.12916227	35.61439689	64.22239664	71.8927522	
1.20_156.0057n	157.0129629	1.199716667	pos							9330.474192	10794.19974	11161.10887	9355.141405	7557.606435	9327.743071	9015.623907	10300.51414	9793.170505	
1.20_171.0624m/z	171.0623549	1.199716667	pos							583.8089254	604.7735702	655.9267435	704.2366349	753.5929091	686.3789867	618.3963861	627.5058262	632.44033	
1.20_174.5772m/z	174.5771702	1.199716667	pos							1412.579644	1875.476697	1456.658729	2086.437086	2220.485117	1973.811198	1631.54241	1593.289278	1532.503105	
1.20_179.9741m/z	179.97415	1.199716667	pos							58.58621742	95.59547254	178.9903451	57.05557606	69.30237365	86.26275703	37.17315256	54.65257263	61.80817172	
1.20_183.0843m/z	183.084278	1.199716667	pos							18913.6527	21747.38479	21703.71697	27927.38033	26446.92973	26713.66602	21810.40574	27221.34926	25121.26685	
1.20_183.0900m/z	183.0900489	1.199716667	pos							1459.962308	1231.941273	1730.175026	2179.791877	1774.141547	1578.026554	1185.692369	1472.619744	1372.381813	
1.20_202.9634m/z	202.9634443	1.199716667	pos							3234.822335	3076.013061	3233.668087	2777.811714	2450.39986	2656.8468	2748.919039	2745.052025	3094.315238	
1.20_203.0556n	204.0628625	1.199716667	pos							5509.083529	6458.420481	6699.584847	8551.960305	8411.298284	8069.548708	7193.117577	8471.730035	7194.117777	
1.20_206.0398m/z	206.0398309	1.199716667	pos							1234.516296	1352.863947	1595.987429	1145.21274	1198.496248	1610.223476	1337.995129	1288.276505	1506.09558	
1.20_217.9802n	218.9874568	1.199716667	pos							12587.87025	13113.73014	13281.27151	9923.277965	9848.985687	9110.328155	12353.46421	12105.9674	11681.18775	
1.20_223.9629n	224.9715508	1.199716667	pos							604.5086898	924.3207292	1055.446299	744.1942258	729.0581638	939.0148598	610.1107023	900.7489036	850.5333305	
1.20_225.9794m/z	225.9794107	1.199716667	pos							37952.4952	39110.36811	38754.85551	32155.14984	31332.72805	33301.85707	34327.6999	36346.81392	35549.0082	
1.20_228.1430m/z	228.1429918	1.199716667	pos							69.96126371	163.0100385	118.2776787	282.5184217	381.8050689	289.693385	0.001403199	359.7845097	133.5201133	
1.20_237.1218m/z	237.1217525	1.199716667	pos							173.3004972	339.5561305	153.0833486	0.001403199	0.001403199	0.001403199	87.32579006	205.5629616	121.754886	
1.20_245.9814m/z	245.981437	1.199716667	pos							468.0913849	1649.604908	1594.082174	594.6094444	780.6116452	710.4204808	592.3020551	1231.216892	1514.213958	
1.20_251.9582m/z	251.9581505	1.199716667	pos							5095.445617	5658.990242	4769.807251	5246.878969	5149.36605	5400.279576	5166.056698	5065.759369	5393.340352	
1.20_280.9983n	282.0056171	1.199716667	pos							3233.609466	3632.8301	3108.315851	3510.439032	3714.28342	3037.191186	3207.320745	3889.5347	3679.814541	
1.20_281.1603m/z	281.1602607	1.199716667	pos							270.5354691	307.9775213	380.069155	0.001403199	0.001403199	92.12095887	96.35724322	0.001403199	148.1002064	
1.20_313.9622m/z	313.9621974	1.199716667	pos							783.6439987	736.3427592	1161.998923	873.9499043	881.8010124	1545.412803	895.1224814	1022.100754	912.7877731	
1.20_333.9674m/z	333.9674297	1.199716667	pos							2491.039695	2757.293483	2641.69838	4568.14646	3676.068263	3945.468561	3012.56309	3532.242825	3522.205866	

1.20_338.9365m/z	338.9365081	1.199716667	pos	2917.492437	2583.458412	2634.740308	2793.085617	2856.630276	2296.775572	2952.373704	3151.742663	3099.818184							
1.20_389.9180m/z	389.9180407	1.199716667	pos	2237.948383	2105.648579	2236.867205	1865.864264	1944.623679	1513.595199	2035.613216	1842.031647	1877.617862							
1.22_127.0188m/z	127.018767	1.22075	pos	606.1493496	634.8777723	689.9459839	268.38616	333.6284932	469.7892233	406.2250224	394.132163	364.0545641							
1.22_130.9771m/z	130.9771176	1.22075	pos	26.90910256	51.85759669	0.001403199	25.34118837	0.001403199	0.001403199	27.89514389	55.78815746	0.001403199							
1.22_194.0182n	212.0526385	1.22075	pos	11767.2114	12930.15889	13522.08694	16296.61765	16402.50873	15887.76387	13730.56132	16532.72944	15515.38445							
1.22_197.5068m/z	197.506803	1.22075	pos	246.8827075	340.1523344	145.3847896	281.6503671	278.1868429	459.0678497	51.43566594	161.4348297	218.4454397							
1.22_201.9990m/z	201.9989817	1.22075	pos	48.7726101	0.001403199	0.001403199	53.09831696	161.4739437	0.001403199	50.46630209	42.91730976	69.43892479							
1.22_204.9639m/z	204.9638699	1.22075	pos	338.9976949	428.2487834	304.820052	214.0863887	269.7097862	566.6842464	385.6060651	452.9723168	407.5686666							
1.22_209.5164m/z	209.5163942	1.22075	pos	201.0158451	203.7980353	118.2187151	533.3864736	273.9575182	261.8337868	0.001403199	185.6484375	216.0742615							
1.22_217.9982m/z	217.998179	1.22075	pos	3907.317587	3858.513965	3752.140058	4314.172774	4214.672721	4427.310002	4037.150528	3641.483176	3827.202841							
1.22_229.5279m/z	229.5278725	1.22075	pos	234.7030292	397.3195757	332.8633878	389.4121206	283.2246936	274.151383	81.09274972	71.94803713	124.1715134							
1.22_303.0683m/z	303.0682586	1.22075	pos	3285.54414	3930.8653	4114.265781	5196.771986	5182.579006	5276.949962	2598.390052	3781.596664	3623.582738							
1.24_157.0858m/z	157.0858388	1.243033333	pos	1172.048404	1002.273328	1058.881138	1034.048796	1126.149961	994.3319734	1059.710824	985.4123597	978.1556326							
1.24_159.5302m/z	159.5301951	1.243033333	pos	1580.70877	1699.408159	1837.766585	2563.226747	2509.083604	2445.661853	1764.69109	1931.740042	1872.992906							
1.24_186.0556m/z	186.0556364	1.243033333	pos	1076.358834	1264.48948	1446.009683	468.4029199	451.5693169	374.4842693	818.3308339	1038.559236	890.4699671							
1.24_190.0297n	208.0635901	1.243033333	pos	68440.19192	74889.07284	77314.49756	46479.32761	42600.92814	43837.50201	42926.94369	50487.47629	47406.13012							
1.24_199.5086m/z	199.5086031	1.243033333	pos	849.3941887	848.8922473	982.959717	1357.675461	1213.658712	1421.20287	966.9808236	895.5666885	1098.624352							
1.24_217.0142m/z	217.0142395	1.243033333	pos	272.3829985	221.7253461	357.1456606	48.18443825	0.341556717	35.97282	123.293145	56.71910233	219.2204598							
1.24_226.9748m/z	226.9747882	1.243033333	pos	7590.042994	8286.229281	7024.167606	8960.759823	8536.254184	8865.630556	8108.825772	8190.593754	7887.196676							
1.24_274.1030m/z	274.1029604	1.243033333	pos	9531.210199	10409.98624	10571.95817	10032.19623	9004.488419	9597.290619	9109.541976	10473.22514	9427.837691							
1.24_275.9732m/z	275.9731647	1.243033333	pos	2849.939507	2587.607767	2430.6288	2827.520802	2810.687065	2840.198566	2934.427425	2975.065136	2954.540983							
1.24_291.9932m/z	291.9931928	1.243033333	pos	2014.61845	2217.344902	2370.726524	1025.901247	759.7702465	799.94067	1600.148059	1997.498684	1932.051701							
1.24_306.0014m/z	306.0013721	1.243033333	pos	8077.505675	9883.582743	9144.954192	14120.95977	14469.44289	13888.80803	9713.917408	13173.72706	10563.82026							
1.24_315.9565m/z	315.9564822	1.243033333	pos	1555.849442	2899.325037	3173.551481	2701.985476	2707.185488	2813.040959	1936.593852	3215.589597	3135.17293							
1.24_373.9865n	356.9832567	1.243033333	pos	12213.23232	12135.52318	12065.70263	13838.51285	13616.01853	13357.27529	9163.767355	11157.74283	9245.806685							
1.24_454.9505m/z	454.9505129	1.243033333	pos	1017.991343	1359.593762	1489.398004	1848.225882	1933.482558	2223.08714	1207.481918	1453.345889	1283.034747							
1.26_156.5229m/z	156.522867	1.264483333	pos	312.8160883	132.9961568	267.0373344	361.5490493	332.5429183	428.1428709	235.1644432	493.2881908	392.3483557							
1.26_164.0170m/z	164.017029	1.264483333	pos	827.7670635	878.9712237	892.0737637	1305.825952	1420.148094	1204.643388	895.7305504	895.2396541	795.1243355							
1.26_164.5188m/z	164.5188031	1.264483333	pos	0.001403199	49.78041648	77.09811367	114.2953193	71.04745972	64.67457459	32.01067888	0.001403199	109.819829							
1.26_169.0858m/z	169.0857544	1.264483333	pos	669.9192567	601.5584914	675.9517857	489.5263692	587.5479971	518.1757609	553.4618692	716.8338848	573.5575644							
1.26_197.9922m/z	197.9921563	1.264483333	pos	999.5311649	852.8639925	717.3790715	752.7523481	690.5694058	771.7293108	838.1529399	699.9672394	734.9726725							
1.26_229.0874m/z	229.0873545	1.264483333	pos	0.001403199	135.1882596	48.94746607	0.001403199	50.10904683	57.78196762	49.68735102	75.87056351	62.97713298							
1.26_235.0187m/z	235.01868	1.264483333	pos	767.0389847	683.2082907	707.7300817	1021.003757	1087.383264	1174.138177	784.5799469	908.0285059	795.7245635							
1.26_239.9950m/z	239.9949673	1.264483333	pos	4195.952146	3973.588369	3748.82641	1344.515598	1582.933281	1908.910813	1464.349028	1487.499573	1393.444188							
1.26_268.9698m/z	268.9697985	1.264483333	pos	18591.07107	19508.6472	17683.54311	9482.859253	8949.425513	9125.591292	9740.430296	8631.031954	9213.4717							
1.26_290.9791m/z	290.9790586	1.264483333	pos	686.0280014	687.561359	574.7360716	995.0918627	712.0531047	769.7758843	658.3536404	658.2193871	720.2847382							
1.26_292.1498m/z	292.1498142	1.264483333	pos	2732.667561	1922.395617	2486.781682	4803.426535	4734.34551	5003.953125	3759.257645	3916.783839	3913.466193							
1.26_360.9782m/z	360.9782135	1.264483333	pos	3757.678867	3267.515723	3517.213482	1035.435355	1069.203118	957.7078866	1027.81652	1245.356538	1309.638465							
1.29_151.0865m/z	151.0864603	1.285033333	pos	374.1565778	205.2930495	234.3869754	199.9935431	200.8119861	211.0393277	275.6874013	233.1638581	143.9968614							
1.29_170.4691m/z	170.4691204	1.285033333	pos	270.6242559	242.8822981	319.9176919	369.7383772	407.2454705	275.5946058	396.8806716	286.2579805	383.3076929							
1.29_173.1171m/z	173.1170762	1.285033333	pos	2249.374831	2420.513139	2393.150896	2096.51392	2027.821628	1719.245218	2068.986791	2142.418162	1961.321209							
1.29_174.4552m/z	174.4551776	1.285033333	pos	1930.127604	2387.582476	2087.513207	2454.118822	2362.90941	2365.672537	2369.773304	2297.913119	2282.041879							
1.29_181.0526m/z	181.052644	1.285033333	pos	560.7811656	925.0093043	995.9010556	615.9039126	624.4956456	599.0349841	834.1973332	973.8857073	974.2071328							
1.29_194.9685m/z	194.9684706	1.285033333	pos	601.3426884	558.5413357	596.4315238	808.2236146	882.6486659	671.1773776	549.9522508	423.8515849	545.098054							
1.29_219.9275m/z	219.9275423	1.285033333	pos	886.6123103	854.0631903	740.6305852	812.3312328	754.8487465	914.4403372	1137.628808	887.5601382	849.4450052							
1.29_261.9076m/z	261.9075519	1.285033333	pos	3872.436746	4359.522101	3848.129669	4471.011724	4312.044176	4144.3834	4397.168858	4096.876294	4307.490179							
1.29_318.8865m/z	318.8864688	1.285033333	pos	1001.07728	671.2965503	842.5411703	679.7791697	927.7603834	946.4440559	1161.658271	624.8376499	911.6318902							
1.29_319.9518m/z	319.9517662	1.285033333	pos	1302.284855	1717.560059	1618.756209	307.1827178	382.5281831	144.6206035	355.4750273	618.6043461	452.359243							
1.29_331.0041m/z	331.0040752	1.285033333	pos	3011.188624	2914.229571	3151.401904	542.8150296	730.0413158	506.5693802	1223.24282	1557.850182	1936.982724							
1.29_416.0268m/z	416.026835	1.285033333	pos	5863.396027	7703.186674	7957.953468	2240.356958	2377.082533	2433.674894	2120.707749	1999.899477	3129.662633							
1.31_119.0254m/z	119.0253613	1.30655	pos	7105.65829	7253.469369	7015.590334	6851.559309	7272.202143	7323.731233	7260.607799	7233.170902	7323.059348							
1.31_167.1064m/z	167.1064442	1.30655	pos	1876.679385	1972.53904	1697.875503	1904.006954	1711.938387	1693.504646	1762.424937	1993.291673	1865.356236							
1.31_197.1170m/z	197.1170075	1.30655	pos	622.145555	915.7708959	645.2897166	577.4985675	509.4218549	513.0734812	681.3060164	521.7660591	584.7019795							
1.31_202.9982m/z	202.9981848	1.30655	pos	287.8809606	348.9100172	428.7099059	495.5679847	343.71804	456.0449326	444.74765	496.5224103	376.265082							
1.31_226.0117m/z	226.0116578	1.30655	pos	1270.056264	1440.884201	1347.156252	842.1559063	777.8920647	861.3177003	1127.567143	1343.04004	1692.022691							
1.31_254.9490m/z	254.9490063	1.30655	pos	107.7586048	477.3370888	123.1903565	123.9679918	159.7228766	220.0167955	217.8881137	156.1012077	109.3245007							
1.31_334.8712m/z	334.8712261	1.30655	pos	19329.9596	20493.49176	18413.86616	19557.29075	22223.87063	21640.5481	22021.67265	21422.6443	20483.94052							
1.31_365.0450m/z	365.0450058	1.30655	pos	481.8540762	1653.522723	1777.248422	284.4241485	294.5033641	563.0568916	263.8881319	682.6070089	675.5037213							
1.31_372.0306m/z	372.030617	1.30655	pos	1316.684863	2195.449433	2325.675171	0.001403199	341.776589	219.1528371	678.5278431	1015.730453	890.4999549							
1.33_108.5170m/z	108.5170299	1.327966667	pos	0.001403199	0.001403199	21.32009933	0.001403199	3.635386312	36.67947262	34.92754496	19.2551918	19.58862684							
1.33_112.0395m/z	112.039454	1.327966667	pos	1195.965556	1503.077731	1213.91649	967.7410977	1049.791174	1061.900633	1185.295739	1168.995567	1119.840333							
1.33_129.0522m/z	129.0521717	1.327966667	pos	1297.543967	1270.865947	1192.03267	1070.526167	1122.08015	1061.385522	1340.496036	1149.061363	1140.370547							
1.33_154.9667m/z	154.9666851	1.327966667	pos	761.1235638	1030.999466	754.9432212	704.2942063	733.8216716	680.3592939	728.2475397	736.9975286	841.7960011							
1.33_168.0310m/z	168.0310006	1.327966667	pos	371.8811733	396.7743946	466.6667112	567.8761128	466.2600991	429.0107832	453.8389837	572.9433043	567.329542							
1.33_168.0878m/z	168.087769	1.327966667	pos	4019.535994	4360.660126	4354.694671	3727.901422	3665.640792	3536.166421	3213.226473	3249.452397	2993.607408							
1.33_173.9846m/z	173.9845891	1.327966667	pos	403.5208166	537.5216762	403.5096685	464.6774772	410.1245423	424.9171465	402.4892799	393.3622894	322.2919195							
1.33_178.9903m/z	178.9902823	1.327966667	pos	1154.776141	1080.120271	998.1160125	1003.794781	932.5785899	1017.243036	1154.8279	964.5928268	978.0170826							
1.33_180.0740m/z	180.0740381	1.327966667	pos	7665.251089	6153.126545	6752.716781	1219.423693	1145.3472	1314.118715	6032.211407	5696.670355	6274.474946							
1.33_215.9794m/z	215.9793618	1.327966667	pos	1843.137491	2170.806028	1730.48267	1623.262137	1623.622532	1644.122763	1821.398813	1654.622725	1621.367878							
1.33_221.0042n	243.9900789	1.327966667	pos	6204.88324	6092.980564	6304.555881	4689.554671	4326.993322	4454.903338	3514.073279	4336.971671	4162.538298							
1.33_230.9457m/z	230.9457325	1.327966667	pos	3531.050454	4009.64129	3368.926647	3325.555071	3679.846103	3600.924127	3746.455081	3757.023087	3519.444948							
1.33_233.5194m/z	233.5193694	1.327966667	pos	1468.721295	1642.898589	1702.014177	1606.895585	1454.042032	1703.969565	1261.290018	1472.281707	1512.828914							
1.33_233.9127m/z	233.9127363	1.327966667	pos	428.5960412	513.9906498	421.7171711	297.2355378	452.9732386	427.2415232	498.0328411	465.0959049	489.6906466							
1.33_234.0210m/z	234.0210112	1.327966667	pos	125.8202304	212.4533451	283.5707838	228.1909036	136.0565481	112.9498414	128.1597472	204.9678593	197.9617628							
1.33_282.9102m/z	282.9101675	1.327966667	pos	2805.797547	2498.899931	2117.197573	2089.799519	1911.943098	2021.31104	2283.849966	1721.272684	2217.841024							
1.35_111.9845m/z	111.9845209	1.350266667	pos	1479.547947	1525.675644	1204.053198	1254.706016	1333.173704	1329.698479	1372.002485	1315.463201	1301.12466							
1.35_174.9975m/z	174.9975204	1.350266667	pos	397.3482312	502.3981535	502.5284907	316.1979331	374.9883803	347.2928712	351.1071255	496.1843078	437.0762069							
1.35_199.1075m/z	199.1074766	1.350266667	pos	530.4078027	435.045325	287.0055429	206.9659321	231.5377078	372.9256841	262.1481273	140.8587742	229.9596329							
1.35_206.0844m/z	206.0844213	1.350266667	pos	0.001403199	66.49461712	96.71878127	95.67664663	71.6893758	0.001403199	0.001403199	85.20517731	0.001403199							
1.35_228.9824m/z	228.9823571	1.350266667	pos	161.2244376	122.0835577	166.8001749	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	87.7275904							
1.35_239.1488m/z	239.1488148	1.350266667	pos	1238.45403	1661.900432	1294.852608	1227.394667	1300.466844	1288.315249	1433.812375	1304.861409	1223.832162							
1.35_243.1593m/z	243.1593114	1.350266667	pos	1579.221906	1466.930697	1887.144366	1909.845653	1783.452882	1805.95939	1456.273915	1291.550117	1902.645125							
1.35_248.9955m/z	248.9954875	1.350266667	pos	1506.650894	1548.587853	1340.394102	1047.115519	883.7001268	1091.235328	1163.710661	1067.744985	1332.047275							
1.35_270.9720m/z	270.9720204	1.350266667	pos	240.1186915	386.2361269	387.1486696	234.4159044	220.8603242	313.100935	349.3941698	368.7916392	212.3803548							
1.35_271.9722m/z	271.9722244	1.350266667	pos	731.7057139	931.7485873	374.7474477	547.3175968	697.7454028	669.3901868	900.0157636	577.3670865	694.5812282							
1.35_291.0696m/z	291.0695679	1.350266667	pos	2157.4821	2695.755338	2950.436395	1980.019998	1749.043304	2092.222997	1402.714343	2326.610993	1922.810479							
1.35_309.0010m/z	309.0010305	1.350266667	pos	3062.623162	2562.398137	2627.094149	2396.289642	2530.719944	2245.826503	2357.282148	2374.005666	2198.336876							
1.35_347.1920m/z	347.1919868	1.350266667	pos	5409.275687	5541.578902	5673.743573	10080.57	9903.917952	9609.747597	6642.325503	8138.24317	7562.082059							
1.37_147.0762m/z	147.0762221	1.372566667	pos	287.8435822	321.7897703	383.0204409	360.7440622	437.7414684	410.2034305	312.0132284	394.715908	420.7481506							
1.37_154.0295m/z	154.0295479	1.372566667	pos	0.001403199	0.001403199	0.001403199	0.001403199	25.33146352	0.001403199	1560.269489	1553.709283	1414.379418							
1.37_170.5203m/z	170.5202626	1.372566667	pos	2426.737581	2150.284791	2609.998672	3299.690684	3199.577155	3338.996601	2835.693206	3464.780829	3492.093278							
1.37_182.0283m/z	182.0283004	1.372566667	pos	5258.665926	4918.320225	4807.752401	6484.589314	6238.726434	6840.701216	6271.518061	7053.655167	6935.910843							
1.37_182.5302m/z	182.530156	1.372566667	pos	426.3266403	553.6637874	550.3157462	768.5288796	861.8471562	735.2418141	763.6390555	740.6626207	740.9125816							
1.37_192.9636m/z	192.9635806	1.372566667	pos	44.56962949	0.431572713	46.36823297	125.2455015	45.806724	121.4112156	38.53021076	50.0557684	28.92619517							
1.37_239.0110m/z	239.0109997	1.372566667	pos	1355.064683	1994.213555	1784.518061	601.1610612	763.0183355	579.6064526	857.7110803	1213.6273	1351.26285							
1.37_271.0411m/z	271.0410686	1.372566667	pos	2923.979669	3888.581382	3974.952983	4621.769958	4416.5428	4801.354554	4909.451206	5006.097342	4903.096901							
1.37_275.9732m/z	275.9732461	1.372566667	pos	3334.225728	3745.006467	3867.900516	4026.252763	4208.819101	3955.922482	4162.238169	4023.185471	3624.956116							
1.37_280.0124m/z	280.0123925	1.372566667	pos	3671.221912	3435.193837	3483.15946	5136.514875	4823.267526	4526.221457	4281.476668	4800.036004	5131.219325							
1.37_310.8503m/z	310.8502515	1.372566667	pos	2002.011909	2063.519661	1743.940656	1848.394168	2232.220018	2118.807975	2184.45065	2160.791832	2238.475423							
1.37_311.8550m/z	311.855038	1.372566667	pos	270.2413029	68.43667077	0.001403199	189.5541787	168.2216273	0.001403199	169.2673683	229.2175713	233.7150759							
1.37_322.0228m/z	322.0228463	1.372566667	pos	13648.71388	13368.90319	14311.61826	19921.83076	18316.18519	18655.46701	17431.52796	20032.36098	19105.84564							
1.39_110.0170m/z	110.0169784	1.39465	pos	0.001403199	13.73411204	0.001403199	40.70103026	10.96209494	20.33020375	30.56678732	0.001403199	0.001403199							
1.39_113.9605m/z	113.9604541	1.39465	pos	418.8860953	294.8151414	276.0498236	495.7094703	411.8305422	476.5299908	431.7124888	474.5362653	363.0917156							
1.39_149.0344m/z	149.0344263	1.39465	pos	207.5893029	216.6163546	192.7654684	214.1656531	219.5283762	97.79283115	177.6112108	69.17895699	126.5850492							
1.39_190.9667m/z	190.9667234	1.39465	pos	5588.450272	5926.579369	6058.218396	7303.696186	7199.699902	6857.93229	6358.644372	6327.347845	6841.895428							
1.39_228.0475m/z	228.0474753	1.39465	pos	1397.731958	1486.525253	1423.929112	1408.351648	1442.92823	1523.715566	1300.258826	1503.727656	1466.075342							
1.42_110.0201m/z	110.020145	1.415933333	pos	253902.2365	254914.3578	236201.4799	247693.0044	256388.7004	243816.8903	271834.923	240827.4202	228748.9872							

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1.66_179.0788m/z	179.0787615	1.655616667	pos
1.66_182.9849m/z	182.9849433	1.655616667	pos
1.66_197.1170m/z	197.1169874	1.655616667	pos
1.68_108.0151m/z	108.0151257	1.6764	pos
1.68_126.0298m/z	126.0297589	1.6764	pos
1.68_128.0048n	167.0560882	1.6764	pos
1.68_130.1225m/z	130.122489	1.6764	pos
1.68_139.9631m/z	139.9630588	1.6764	pos
1.68_141.0537n	124.0504528	1.6764	pos
1.68_152.0218m/z	152.0218132	1.6764	pos
1.68_158.9617n	141.9584258	1.6764	pos
1.68_181.9771m/z	181.9771315	1.6764	pos
1.68_227.0148m/z	227.0147621	1.6764	pos
1.68_266.9806m/z	266.9806437	1.6764	pos
1.68_284.0752n	285.0825052	1.6764	pos
1.70_150.0890n	173.0781322	1.697866667	pos
1.70_154.0690m/z	154.0689677	1.697866667	pos
1.70_171.0622m/z	171.0622469	1.697866667	pos
1.70_196.1541m/z	196.1541228	1.697866667	pos
1.70_201.0731m/z	201.0730578	1.697866667	pos
1.70_282.9756m/z	282.9755877	1.697866667	pos
1.70_304.9574m/z	304.957432	1.697866667	pos
1.70_419.0137m/z	419.0136732	1.697866667	pos
1.72_110.0169m/z	110.0169254	1.7202	pos
1.72_125.9862m/z	125.9861606	1.7202	pos
1.72_151.0274m/z	151.0273966	1.7202	pos
1.72_283.1396m/z	283.1396151	1.7202	pos
1.74_107.5175m/z	107.517534	1.741883333	pos
1.74_129.0522m/z	129.0521592	1.741883333	pos
1.74_130.9772m/z	130.9772434	1.741883333	pos
1.74_159.0682n	160.0754376	1.741883333	pos
1.74_172.9561m/z	172.9561335	1.741883333	pos
1.74_179.0804n	180.0876854	1.741883333	pos
1.74_199.9751m/z	199.975109	1.741883333	pos
1.74_224.9327m/z	224.9327426	1.741883333	pos
1.74_253.9098n	276.8963074	1.741883333	pos
1.74_288.1437m/z	288.1436723	1.741883333	pos
1.74_304.8916n	287.8883602	1.741883333	pos
1.74_328.9149m/z	328.9148592	1.741883333	pos
1.76_115.9620m/z	115.9620234	1.76405	pos
1.76_140.9510m/z	140.9509644	1.76405	pos
1.76_179.4929m/z	179.4929092	1.76405	pos
1.76_186.1121m/z	186.1121495	1.76405	pos
1.76_215.0887m/z	215.0886714	1.76405	pos
1.76_217.9982m/z	217.9981667	1.76405	pos
1.76_220.4290m/z	220.4289761	1.76405	pos
1.79_111.9845m/z	111.9844989	1.7859	pos
1.79_148.9329n	149.9401388	1.7859	pos
1.79_155.9741m/z	155.9740556	1.7859	pos
1.79_167.1064m/z	167.106425	1.7859	pos
1.79_178.9903m/z	178.9902681	1.7859	pos
1.81_113.0347m/z	113.0346694	1.807733333	pos
1.81_154.9849m/z	154.9848835	1.807733333	pos
1.81_158.0082m/z	158.0082012	1.807733333	pos
1.81_158.5100m/z	158.5099765	1.807733333	pos
1.81_168.0308m/z	168.0308199	1.807733333	pos
1.81_178.5214m/z	178.5214004	1.807733333	pos
1.81_193.0831m/z	193.0831395	1.807733333	pos
1.81_200.1158n	223.1049525	1.807733333	pos
1.81_214.4863m/z	214.486314	1.807733333	pos
1.81_221.0604n	244.0496025	1.807733333	pos
1.81_227.9826m/z	227.9826152	1.807733333	pos
1.81_228.4838m/z	228.4837958	1.807733333	pos
1.81_241.0380n	242.0453101	1.807733333	pos
1.81_246.9962n	229.9929195	1.807733333	pos
1.81_290.9851m/z	290.9850887	1.807733333	pos
1.81_298.0596n	299.0668352	1.807733333	pos
1.81_332.0147m/z	332.0146535	1.807733333	pos
1.81_341.9700m/z	341.9700069	1.807733333	pos
1.83_129.9539m/z	129.9538588	1.829866667	pos
1.83_142.9665m/z	142.966496	1.829866667	pos
1.83_182.0784m/z	182.0783869	1.829866667	pos
1.83_209.0781m/z	209.0781036	1.829866667	pos
1.83_220.9614m/z	220.961443	1.829866667	pos
1.83_261.1304m/z	261.1304075	1.829866667	pos
1.83_339.0682m/z	339.0681662	1.829866667	pos
1.85_128.0423m/z	128.0423198	1.8515	pos
1.85_197.0119m/z	197.0119312	1.8515	pos
1.85_202.9509m/z	202.9508651	1.8515	pos
1.85_300.8797m/z	300.8797398	1.8515	pos
1.85_300.9202m/z	300.920201	1.8515	pos
1.85_306.8937m/z	306.8936995	1.8515	pos
1.85_319.2258m/z	319.2257937	1.8515	pos
1.87_201.0730m/z	201.0730142	1.872316667	pos
1.87_239.9949m/z	239.9948913	1.872316667	pos
1.89_142.0609m/z	142.0609114	1.894366667	pos
1.92_124.0505m/z	124.050494	1.916533333	pos
1.92_130.9772m/z	130.9772237	1.916533333	pos
1.92_139.9820m/z	139.982	1.916533333	pos
1.92_168.5355m/z	168.5354808	1.916533333	pos
1.92_188.0308n	189.0380323	1.916533333	pos
1.92_193.0962n	194.1034691	1.916533333	pos
1.92_250.9593m/z	250.9592812	1.916533333	pos
1.92_263.0110m/z	263.0109936	1.916533333	pos
1.92_266.9807m/z	266.9806636	1.916533333	pos
1.92_308.0070m/z	308.007045	1.916533333	pos
1.92_371.1006m/z	371.1005967	1.916533333	pos
1.94_161.9731m/z	161.9730936	1.938766667	pos
1.94_302.9454m/z	302.9453767	1.938766667	pos
1.94_306.5824m/z	306.5824101	1.938766667	pos
1.96_171.0623m/z	171.0623021	1.961133333	pos
1.96_199.6050m/z	199.6050318	1.961133333	pos
1.96_282.9101m/z	282.9100734	1.961133333	pos
1.96_286.0691m/z	286.0690758	1.961133333	pos
1.96_288.1434m/z	288.1433734	1.961133333	pos
1.98_140.9510m/z	140.9510422	1.982566667	pos
1.98_199.0823m/z	199.0823308	1.982566667	pos

1542.937529	1412.545268	1606.928636	806.263905	783.3513412	779.4107202	1423.168777	1433.034664	1564.359108
3161528.404	3046501.043	2917196.465	2979036.03	3139001.259	3066723.072	3252918.601	2977603.965	3083600.242
620.894436	578.7520712	586.3136471	529.2714423	526.8184701	446.367565	453.9777818	555.7927416	510.0823998
584.4113968	695.3536713	767.8737972	1126.551544	1219.369309	1177.151065	781.1746954	974.6099548	1016.60187
88.18931984	107.5607854	88.1628196	97.82803235	146.4306366	128.1772369	147.5008357	79.3978653	110.7772938
52528.74617	55752.05967	57928.26938	73913.49683	69866.49272	71511.56725	60261.93522	66975.94797	65970.47002
329.1418177	291.9840821	340.2131472	339.8791528	336.2242333	398.1896446	383.6920015	337.6907099	363.9653175
68565.68642	65487.56722	63279.33442	66212.43614	68531.29768	67448.23106	70121.16311	64709.03314	67003.7148
538.6966423	553.3855113	663.8868029	758.6571698	760.6669263	794.112615	646.8552573	614.880382	580.8882659
481.5148678	641.9238692	560.2612122	499.3488538	427.0536881	416.3847014	396.9683929	476.949021	377.738585
1980096.848	1888358.122	1855467.389	1941234.804	2036673.826	2015264.4	2064494.098	1914161.504	1993203.659
5447.873097	5220.616862	4999.934855	4422.754649	4703.745647	4387.385048	5500.624009	4863.009856	4684.75207
4719.395248	4717.110945	5371.587856	5467.502644	5711.194417	5967.854636	5631.520784	5704.51675	5589.342134
2166.229022	1995.180053	2479.768351	2651.699246	2517.874348	2717.78464	2309.768687	2577.990227	2744.59406
16808.45704	18154.11696	18701.92122	14255.83761	13165.87049	13301.021	12231.56499	13837.34751	13571.85514
43781.51328	33196.66887	31009.9239	30135.63552	30980.94625	32962.24386	36338.68058	33415.76092	34678.34197
0.001403199	21.88329606	21.37662907	405.5570592	409.9842998	410.3213158	94.21490431	129.7377367	54.6128838
490.5039848	471.2389809	583.2550038	480.9357506	502.7673473	483.7555809	532.6270035	459.9464883	506.8950431
2633.080079	2166.106795	2126.789557	1710.82978	1852.209594	1664.870557	1971.383167	1930.571429	2021.014237
1165.353223	1082.885055	1111.519071	875.7703396	1015.838137	905.2055296	973.4182353	1119.042695	1154.949626
10778.12244	10490.33095	11563.65478	11758.90308	11945.31362	12122.66233	10720.84702	12594.60072	11621.71562
1836.663265	1158.250959	2013.694409	695.0765855	1397.421962	1595.87947	1732.635232	2445.987983	2096.959504
1430.829022	1180.412195	1566.983199	1676.965002	1455.194551	2057.700885	1414.164504	2004.681536	1884.236597
11.93894499	0.001403199	0.001403199	24.72430073	22.62822704	0.001403199	0.001403199	0.001403199	0.001403199
5644.468855	5282.197422	5473.539599	5357.054925	5983.69798	5299.381799	5807.357093	5635.16452	5262.384569
170.3421465	92.06071035	106.6977886	46.52972729	38.88214015	114.6649301	170.7437984	141.4200476	91.67864101
2227.949069	2308.421178	2221.771003	262.6984951	222.7126964	250.6249796	749.6997572	801.0310364	784.6659501
162.1168672	132.9636606	126.5754859	144.4471315	144.3249218	137.1660521	148.1596882	150.5133851	148.6740112
723.1065666	683.3560473	603.9360994	585.0634859	589.9077826	573.573491	709.6416283	599.8082424	646.5304336
0.001403199	0.001403199	49.4994675	0.001403199	0.001403199	17.84180895	22.66728701	28.41448021	31.42889861
3119.105915	3057.46975	2877.610836	3061.787074	3025.520125	2869.64595	2813.179998	2955.683948	2766.432925
326523.0225	315746.2078	300336.7839	304604.2149	320819.3104	318029.1736	342434.4575	310380.1163	321872.1996
5738.000608	5958.530965	6074.054167	3427.327815	3763.644647	3571.785836	5004.600297	5157.447837	5183.208923
135286.3937	127856.4618	123342.7145	130581.338	139693.4113	136516.8849	142126.1772	127554.4247	134657.531
1381.964477	1079.768351	1139.814138	1070.715041	1246.746559	1260.022945	1237.524449	1057.772211	1281.985298
102129.9743	93324.53026	89662.03731	91369.43358	96251.69879	95925.84317	97449.4399	93433.67643	97754.72536
1899.329159	1933.174743	2114.484855	3396.736916	3252.20951	3031.235326	2055.851244	1976.640767	2272.994099
141154.577	134309.2597	130272.7639	133579.5872	143416.5477	139359.7496	144051.4825	132973.5251	141264.633
106663.983	100728.9568	94903.20432	96408.41	102485.934	99074.8921	106846.2012	102621.65921	101509.5938
18.73323073	71.13747464	164.6942651	98.99643098	89.70800658	120.1431496	107.7744556	265.5954476	133.3369184
735.5042609	675.0270701	628.2488032	612.8571293	719.7045482	703.4848063	649.7811888	684.9008865	736.0892293
33.0744692	34.99738511	63.96283863	67.11543414	161.8208541	97.79680781	102.0291355	26.93410681	81.35804942
2415.59657	2412.178251	2498.42236	2146.841379	2493.748511	2253.903203	2308.698668	2369.930453	2368.026382
436.4703085	464.4152757	505.5539076	430.9663998	417.3905713	437.7900293	496.8786812	565.3839132	523.6831454
1246.625176	1154.547462	1279.821581	1280.269376	1342.504572	1303.041125	1166.097527	1364.408224	1250.219198
90.57483835	71.13926054	89.3393367	53.50771868	82.09803477	79.03290296	133.6407027	35.04134369	127.9808433
1559.373885	1477.744966	1553.402091	1405.833693	1550.452489	1438.133642	1541.018732	1604.036737	1506.180769
10228.24844	10595.81939	10189.33985	10187.0122	10285.92603	9375.471668	11388.99583	10232.88293	9989.244632
828.9759915	896.6350665	866.0136128	756.2036097	841.7913773	793.9788914	847.6263338	835.7910867	854.4540459
1872.545944	1769.564031	1896.678679	1706.957911	1763.718041	1738.363566	2051.425137	1741.382339	1568.935629
1589.185014	1557.669051	1466.190896	1541.894928	1508.638021	1496.118495	1390.992118	1494.894836	1539.538916
7161.258141	6637.356133	6565.408909	6904.955927	6964.136257	7130.583901	7371.107145	7045.215012	7028.384288
76.98827201	125.8407612	146.4713675	0.001403199	0.001403199	51.54248251	201.6424929	103.1011581	50.87480755
3849.568936	4057.437638	4388.586436	2519.680566	2782.658693	2819.171675	4148.718007	4774.871237	4418.767502
355.0267128	410.3540209	433.2692397	232.4554177	170.1243251	203.0937307	328.3518864	417.3265581	453.4682893
324.7817329	569.712327	643.3850505	776.9324227	1016.436537	749.7765321	710.8860658	510.5268961	648.8579929
1137.066767	1253.358191	1254.840738	720.5922758	664.2312503	646.5916408	1112.846877	1333.175205	1159.89588
2217.909453	2148.797373	1989.103478	1760.411637	1709.08836	1763.923178	2090.844207	1791.411024	1701.390793
27475.12193	30291.99201	31166.86487	36403.64807	34444.28393	34076.60388	23704.96041	26781.45639	24984.01114
218.6889977	175.0512241	116.5928583	0.001403199	58.08429768	88.55984512	127.6426142	211.9685726	146.6883581
505.3719677	481.1338433	364.3075627	194.5477028	128.2196352	237.1414689	536.4783717	573.1379691	532.8584118
1825.48133	2050.236497	1937.702824	1915.601178	2112.660025	1859.598365	1860.224447	1807.398296	1817.80316
163.179463	36.07173583	325.7296783	98.38596406	223.3647233	148.3446011	235.6425959	240.4686347	304.5233404
94337.30377	102667.4033	104224.3819	63557.59462	61200.26884	60423.5357	103576.8367	117716.6598	110118.5814
7383.665933	7810.555097	7833.423279	4270.931221	4315.597937	4328.752441	7392.273066	9046.535434	8449.870594
1491.741422	1803.692652	1514.678965	1137.274128	993.8273955	894.7883197	1625.930248	1692.352592	1534.202358
7748.657627	7704.694082	8537.200419	3480.769898	3283.845743	3459.370842	5150.487481	5351.5592	5171.369436
2284.758412	1840.582523	2381.931044	1048.647809	1142.172267	1065.220983	2755.119999	2971.225882	2712.275716
3370.759601	2922.5012	3544.699969	1833.621577	1771.576319	1780.495368	3744.273897	4329.532136	3799.476215
259.4952262	200.4032202	294.6355232	237.3797204	318.029137	249.4750625	293.805409	174.615274	244.2120088
2884.010082	2607.982163	3089.585133	2912.007526	3368.359129	3213.803735	3267.086367	3100.380563	3277.256549
646.4006335	560.9521674	619.7512488	610.3821305	771.3610313	737.330156	710.6403247	699.4396122	665.2836977
1308.848784	1266.739306	1062.089832	1155.269425	1207.046959	926.2521722	1291.306684	896.659282	1054.291971
2776.518275	2773.872221	2514.801632	2344.637354	2881.097355	2867.763115	2755.37003	2446.257708	2248.247874
1056.29408	1109.992358	981.1429374	844.1372653	900.6408222	902.88249	978.3301662	907.8010324	606.3498444
4025.855622	4136.647744	5282.456869	601.8221208	413.3403348	710.1269414	1209.959131	1862.811221	1472.210772
18.0658134	30.3505368	15.23891214	0.001403199	0.001403199	0.001403199	0.001403199	25.59501862	31.25173156
47.46530721	0.001403199	77.51115649	285.63503	262.0385775	255.3846618	122.3594551	172.0307893	146.3672187
280290.1038	270633.5207	264874.2524	278457.7951	295990.4899	295784.4262	301597.5426	275731.8221	286727.1234
386.9698788	258.1485073	345.5777383	401.4847402	481.5406598	381.3141681	520.6792835	201.6631438	319.4448271
1364.689371	1323.47668	1250.857247	1244.931628	1456.815266	1206.65234	1441.181624	1164.43559	867.6939669
1040.904128	1157.592695	1043.302164	1064.678684	1619.768866	1316.769154	1305.225129	1139.471167	1201.666593
879.6803436	814.1661787	596.0822123	447.961707	502.0369322	329.7582281	536.3391681	364.1677033	435.3555307
2975.045791	3093.599335	2972.43832	3084.458997	3026.760913	2926.789701	3067.48447	3561.975176	2825.877761
1478.83851	1669.068197	1646.086397	2104.521347	2080.873009	2028.012715	1500.607331	1533.766893	1027.950001
207.4791201	277.0326566	314.6848915	348.9459944	399.0829031	318.1847731	318.5646776	261.4229813	310.9160272
75.52936605	40.00017069	87.01030818	62.20029342	89.99723124	69.72634175	59.29237111	97.95827327	69.80431392
0.001403199	29.93239193	42.52958154	40.70939033	39.39725271	0.001403199	0.001403199	25.92985563	0.001403199
4910.031345	5184.997927	5141.657335	5165.52041	5392.694307	4911.839662	5751.681206	5229.077656	5081.57939
25.31057475	30.27087589	143.0027164	191.8003379	162.8494973	150.4023469	114.0787377	163.8766065	168.7977058
1577.426098	1404.654525	1399.824343	1635.316362	1623.927662	1680.609382	1618.432643	1741.03214	1511.694039
3324.233267	3191.296694	3777.473225	2502.916351	2674.990479	2671.045664	3096.500772	3575.732097	3429.910595
7340.930127	8004.775095	7568.030626	1446.335556	1276.933552	1410.642078	6127.381054	7478.171577	6310.992144
3608.751411	3873.202386	3670.959036	554.3888768	763.9059293	535.1544313	2860.570071	3069.739676	2532.207442
1492.983296	1998.546333	2025.325964	2370.981024	2307.974925	2123.095265	1802.839133	2274.503195	2005.660201
2203.802154	2071.619644	2325.629073	2964.59293	2768.805809	2549.20457	2195.172019	2676.121394	2522.956832
1315.440938	1214.407091	932.5323455	726.6963908	1062.804621	920.447741	866.0327254	940.0835072	938.2363695
0.001403199	0.001403199	42.05010684	33.41328465	87.77578047	0.001403199	0.001403199	24.13847938	0.001403199
2081.645342	1831.723461	2085.196371	0.001403199	0.001403199	0.001403199	0.001403199	402.9020401	486.1463814
1296.131206	1175.504285	1779.623245	0.001403199	0.001403199	0.001403199	840.9784824	1128.457485	1092.819351
839.4174555	1144.199466	1101.256577	720.7839961	817.6403363	614.8272814	891.6439553	799.7590494	829.1605097
64.77862815	88.50559712	178.0127981	33.58309411	0.001403199	113.9541272	126.2546668	118.341032	70.30826246
3567.568067	3513.524571	3286.347438	2943.327761	3229.830749	2631.455451	3533.108731	3349.779599	3457.665914
459.7986445	348.7935983	484.1515971	0.001403199	0.001403199	0.001403199	273.2497485	786.8052798	772.2718846
1244.557129	1249.236777	1552.036445	1822.785554	1790.877514	1886.17391	1330.443248	1721.385146	1489.408852
1321.872638	1358.132352	1547.335307	1458.549662	1617.688157	1321.132284	1664.687056	1445.327116	1178.577499
1221.297189	1259.027238	1326.548985	1481.563325	1664.812678	1983.443597	1478.712509	1798.780739	1506.358744

1.98_203.9711m/z	203.9711385	1.982566667	pos							114.8178552	250.1851188	285.3539225	185.2705397	228.5555518	140.7228152	155.7497397	244.2532101	277.1512116	
1.98_217.0141m/z	217.0141431	1.982566667	pos							36.75867638	76.90386321	37.93716209	112.2786098	0.001403199	45.91703017	0.001403199	29.13606353	0.001403199	
1.98_217.9981m/z	217.9981196	1.982566667	pos							1067.6971	1121.558626	968.8215494	934.6973125	1029.400783	850.7252542	1200.683935	1138.898582	1174.672497	
1.98_240.4407m/z	240.4407364	1.982566667	pos							530.9538961	446.843928	630.6789441	536.6846557	675.2673059	458.4100949	689.3518842	399.4209807	539.2840323	
10.00_100.9570m/z	100.9569669	10.00346667	pos							647.1647688	821.7144648	692.1749265	822.8432783	670.3041213	801.9010527	830.9014787	806.0138443	811.648129	
10.02_114.5585m/z	114.5584641	10.01541667	pos							215.8645416	333.3464854	319.5173208	343.9034166	215.3875395	273.3304694	313.2665125	339.7376032	313.6803841	
10.02_278.2473m/z	278.2473144	10.01541667	pos							2406.346753	2897.609876	2350.026714	2587.604604	2294.082552	2321.435719	3160.604584	2552.315711	2960.061065	
10.02_360.7827m/z	360.7827019	10.02403333	pos							1466.073459	1641.47857	1014.07373	1460.841149	1306.578316	1294.640557	1578.27492	1307.431997	1654.588687	
10.02_838.5549m/z	838.5549208	10.02403333	pos							4890.863643	3465.269012	2503.259128	690.4431014	343.133389	1276.982653	2614.670711	2337.051892	1210.307612	
10.04_112.9669m/z	112.966865	10.03561667	pos							9841.375778	9618.012675	9438.77477	9754.528879	10365.21162	10408.9824	9635.367285	9639.022215	9891.778815	
10.04_118.9599m/z	118.9598555	10.03561667	pos							1611.866669	1555.258084	1568.020422	1432.882236	1671.056975	1500.972198	1445.154849	1592.523511	1404.428541	
10.04_324.9028m/z	324.902766	10.03561667	pos							1286.102886	1662.300164	1616.546258	1510.247198	1538.780347	1541.084285	2045.585247	1497.72316	1716.592948	
10.04_395.8132m/z	395.8131907	10.03561667	pos							2271.071851	2282.111284	2677.246014	2143.020307	2362.167117	2544.855665	1934.29017	1820.837673	2064.499072	
10.04_442.7415m/z	442.7415367	10.03561667	pos							1713.365904	1879.166692	2003.68303	2191.888315	2290.9317	1648.262595	2267.903262	1926.322632	1734.155154	
10.04_840.5716m/z	840.5715534	10.03561667	pos							4779.145436	5490.767297	4610.338735	3435.122243	2702.676737	2615.138289	4486.5408	3749.175629	4143.913946	
10.04_841.5739m/z	841.5739321	10.03561667	pos							1770.743628	1782.778114	3239.20051	632.3726206	725.7981724	1049.887597	998.3071218	671.5364075	1031.541342	
10.05_193.5037m/z	193.503741	10.04765	pos							421.8231262	587.444279	252.5384211	569.911873	527.5608285	498.6834307	523.0449811	405.1726813	453.1389751	
10.05_203.9711m/z	203.9710834	10.04765	pos							1003.495474	1134.716671	1147.282276	1219.827726	1139.877763	1084.841413	1325.655368	1263.743052	1308.908159	
10.05_299.1056m/z	299.1056123	10.04765	pos							751.0469368	924.8489408	889.5718998	835.1743735	860.2666712	865.7437712	1034.021676	910.2425944	1047.538157	
10.05_329.9299m/z	329.9299047	10.04765	pos							262.6076525	164.2684585	178.5063439	168.5354805	294.3189229	95.91017582	279.3370555	387.1377739	236.8070314	
10.06_284.8136m/z	284.8135514	10.06391667	pos							2523.504518	3075.229179	3117.067741	3055.276165	3003.212234	2409.939248	3102.488233	2722.515821	2597.144061	
10.08_242.8471m/z	242.847148	10.07595	pos							2226.731995	1975.866195	2094.994611	1784.101939	2206.316964	1950.040596	2015.102185	1878.655066	1767.418837	
10.08_281.9130m/z	281.9130358	10.07595	pos							5733.710316	6892.352695	6088.233134	6272.704575	5753.750802	6234.128529	6988.447144	6129.380313	6061.807174	
10.08_306.8942m/z	306.8942323	10.07595	pos							15719.53289	14817.76433	15452.02455	14737.62727	18368.52829	15907.18742	17271.05084	14747.09807	16048.70076	
10.08_815.5592m/z	815.559164	10.07595	pos							3247.39846	1084.303962	1827.505614	231.6478693	316.4509055	0.001403199	665.9587138	1168.318726	1465.765976	
10.09_130.0347m/z	130.0346781	10.08803333	pos							569.6840499	390.443993	496.3726527	335.3139571	512.3367318	422.4946857	432.3695593	403.538316	442.6163073	
10.09_323.8843m/z	323.8843175	10.08803333	pos							5154.353866	4654.470361	5508.641784	4861.477054	6704.220997	6108.74267	5582.359703	4717.677867	4658.846629	
10.10_314.8740m/z	314.8739653	10.08901667	pos							2025.981349	1805.000842	1743.092444	1513.879852	2154.780339	1694.219743	1787.474888	2175.978559	1876.767433	
10.10_360.7828m/z	360.7828106	10.08901667	pos							2142.709351	1663.83692	2063.559146	1591.964452	2173.840341	1930.503146	1600.791797	1647.605511	1832.612462	
10.10_406.8413m/z	406.8413247	10.08901667	pos							1236.731864	832.4582893	1073.461574	1211.844346	1216.421836	1401.751746	248.7441217	1041.345443	1058.565576	
10.10_605.5494m/z	605.5494353	10.08901667	pos							12343.43869	9038.222678	10268.20843	6466.327266	8306.303391	6019.477522	9498.173383	8014.046215	7718.607545	
10.11_435.8065m/z	435.8064966	10.11105	pos							689.3591687	490.1971103	374.1888087	111.6988091	257.2944826	0.001403199	619.4493435	782.6694141	412.1456238	
10.11_442.8689m/z	442.8688724	10.11105	pos							2601.884063	1796.625527	3267.612026	2206.270801	2927.282262	2716.620159	2418.223431	2205.377279	2451.57002	
10.11_478.7479m/z	478.7479054	10.11105	pos							633.8159856	511.2037308	962.9092114	516.1781379	888.8939062	428.5638529	589.1222327	602.5238579	910.1299583	
10.12_111.0171m/z	111.0171438	10.12261667	pos							763.2048617	1550.149164	574.9619903	1064.141155	1543.074671	762.541625	1375.969143	1341.336346	1421.818238	
10.14_100.9569m/z	100.9569203	10.14475	pos							1348.85713	1181.327222	1269.984561	1149.243277	1433.155626	1484.819091	1161.566239	1059.907179	980.2981112	
10.14_114.5585m/z	114.5584634	10.14475	pos							721.4499903	556.4201396	702.9895496	424.8964834	633.3999099	532.3601579	552.2346123	527.5408211	565.8940061	
10.14_157.9937m/z	157.9937416	10.14475	pos							108364.8269	107603.4898	103484.9565	107461.5358	110646.9047	110646.004	111922.1553	106964.927	109715.5458	
10.14_271.2413m/z	271.241301	10.14475	pos							1522.982111	681.2292501	392.7149987	81.75774	195.4980484	0.001403199	169.8310009	0.001403199	146.5301241	
10.14_322.8870m/z	322.8870246	10.14475	pos							338.3459951	281.7920274	562.4025635	288.5498647	431.6395754	334.4638846	408.290993	373.9602715	520.927941	
10.16_329.9299m/z	329.9298863	10.16326667	pos							110.4113209	202.9713072	0.001403199	192.4936542	215.3486317	75.29266404	99.52513407	283.2899528	88.78423238	
10.16_335.2432n	318.2398911	10.16326667	pos							85186.52013	83485.16497	77337.60932	87961.56495	92468.89137	84217.59626	82175.80893	78599.66004	98729.54025	
10.19_115.9641m/z	115.9641353	10.1851	pos							218859.1831	217185.5354	213543.3549	221904.7803	232105.0418	228081.6587	228282.0184	218044.3345	225385.108	
10.19_119.0833m/z	119.0833182	10.1851	pos							130.1990697	160.1914592	117.4835333	161.3509461	152.6834965	216.9465883	117.5690817	139.0534887	161.6363182	
10.19_120.0255m/z	120.0254988	10.1851	pos							2182.708716	1909.96919	1709.264709	2011.901155	2079.027121	2095.769135	1943.828692	1855.906155	2031.908299	
10.19_131.5292m/z	131.5291667	10.1851	pos							0.001403199	0.001403199	14.39201193	40.1184368	21.84527169	20.03639298	20.20875333	47.39327526	9.791926373	
10.19_154.0430m/z	154.0429983	10.1851	pos							99.78708013	62.83250813	28.51692589	0.001403199	67.76217743	0.001403199	38.59133891	33.71087837	43.18416367	
10.19_256.5821m/z	256.5820517	10.1851	pos							4809.401054	5298.126423	3593.728924	4462.121021	5501.702425	5459.267214	3599.338215	4146.844179	5255.221277	
10.19_257.0837m/z	257.0837294	10.1851	pos							868.5157588	1028.586423	880.2628256	1030.251384	1430.298379	1241.846889	795.1664897	1114.98312	1494.626598	
10.19_277.5971m/z	277.5971452	10.1851	pos							1926.767279	2291.543625	1462.311073	2089.172164	2267.263282	2324.272893	1595.692311	1947.962546	2306.580204	
10.19_445.2456n	446.2528838	10.1851	pos							2767.208063	3028.673043	2498.31559	3230.156302	3912.358981	3860.145646	3658.321446	2508.441138	2543.331802	
10.19_517.1360m/z	517.135994	10.1851	pos							3137.542607	4955.042187	3421.649595	4741.17978	5001.276941	6007.87847	4085.443748	4574.714731	5772.297917	
10.21_332.8193m/z	332.8193228	10.20726667	pos							1268.601039	1278.35472	1124.787261	1698.522067	1527.740028	1366.506929	1535.730428	1097.746068	1137.541159	
10.23_217.9791m/z	217.9791162	10.22606667	pos							4466.667091	4972.154137	5111.906984	5098.494659	4948.428698	4973.914228	4821.931546	4397.623932	5449.963935	
10.24_299.9376m/z	299.9375575	10.24246667	pos							1253.865814	1356.893695	1374.89518	1313.637833	1212.422395	1284.755445	1015.698218	1013.200894	1488.893039	
10.24_324.9030m/z	324.9029667	10.24246667	pos							1373.796258	1105.514446	1242.610602	1240.437852	1427.142267	1074.022268	1071.751985	1317.705964	1505.209177	
10.26_159.9892m/z	159.9892187	10.25745	pos							2350.451242	1583.108666	1999.368408	2181.408346	2029.221306	2017.871656	1856.914631	2028.466145	2381.823505	
10.26_271.2415m/z	271.2415276	10.25745	pos							773.4446914	464.1463019	360.1779466	67.88344283	71.9375126	0.001403199	224.8501253	115.6423454	267.0316448	
10.26_281.9132m/z	281.9131887	10.25745	pos							2768.95519	2832.32295	2548.780984	2964.128293	2928.975983	2424.762593	2348.020616	2475.800882	2566.506319	
10.27_100.5102m/z	100.5102018	10.2673	pos							45117.2219	46228.00544	46452.99123	46856.92352	50834.63532	49359.72873	48976.04216	46242.51628	48873.22801	
10.27_243.9413m/z	243.9412878	10.2673	pos							1405.095892	1024.822866	1371.587239	1534.197195	1545.174187	1550.879551	1126.693713	1448.913312	1492.055938	
10.27_388.8506m/z	388.8506084	10.2673	pos							7026.740051	6992.083823	7588.855362	8558.762054	8187.180319	7848.846775	7459.606076	7195.810294	8520.796519	
10.27_398.3400m/z	398.3399574	10.2673	pos							2131.317444	2197.151781	2389.906181	1048.54205	477.4922102	108.2777529	2140.300628	1553.419537	1588.704373	
10.28_124.9643m/z	124.9642701	10.27931667	pos							5575.481753	5570.783201	5191.8673	5710.131113	6028.133894	5601.109269	5504.33366	5745.591944	5815.626821	
10.28_442.7418m/z	442.7417547	10.27931667	pos							5973.388748	4502.597741	6374.652297	6154.17551	6643.827627	5829.135188	4842.002361	5781.575386	5810.800562	
10.28_444.7570m/z	444.7569848	10.27931667	pos							3620.617596	3678.401889	4167.072318	3202.302664	2694.837448	2296.875367	3129.655978	3377.86723	2720.79292	
10.29_162.9830m/z	162.9830219	10.28965	pos							5247.232266	5051.927951	5640.342967	5442.34901	5590.335585	5861.668039	5303.425615	5182.328891	5557.511287	
10.29_178.9904m/z	178.990436	10.28965	pos							1821.482862	1578.202586	1958.774968	1910.779477	2143.692412	2067.862409	1463.352074	2145.455755	2342.606342	
10.29_306.8942m/z	306.8942477	10.28965	pos							15771.67262	17861.00583	17418.09763	20278.51342	17899.65791	19929.54091	20389.84712	17790.91616	21032.32295	
10.30_154.0431m/z	154.043146	10.30121667	pos							56.49205321	0.001403199	21.57228021	125.8053409	33.87509645	21.30548829	29.13509862	0.001403199	43.80473186	
10.30_213.0098m/z	213.0097852	10.30121667	pos							539.3082144	657.3227374	827.8452903	787.0614888	766.5902742	785.189509	559.0526018	772.2605268	881.7692762	
10.30_292.2245m/z	292.2244639	10.30121667	pos							2952.237577	2630.442954	3012.776274	3096.676187	3408.543954	3224.402307	2989.942197	3088.823687	3454.717214	
10.30_324.8060m/z	324.8060365	10.30121667	pos							1729.767803	1583.653301	2158.470878	2403.549804	2243.990647	2491.373643	1768.703881	1884.875728	2625.913306	
10.30_328.9332m/z	328.9332006	10.30121667	pos							2607.71118	2056.276117	2477.853735	2044.887579	2814.77391	2223.519814	2443.648588	1834.306786	2435.683995	
10.30_442.8691m/z	442.8691438	10.30121667	pos							1967.370387	1836.5249	2560.787517	2430.626746	2646.699805	2872.271098	1931.079387	2752.103397	2501.589609	
10.31_111.5219m/z	111.5219297	10.30981667	pos							908234.7001	892845.7014	881365.2989	923691.6939	953546.1209	942161.8756	957239.8288	914868.4667	947850.0162	
10.31_158.9859m/z	158.985862	10.30981667	pos							892245.7751	876616.9331	851974.1065	882132.627	915188.4955	893596.9976	911428.0948	870775.702	908382.451	
10.31_468.7940m/z	468.7939966	10.30981667	pos							2374.45792	2437.303232	2331.590805	3325.753372	3427.774889	3083.02451	1971.044261	2933.314892	3030.501965	
10.31_836.5409m/z	836.540909	10.30981667	pos							5585.814653	4401.451188	4003.657519	2426.455468	2766.380333	2004.217732	3197.368162	3238.674	3047.654605	
10.32_100.9569m/z	100.956914	10.32015	pos							1676.716617	1951.881984	2017.56841	2146.31164	2083.275604	2176.00337	2166.825626	2127.756981	2304.052881	
10.32_138.9799m/z	138.9798977	10.32015	pos							11875.40645	12032.84624	11464.95902	12283.56029	12044.2749	12609.2854	12685.30432	12279.87315	12376.28283	
10.32_139.9877m/z	139.9876899	10.32015	pos							3427938.271	3363143.512	3300033.561	3433374.895	3584812.829	3556504.579	3566676.668	3426202.24	3533304.984	
10.32_186.9808m/z	186.980761	10.32015	pos							323789.5907	316846.3287	308478.4676	323690.0664	338011.4399	328761.632	336992.3098	328711.1319	332811.5246	
10.32_302.8243m/z	302.8243321	10.32015	pos							5876.495143	5557.880113	6024.045684	5990.102685	6241.800503	5967.535823	5000.270344	5751.063018	6685.609691	
10.32_407.3451m/z	407.3451024	10.32015	pos							969.4577974	489.0190733	575.9418991	298.6227372	295.3115609	0.001403199	1309.500247	261.1851883	836.3414782	
10.33_134.0284m/z	134.028399	10.32873333	pos							0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	65.48444831	0.001403199	36.97426591	
10.34_180.0993m/z	180.0992943	10.34366667	pos							147.5983343	165.8352414	139.5832641	280.1245073	132.6616226	281.4849159	216.9133049	179.0860214	315.8545297	
10.34_281.9127m/z	281.9127352	10.34366667	pos							1156.676929	980.5703782	1509.917734	1612.010715	1166.556096	1998.20162	2367.352442	1936.884209	1731.72206	
10.34_424.7307m/z	424.7307387	10.34366667	pos							774.433273	962.6917605	1306.59511	1681.489793	1300.397588	1995.619932	2343.142351	1879.246392	1787.015879	
10.34_841.5746m/z	841.5745971	10.34366667	pos							1839.553435	2127.531214	844.7189911	872.3707788	299.4072158	689.3448176	2116.136452	1376.151787	868.8938095	
10.36_111.0171m/z	111.0171497	10.36036667	pos							2020.397006	2741.759769	3053.543561	2373.26517	3503.650832	3281.257242	2140.912455	2929.717923	3605.806826	
10.36_111.0204m/z	111.0203504	10.36036667	pos							11284417.37	11184999.16	11043608.26	11498454.71	11926308.35	11829163.97	11968684.09	11420299.33	11876528.36	
10.36_131.5292m/z	131.529184	10.36036667	pos							93.23827638	164.8919521	164.2520585	106.7396688	181.5041324	129.7546734	41.55756175	148.6768699	230.6512639	
10.36_132.5363m/z	132.5363239	10.36036667	pos							0.001403199	0.001403199	0.001403199	204.8869821	183.4825044	0.001403199	0.001403199	350.9590759	0.001403199	
10.36_141.9832m/z	141.9831731	10.36036667	pos							1275812.133	1239822.72	1225574.543	1293888.573	1339513.91	1336571.101	1321808.183	1278162.269	1320655.84	
10.36_201.9754m/z	201.9754215	10.36036667	pos							24581.36839	26484.77355	24317.8513	26105.5891	26931.75361	26580.98447	26769.69353	25136.81894	28526.77658	
10.36_400.8063m/z	400.8062805	10.36036667	pos							5440.408727	6509.701198	5197.28063	6187.968311	5741.872712	6777.317788	6457.155074	5738.219868	7055.508377	
10.36_422.7730m/z	422.7730164	10.36036667	pos							699.8416176	1095.003992	1041.056883	879.5369415	794.8960135	868.5111713	1257.633379	1236.499881	1313.652157	
10.37_283.8765m/z	283.8765401	10.37066667	pos							3096.903074	2806.636858	2037.649615	2605.824536	2739.321039	2346.538936	2525.933232	2613.075882	3353.597839	
10.37_402.8019m/z	402.801892	10.37066667	pos							3207.683099	2745.92433	2867.524064	2965.152031	3363.98006	3379.668068	2934.896336	2922.968662	4306.63721	
10.38_142.9909m/z	142.9909101	10.38436667	pos							525.0556718	629.3094279	499.6556411	627.0500079	495.451803	518.7111837	533.7878108	458.2338971	757.1652011	
10.38_286.9058m/z	286.9058066	10.38436667	pos							154643.2759	151269.9131	150347.2563	158641.1299	164796.891	160493.5831	165946.6481	154234.5887	160681.8386	
10.38_398.8676m/z	398.8675657	10.38436667	pos							9054.72602	7927.543029	8791.505275	7945.01257	8077.151167	7988.3868	8670.311419	7422.384552	9221.945927	
10.40_395.8133m/z	395.8132702	10.40298333	pos							3121.340467	3209.782477	3206.550439	3461.604837	3186.104525	3195.560319	3060.76355	3446.912467	3202.678081	
10.42_217.9791m/z	217.9791108	10.41986667	pos							7093.822565	6565.750489	5906.109515	6267.715931	5932.605633	6253.579571	7427.216883	6764.043762	7932.165174	
10.42_444.2558m/z	444.2557856	10.41986667	pos							4221.33915	3708.30639	2420.566919	1272.026842	1651.01311	1566.463111	2618.370372	2108.910386	1799.685057	
10.43_120.0255m/z	120.0255204	10.4331	pos							817.7034667	661.3586173	690.5614794	554.6536311	729.6177589	534.8277493	704.1363096	722.9655569	761.831	

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11.30_283.8764m/z	283.8763895	11.29856667	pos
11.30_390.7779m/z	390.7778847	11.29856667	pos
11.30_405.8406m/z	405.8405824	11.29856667	pos
11.30_553.7705m/z	553.7704776	11.29856667	pos
11.31_297.9421m/z	297.9420796	11.31071667	pos
11.31_419.8491m/z	419.8490552	11.31071667	pos
11.33_395.8128m/z	395.8128297	11.32543333	pos
11.33_397.8094m/z	397.8094497	11.32543333	pos
11.33_603.5331m/z	603.5330696	11.32543333	pos
11.34_100.9569m/z	100.9569391	11.33928333	pos
11.34_409.7838m/z	409.7838238	11.33928333	pos
11.34_435.8068m/z	435.80682	11.33928333	pos
11.34_444.7565m/z	444.7564656	11.33928333	pos
11.34_604.7683m/z	604.7682623	11.33928333	pos
11.35_324.9029m/z	324.9028898	11.34963333	pos
11.36_305.8431m/z	305.8431161	11.35961667	pos
11.36_414.7749m/z	414.7748681	11.35961667	pos
11.36_482.7623m/z	482.762262	11.35961667	pos
11.36_786.5988m/z	786.5987733	11.35961667	pos
11.36_814.6309m/z	814.6308539	11.35961667	pos
11.37_799.5433m/z	799.5433051	11.37301667	pos
11.39_113.5153m/z	113.5152664	11.38858333	pos
11.39_419.7922m/z	419.7921512	11.38858333	pos
11.42_360.2144n	383.2033956	11.41601667	pos
11.42_385.2088m/z	385.2088227	11.41601667	pos
11.44_202.0530m/z	202.0529539	11.43665	pos
11.44_338.0751n	361.068682	11.43665	pos
11.44_405.7835m/z	405.7834882	11.43665	pos
11.44_406.2794m/z	406.2794078	11.43665	pos
11.44_414.7751m/z	414.7751052	11.43665	pos
11.44_442.8687m/z	442.8686929	11.43665	pos
11.44_468.7939m/z	468.7939038	11.43665	pos
11.44_524.6570m/z	524.6570358	11.43665	pos
11.46_201.5512m/z	201.5512442	11.45555	pos
11.46_209.5712m/z	209.5711856	11.45555	pos
11.46_229.5826m/z	229.5825775	11.45555	pos
11.46_230.0843m/z	230.0843116	11.45555	pos
11.46_305.0062m/z	305.0062468	11.45555	pos
11.46_327.6317m/z	327.6317055	11.45555	pos
11.46_346.7880m/z	346.7880082	11.45555	pos
11.47_216.9864m/z	216.9863784	11.47106667	pos
11.47_332.8190m/z	332.8190364	11.47106667	pos
11.48_283.8764m/z	283.8763681	11.47973333	pos
11.48_299.9375m/z	299.9375201	11.47973333	pos
11.48_374.8817m/z	374.881739	11.47973333	pos
11.48_394.8054n	395.8126496	11.47973333	pos
11.48_467.7425m/z	467.742525	11.47973333	pos
11.48_482.7624m/z	482.7623665	11.47973333	pos
11.48_513.7894n	536.7811054	11.47973333	pos
11.49_238.9069m/z	238.9069458	11.49356667	pos
11.52_327.9324m/z	327.9323588	11.5155	pos
11.52_402.8019m/z	402.8019037	11.5155	pos
11.52_760.5823m/z	760.5822598	11.5155	pos
11.53_364.9302m/z	364.9302417	11.5276	pos
11.53_443.2481m/z	443.2480972	11.5276	pos
11.53_494.7187m/z	494.7186971	11.5276	pos
11.53_799.5443m/z	799.5442577	11.5276	pos
11.54_285.8717m/z	285.8716731	11.53753333	pos
11.54_309.1304m/z	309.1304474	11.53753333	pos
11.54_319.0747m/z	319.0747311	11.53753333	pos
11.55_144.9775m/z	144.97746	11.54626667	pos
11.55_397.8671m/z	397.8671317	11.54626667	pos
11.55_448.8063m/z	448.8062955	11.54626667	pos
11.55_498.9005m/z	498.9005085	11.54626667	pos
11.56_125.9723m/z	125.9722642	11.5567	pos
11.56_298.9416m/z	298.9415527	11.5567	pos
11.56_305.8431m/z	305.8431183	11.5567	pos
11.56_342.7722m/z	342.7722203	11.5567	pos
11.56_404.7483m/z	404.7483164	11.5567	pos
11.56_436.7812m/z	436.7811904	11.5567	pos
11.56_446.8094m/z	446.8093678	11.5567	pos
11.56_485.7839m/z	485.7838977	11.5567	pos
11.56_592.8128m/z	592.8128141	11.5567	pos
11.57_238.9069m/z	238.906851	11.57015	pos
11.57_463.7998m/z	463.7997924	11.57015	pos
11.57_528.7668m/z	528.7667699	11.57015	pos
11.58_414.7754m/z	414.7754039	11.58235	pos
11.59_308.8897m/z	308.8897215	11.59231667	pos
11.59_324.8826m/z	324.8826008	11.59231667	pos
11.59_409.7834m/z	409.7834056	11.59231667	pos
11.59_444.2562m/z	444.2561878	11.59231667	pos
11.61_283.2633m/z	283.2632606	11.61258333	pos
11.61_346.7880m/z	346.7879927	11.61258333	pos
11.61_604.7687m/z	604.7686855	11.61258333	pos
11.62_382.7648m/z	382.7648054	11.62466667	pos
11.62_477.7405n	478.7478125	11.62466667	pos
11.62_838.5566m/z	838.5566021	11.62466667	pos
11.64_283.8763m/z	283.8762832	11.63681667	pos
11.64_285.8716m/z	285.8715714	11.63681667	pos
11.64_562.7061m/z	562.7061248	11.63681667	pos
11.65_422.7362m/z	422.7362278	11.65071667	pos
11.65_443.2476m/z	443.2475911	11.65071667	pos
11.65_494.7186m/z	494.7186434	11.65071667	pos
11.65_514.7968m/z	514.7968368	11.65071667	pos
11.66_131.5293m/z	131.5293184	11.66275	pos
11.66_315.8717m/z	315.871708	11.66275	pos
11.67_220.8653m/z	220.8653492	11.67456667	pos
11.67_305.8430m/z	305.843006	11.67456667	pos
11.67_307.8400m/z	307.8399587	11.67456667	pos
11.67_356.8404m/z	356.8403817	11.67456667	pos
11.67_528.7676m/z	528.7675662	11.67456667	pos
11.67_540.7212m/z	540.7211532	11.67456667	pos
11.69_218.9195m/z	218.9195485	11.688	pos
11.69_326.8983m/z	326.8983115	11.688	pos
11.69_422.7729m/z	422.7728621	11.688	pos
11.70_307.8539m/z	307.8539004	11.69673333	pos
11.70_324.9030m/z	324.9030079	11.69673333	pos

4618.152999	5169.187393	5477.969066	5661.209193	6894.8057	5822.118539	5247.916558	5319.311729	5270.991365	
1029.107454	780.6011211	1284.023115	853.7422552	1908.678827	1360.254848	1535.037548	1512.462119	1618.945504	
16011.18874	15160.64856	16638.73214	16669.6805	20634.64407	19164.61431	17935.51983	16832.81848	18295.33305	
444.5152062	523.2808068	810.9198896	725.3399642	1176.537366	1265.891914	748.9497942	805.3950819	974.8158933	
189184.1279	184371.6706	185377.8598	189312.6522	196440.9922	191630.926	201606.6635	188286.3401	196674.4344	
901.8495482	673.7721937	960.5535011	821.8823399	1368.390167	966.218351	1196.603536	727.4602468	1361.536294	
10202.16417	11094.96885	8549.770341	10503.82592	10869.49369	9099.324659	9887.741323	9490.402205	9976.461031	
754.7070084	1016.525259	1032.141075	1233.180768	1985.954748	1139.99319	1236.104823	945.3390956	1232.253863	
3015.079777	2781.875148	2001.838452	1993.978513	2243.548557	1238.979452	2679.164708	2628.678407	2207.563016	
690.8348689	599.7063063	539.3613595	507.9872727	803.1018903	651.0364709	649.0057063	550.0235715	699.9231465	
1275.954	1841.693443	1561.94579	1297.420077	2507.560385	1806.730865	2322.138271	1817.224449	2165.476801	
33243.01888	28033.51193	29597.04842	12980.135	9104.102453	6340.669544	31867.19706	22598.77224	18034.79593	
2723.163147	2374.431703	1502.068636	1409.535221	2228.312319	1898.746422	1777.647936	2001.145042	2425.463822	
4216.116901	4921.868318	5110.337331	5778.859547	6698.954604	5686.40958	5483.874295	5150.050358	6602.978798	
4096.427452	4887.913264	4742.754485	4675.832829	5654.586209	5095.695022	4145.492392	5335.067114	5554.99626	
1015.623732	1198.864412	446.7586445	871.4880874	976.4172223	655.761275	751.525327	1008.490545	1208.673281	
2144.92584	4240.537376	2469.029261	3244.124327	3469.895352	2621.11416	3259.275369	3254.401612	2866.187964	
2115.809485	3347.937583	1646.974408	3019.27614	3045.814441	2493.549514	1854.591432	2866.866837	2487.561206	
6637.943355	6771.59989	4685.76766	4693.594686	4759.639833	3607.458146	5194.667385	3792.818579	4187.187862	
13422.09386	11677.64514	6721.650571	3828.500441	3486.650911	778.9079538	8037.571038	7129.616626	4098.366609	
10719.7554	12046.97877	9982.042456	7254.62821	7012.664111	6253.315825	9658.973838	8143.942276	9086.472445	
0.001403199	0.001403199	0.001403199	0.001403199	24.91734115	0.001403199	35.18048384	0.001403199	31.98460722	
238.2268382	344.9397012	653.4649396	593.6432282	633.0169138	418.0699703	588.0648586	638.8378854	578.937931	
66201.02551	56339.30456	57387.61537	70666.86539	56395.42921	59326.93053	58425.05093	54728.01702	62526.55239	
784.4662457	696.3707641	551.4161285	812.523451	728.5862571	495.5100812	598.0235432	448.7061729	505.6703902	
137.8878119	67.51821053	247.6058013	172.696627	203.2634537	301.2109113	180.9889249	151.73527	0.001403199	
4253.052363	4160.679802	4091.760629	4358.073888	4115.836371	5358.158316	4234.696226	4390.486899	5516.98767	
9428.380342	9854.476049	10585.46303	10302.02863	12852.7005	11338.82978	10991.25092	10772.77469	12510.02596	
1146.982357	1024.662441	992.3665665	1109.750809	590.3942894	1074.723833	610.4280319	1195.114803	909.8772131	
2322.050333	1833.734402	2986.023669	2035.011653	2551.899008	2862.86819	2190.850759	2064.769944	2748.785375	
7009.442696	7514.275842	7731.568437	9776.226539	8926.696548	8955.841165	7970.895734	8395.946564	9531.890658	
8356.485152	9499.185579	10283.48961	11151.50156	10148.00201	11487.7875	9371.964707	9416.04905	11777.28819	
552.4920356	1050.042422	942.4260191	1200.344467	1037.559133	1110.440332	705.3931946	317.0392168	385.285859	
2591.057239	1912.355093	2487.403708	2623.140709	3404.71411	2925.280221	2501.918936	2388.349819	2642.628708	
891.1781833	876.9409407	843.3180533	1032.464404	1012.854204	1506.956418	820.9718518	896.0807593	1002.804521	
19589.85306	15558.42775	17023.75118	20654.4401	20606.64126	21045.51959	18178.49904	18120.15484	20601.19666	
3845.287494	2881.645359	3208.878734	4278.734274	4089.493003	4096.480893	3850.053522	3345.191285	4260.029814	
1495.155277	1374.605022	1855.440472	1677.13164	1610.041419	2132.133631	1751.537793	1819.847423	2008.527781	
1118.325184	1588.052148	1758.265556	2019.539144	2049.541165	2207.016518	1450.40338	1540.605278	1754.69957	
3518.491469	2528.325585	4598.562424	3924.45633	3187.268655	3797.996614	3939.739344	3414.316684	5041.763915	
55.24602216	0.001403199	0.001403199	0.001403199	79.31303405	61.92656859	0.001403199	50.8776356	65.11180394	
25545.76125	25869.36119	28066.09042	29773.11974	31730.148	29820.12594	29707.60925	28384.92382	29749.40433	
2184.139264	1483.630874	2867.006426	2061.504032	1719.407142	2366.431201	2702.41796	2291.502451	3463.327641	
51661.21963	51692.77922	52657.51686	55218.42734	57432.89583	58152.03342	59816.42019	54949.1676	56914.7136	
5691.638246	2888.32832	5179.122625	4722.557005	3913.289406	4772.552398	5009.987207	5009.987207	6715.496529	
7980.351898	6248.746388	8957.358394	8246.283105	8368.188408	8745.995794	7604.346586	8607.40505	9478.274377	
1459.399537	957.7009121	1907.606599	1618.471466	1543.234691	2326.078691	1039.955654	1690.323878	2390.353825	
6663.397629	4802.167221	6733.449008	6081.014772	7727.125776	7586.020525	6492.280357	6426.492762	8267.306359	
16522.33848	15184.76879	17138.7467	19391.30285	19459.97949	19064.55934	17298.68444	16656.91157	19767.16192	
1994.094429	782.0770966	2080.689635	1242.430607	1188.422934	1733.122484	1706.223685	1769.847519	2563.640079	
13680.77845	13014.69227	13492.28562	16145.16231	15068.62747	15681.40906	13876.67101	15232.1461	15778.01227	
1422.779748	835.1154108	1168.989936	1034.590189	1348.679401	1249.101185	1224.07941	1305.851166	1689.63369	
7326.228286	4324.685316	5470.839413	2779.544835	3652.641975	4017.409	5260.766438	5479.416482	5916.38213	
146.7538399	0.001403199	68.49009516	91.04023535	78.37692272	87.74383331	108.043589	143.4850605	0.001403199	
509.6865086	381.8705123	329.7235332	0.001403199	0.001403199	141.8442169	0.001403199	229.1039886	0.001403199	
964.1803233	435.6253994	620.1953878	802.7245614	1215.215534	619.3482965	737.153619	1237.334157	796.0759931	
7543.963519	4969.713718	6845.154161	4550.447163	4198.448791	4459.634107	5657.602707	3866.871921	6732.271156	
928.8535531	608.3602877	623.9862829	725.5213569	930.7798357	738.2146972	1034.620409	1015.922044	709.0714604	
6178.491989	5514.6195	5817.097122	6756.158046	6207.055524	6414.923919	5956.689916	6242.133932	6447.641222	
371.5159421	312.3470455	325.7057166	323.8682323	530.5875064	282.7931615	486.6588369	464.8932942	240.7510905	
0.001403199	0.001403199	0.001403199	10.00432293	0.04944079	10.3987257	0.001403199	25.36192322	0.001403199	
99642.96489	103622.2921	107186.1602	117036.3694	122249.3439	121372.5437	120065.5012	115214.7629	124061.9543	
2762.152903	2563.362761	3721.324432	2410.336003	3179.112989	2542.668259	3120.666292	2916.135406	2838.318356	
131675.4077	134760.4887	138739.2317	149740.777	157736.2597	152699.0466	153595.8949	143933.2243	156514.9894	
315.8263041	217.9601731	240.8149368	302.8714858	330.8390511	271.8904002	304.9559219	336.4253277	333.9186245	
795.6202684	801.6737837	446.3190195	849.1079703	1034.058478	690.0378723	644.8552363	817.5530594	598.842062	
1282.873457	1389.979402	1170.952075	1649.863269	1952.039949	1561.917512	1492.869397	1417.266286	1597.431997	
977.7389957	839.247803	837.9848819	750.0144134	1260.41306	848.6489293	1129.085633	1097.713795	750.6385964	
3336.905405	3213.72794	3493.878147	4136.710459	3986.869393	3807.554174	3454.874899	3683.506209	4074.161426	
1659.504712	2341.535637	1908.428024	2205.185845	2388.600912	2963.922395	2140.300126	2454.948836	2210.634261	
41722.30896	40041.01732	42321.18186	46076.17174	45906.97441	46227.64652	42224.24773	42644.27098	46589.97837	
794.9469795	1131.974918	842.8083777	888.7693362	1516.41893	1277.294388	1143.832243	1084.152687	925.1104878	
4239.529546	4710.605016	4712.374166	4500.545444	6768.985648	5900.729063	4893.491005	5475.545568	4825.476003	
4003.585722	4342.600899	3642.062743	5163.913099	5335.017791	4760.505581	4023.041471	4449.65888	4426.76312	
6881.128647	5315.809995	6081.816971	6909.405937	7166.66902	6707.233173	6141.057843	6708.392557	7218.139482	
6620.378586	6388.606801	7143.724862	8866.592622	8715.292446	8093.488425	7840.723958	6757.719544	8331.247038	
5065.200667	4183.733666	4056.235152	4596.491957	5459.140928	3961.563627	4110.044467	5010.261943	4147.852449	
3654.859443	4393.014318	3782.74845	5074.554988	4863.944673	4142.323408	4073.521231	3918.50652	3886.682729	
193.3472738	175.9603912	120.9654755	340.1935824	409.9694874	625.2042149	300.8536151	433.6072636	359.9687593	
2086.701674	2588.74221	2262.779018	3294.842029	3336.049689	2713.363712	2268.036766	2505.902043	2401.588102	
6654.295899	5260.956329	4380.553725	3762.357218	3417.082325	3507.175334	5517.692902	4536.472282	5423.058029	
3986.186532	3783.338969	3392.658972	4140.716132	4315.690721	4194.724048	3723.211497	3886.031115	3265.721814	
3315.661197	3614.078616	3328.428988	4803.167836	4460.547036	4460.570091	3987.326104	4083.843768	3688.921179	
4011.246764	2853.314027	3792.41194	5426.525248	5571.925364	4720.148439	4669.926754	3736.725987	4604.600419	
890.4945745	1301.412705	977.4525033	1615.746455	1544.304323	1432.129026	1609.555549	1153.604281	1464.332196	
134507.8741	140090.1285	146696.5726	163813.9805	171734.4367	165901.7574	164515.0346	156175.4194	168135.5739	
8401.206323	8288.886981	5422.461418	3020.683741	2845.636921	2055.785817	4340.790425	3669.314016	3601.537794	
2267.058678	2428.270296	2616.282902	3274.7917	3917.146025	3260.572073	2449.267041	2904.219334	2904.157995	
931.2890073	841.888685	1070.813275	1389.658624	1171.650255	1206.501868	1086.899876	926.362345	1211.381943	
2087.322301	1593.357295	2492.255767	3495.345258	2981.979321	3776.707283	2540.557922	2625.393944	3842.496849	
1761.958677	1540.396656	1401.707565	1716.392911	1357.416123	1643.53808	1852.04425	1334.925835	1763.485911	
781.0439469	615.9783654	82.56514337	75.23161672	0.001403199	113.0880958	330.9734309	242.8615341	0.001403199	
1575.553991	2515.247734	1123.636814	3260.00578	3138.923642	3570.152477	2027.736355	2198.46759	3086.179343	
5194.549182	5569.231628	4864.088214	7055.485427	6501.786478	8097.596292	5472.026297	6006.867031	7011.381376	
13.13267133	27.54935184	31.07696175	93.98748283	37.75902955	89.78086443	60.49222536	22.2799964	75.73862189	
35199.20953	35093.48745	36899.03101	39892.12784	41613.06692	39050.95255	38639.29017	37882.99004	39385.52821	
1518.209787	1426.91237	1296.999111	1432.80603	1566.166501	2039.302172	1548.456711	1457.014391	1774.493512	
3075.963903	2097.77121	2153.677708	2716.914381	3078.064102	3391.083326	2761.12195	3218.825442	2670.174415	
400.5315729	680.6362707	360.5812603	512.1732688	588.6637566	802.9094837	352.9029917	533.0804777	535.4205964	
81199.56603	82188.45346	84310.11874	95127.5849	100410.6896	98387.51487	94995.40837	91362.15302	96464.60516	
11442.2555	10751.21339	11501.19253	13448.73675	13595.24006	14043.29281	12800.6032	13288.43138	13263.60512	
823.2010478	949.7377728	795.1283768	1227.961898	1185.617713	1600.553012	521.9415497	738.3386574	1356.056782	
2872.289558	2407.07101	2963.601118	3275.898187	2805.611137	3117.996884	3072.639672	2919.025734	2865.293241	
761.9227922	640.4193019	425.6832077	453.8874579	530.789885	892.0015894	769.0425245	692.7267198	667.1351377	
8993.638065	8326.102158	7413.835604	6605.028976	6218.124969	6273.141021	7586.465049	6944.347522	6018.62264	
273.7033079	365.4038805	447.8853767	472.1821837	500.8887019	632.4472231	612.0597153	557.451046	359.2285123	
1737.429662	2157.114616	1350.23853	1606.341232	1375.711844	2353.434197	2002.932884	1912.099808	1775.182121	

11.70_374.8817m/z	374.8816957	11.69673333	pos							5821.853859	5287.184711	5456.825671	6755.246324	6321.307486	7374.628027	5634.751005	6513.958023	5775.851594	
11.70_707.1677m/z	707.1677337	11.69673333	pos							24875.37112	37890.02516	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	51.50684455	0.001403199	
11.71_144.9775m/z	144.9774636	11.70886667	pos							31.23692106	0.001403199	14.26943597	10.12367951	31.61036106	25.53409567	0.001403199	11.37739849	0.001403199	
11.71_305.8581m/z	305.8581088	11.70886667	pos							1337.727255	997.6103792	1362.274299	1415.907692	1531.335258	1780.841638	1688.119039	1845.331994	1161.933589	
11.71_341.8931m/z	341.8931249	11.70886667	pos							999.6395802	608.5028429	702.1676346	734.1946102	742.9857574	858.6553727	888.361239	932.3514879	817.1332992	
11.71_840.5723m/z	840.5722552	11.70886667	pos							13459.93503	9660.091571	8205.234349	7762.140915	7783.74282	6802.50781	9552.014351	8462.846998	7132.297986	
11.72_406.7833m/z	406.783328	11.71891667	pos							127.3546572	177.8191681	284.4611948	506.3882045	831.9831069	773.073029	333.5597203	880.1054897	398.6763952	
11.72_839.5609m/z	839.5608826	11.71891667	pos							2228.820732	2044.579124	1790.420918	0.001403199	807.367639	224.0832607	975.4755654	1427.01162	375.2531184	
11.73_309.1305m/z	309.1305152	11.72773333	pos							2719.725244	2121.445203	2343.057377	2430.155863	2688.765001	3437.672442	3087.370294	2828.419437	2324.49083	
11.73_402.8016m/z	402.8016223	11.72773333	pos							2165.465674	1821.138655	2203.466801	1861.12205	2390.335137	2233.900666	2234.356549	2473.436391	1763.421325	
11.73_417.7966m/z	417.7965755	11.72773333	pos							3919.477304	4050.625723	4554.290226	6473.918148	6170.119724	6350.165358	4610.519559	5704.254705	5172.350738	
11.73_428.7755n	446.8093689	11.72773333	pos							23535.00467	23718.12714	25382.45606	26889.89002	28661.88613	30682.75372	24225.81069	27232.07655	25394.85362	
11.73_550.7507m/z	550.750695	11.72773333	pos							2015.593224	1231.373503	1304.630987	1629.479559	2635.382461	2148.354321	2244.736515	2250.866992	2145.048993	
11.73_556.3501m/z	556.3500655	11.72773333	pos							1810.746674	1401.460851	1269.191149	985.0515059	2096.871729	2072.319799	1266.100268	1507.703455	622.9907089	
11.73_556.8579m/z	556.8579003	11.72773333	pos							2030.343408	1478.252474	1522.100025	1816.746866	2864.514728	1846.891808	1613.965614	2390.9487	1789.888126	
11.74_334.8147m/z	334.8146867	11.73825	pos							1009.725229	918.8326872	830.8870861	1076.827391	1493.601095	1199.024671	1321.760152	1242.241531	831.4361978	
11.74_604.7680m/z	604.7680174	11.73825	pos							2187.360645	1256.123962	1358.963341	1693.301725	2182.693385	1590.934878	2165.81125	2474.971689	1662.152655	
11.75_217.9793m/z	217.9793414	11.7471	pos							1133.55559	1162.383115	879.2784674	1058.856141	1276.266729	1413.183147	1440.883599	1521.763715	1259.31449	
11.75_308.8898m/z	308.8897932	11.7471	pos							2253.449543	2316.12594	2290.20187	2469.946166	2628.962123	3207.684492	2357.171174	3099.335151	1635.627119	
11.75_414.7753m/z	414.7752703	11.7471	pos							8493.715469	7848.092838	8134.04813	9455.39116	9365.748934	10963.7748	8440.302572	8932.223082	7898.140011	
11.75_514.7968m/z	514.7967542	11.7471	pos							4729.280107	5327.402824	5709.769863	5913.37758	6679.719679	6813.068796	6683.74943	6473.814165	4950.426031	
11.75_531.8592m/z	531.8591545	11.7471	pos							9647.084441	7736.916705	7638.921554	8348.613348	8884.351133	7910.970869	9035.557663	9215.291449	8844.933418	
11.75_534.3367m/z	534.3366822	11.7471	pos							6731.277641	6385.084333	5771.517509	6601.776476	5360.283611	8009.424025	5765.122075	5963.51632	6019.316274	
11.75_553.8723m/z	553.8722616	11.7471	pos							4507.332278	2496.18356	3380.037581	3572.323151	4296.168509	3187.701422	4067.971481	3733.297142	3559.427141	
11.76_244.8443m/z	244.8443173	11.7576	pos							1092.326787	1672.097165	1361.51357	867.4398739	1173.579319	1490.434993	1210.567597	1430.2301	871.7470816	
11.76_283.8764m/z	283.8763655	11.7576	pos							1370.190305	1590.383039	1606.838398	1679.553498	1853.253342	2357.03458	1694.18631	2139.997467	1207.958716	
11.76_346.7879m/z	346.7879424	11.7576	pos							5633.867366	5599.094738	4994.067453	4836.309059	5815.93696	7189.548258	6390.665353	6487.344477	4920.826051	
11.76_511.8493n	534.8385655	11.7576	pos							4139.881124	3248.820661	3717.533091	2838.077081	3429.877898	3505.362495	3596.536496	4358.411955	3999.549382	
11.76_529.3814m/z	529.38144	11.7576	pos							2279.808548	2468.662997	2311.89853	2630.584833	2028.369323	2236.270672	3145.093126	2585.225247	1875.135426	
11.76_532.3606m/z	532.3606046	11.7576	pos							3803.270625	3044.439486	3797.40916	4359.579181	3646.069207	3777.501162	3541.902241	3966.66571	3445.650232	
11.76_554.3735m/z	554.3735193	11.7576	pos							1980.490619	1402.345081	1415.402673	1758.865848	2095.005644	1978.874291	1625.244022	2088.927667	1897.932507	
11.77_327.8249m/z	327.8248997	11.76641667	pos							1559.916865	1820.207233	1248.687696	1216.655748	1696.650219	1772.523032	1651.3028	1842.257051	1321.320319	
11.78_305.8582m/z	305.858169	11.78391667	pos							1498.104797	1664.433835	1376.508151	1383.726851	1338.020435	1535.207908	2124.48411	1641.85472	1268.685914	
11.78_329.8222m/z	329.8221628	11.7715	pos							483.5190716	536.5991076	498.0905111	348.3931854	518.2923854	675.0767553	514.1358579	619.3421969	510.9426589	
11.78_384.2347m/z	384.2347214	11.78391667	pos							536.0443176	788.8628243	903.4953565	762.4503185	596.2449015	1003.148027	807.431287	784.416187	691.0416776	
11.78_404.7481m/z	404.7480904	11.78391667	pos							3626.335989	3407.67279	4432.995531	4634.770331	4786.13397	5054.281836	4341.345501	4372.019045	3997.670373	
11.78_489.3345n	512.3236826	11.78391667	pos							14598.17451	16799.06795	15575.01834	16524.97919	14270.94286	15323.70958	17310.17609	16518.21838	15259.02343	
11.78_509.8462m/z	509.8462291	11.78391667	pos							10999.33989	12725.10949	11276.32547	11617.65961	10726.88884	12094.02573	13252.49472	11983.47991	12447.46379	
11.78_531.7866m/z	531.7865918	11.775	pos							1319.035074	1464.282957	2314.479061	1574.106896	1767.105841	1818.868896	1864.537878	1740.494515	1512.541469	
11.78_562.7063m/z	562.7063032	11.78391667	pos							1730.053609	2346.809274	2784.857415	2976.66527	3485.001796	3163.217261	3140.257629	3558.358031	3108.005826	
11.79_420.7892m/z	420.7891613	11.7945	pos							883.4166309	1071.267793	1066.549487	877.6513749	1092.361487	908.2317975	1445.762622	1445.063034	1178.585335	
11.79_473.8282m/z	473.8282448	11.7945	pos							4313.670051	6018.051744	6398.292397	7069.913083	6134.320832	5589.777281	7912.123985	6076.879587	6025.056755	
11.79_489.8369n	512.8255758	11.7945	pos							5593.821743	7365.140572	5847.777604	7763.497916	5701.409772	7149.619171	6157.872142	6862.856486	6515.308455	
11.79_510.3479m/z	510.347905	11.7945	pos							5888.545495	6954.615719	6310.128079	6471.524145	5237.390969	5892.351593	7561.848681	5177.081503	6923.889254	
11.79_510.8556m/z	510.8556243	11.7945	pos							3498.856007	4658.696575	4634.419956	4300.883007	4181.419055	4061.078961	4367.231721	4157.506397	3472.919485	
11.81_218.9195m/z	218.9194663	11.81006667	pos							2148.109926	2726.686567	2930.640969	2390.332252	2435.801045	2334.234552	2553.322468	2768.398618	2278.900225	
11.81_220.8653m/z	220.8653326	11.81006667	pos							1105.327915	1648.796576	1787.989092	1499.16279	1556.352969	1338.091635	1420.976427	1437.369855	1285.827719	
11.81_222.8624m/z	222.8624173	11.81006667	pos							297.0401236	477.2643153	457.127875	371.3455111	438.3544716	356.131573	388.1206659	411.2398491	364.1311344	
11.81_229.5828m/z	229.5827538	11.81006667	pos							370.2931725	522.6822212	413.9979476	397.6240458	449.3592607	444.5926716	585.3107399	466.1967356	641.0793019	
11.81_382.7647m/z	382.7647191	11.81006667	pos							7675.368524	7788.123824	8881.329483	10349.92858	10731.71925	9734.649207	10223.81065	10001.72886	10937.09786	
11.81_467.3216n	490.3106103	11.81006667	pos							18095.07392	22529.26208	21620.00045	23123.28322	19823.33076	21663.49265	21131.29026	19334.27924	22939.0794	
11.81_467.8230n	490.8128913	11.81006667	pos							8268.634657	10832.81482	10140.40798	11393.60458	10964.15167	10425.31981	10727.53074	9888.774046	12109.86197	
11.81_487.8329m/z	487.8329119	11.81006667	pos							17480.99108	18969.25973	20059.48314	20514.66833	18514.47506	18006.45523	19727.82743	18326.39406	19071.57041	
11.81_604.7679m/z	604.7679061	11.81006667	pos							1599.308157	2103.965247	2465.286691	2771.39958	3421.148834	2020.231961	3434.497695	2754.348343	3539.955494	
11.82_494.7186m/z	494.7185776	11.8223	pos							1940.799535	2154.966431	2153.015748	2210.89527	2658.299168	2102.979476	2393.171014	2138.103805	2502.564085	
11.83_142.9802m/z	142.9802096	11.83283333	pos							0.001403199	0.001403199	16.33871363	0.001403199	0.001403199	26.43725831	26.03699968	18.06834647	0.001403199	
11.83_374.8817m/z	374.8817286	11.83283333	pos							2221.26219	3487.735144	3032.948814	5130.938729	3520.922131	2922.342467	3904.975354	3297.046617	4250.86442	
11.83_445.3081n	468.2975966	11.83283333	pos							21012.62074	21685.41869	22787.89829	22976.98984	23561.46606	20808.38662	23733.38392	20032.74541	24088.83925	
11.83_445.8099n	468.7957341	11.83283333	pos							21360.14355	22392.80343	24697.93035	24847.43713	26721.07309	22273.56204	26689.87527	24147.09085	26550.11573	
11.85_395.8126m/z	395.8125763	11.84828333	pos							4450.675289	4687.606501	5115.77491	5237.487657	5602.150509	4543.755263	6656.928182	5121.530228	5925.526284	
11.85_397.8093m/z	397.8093237	11.84828333	pos							1710.336776	1379.372382	2195.169356	2360.748738	2282.025576	2053.449528	2757.108301	2035.598574	2263.555453	
11.85_465.8199m/z	465.819853	11.84828333	pos							21603.70777	22847.3137	22333.60246	23051.09201	24218.07344	20743.13176	24327.10274	22744.7566	24127.0249	
11.85_466.3218m/z	466.3217813	11.84828333	pos							8024.475811	7901.94768	8956.768681	9740.708286	8513.841352	8250.324383	8920.280158	8507.710864	10587.15995	
11.86_341.8930m/z	341.8930304	11.8588	pos							638.2969856	360.5959926	666.6246942	694.698848	844.5498046	511.6048238	770.6024944	599.4385986	885.6469898	
11.86_348.2867m/z	348.2867328	11.8588	pos							477.3029361	824.9171567	840.2880483	785.6892687	852.2751683	420.7994989	1209.114396	887.048289	1105.893036	
11.86_402.8020m/z	402.8019747	11.8588	pos							3223.823447	2655.282941	3334.172817	3596.797473	3316.626268	3403.131383	3997.739062	3808.113564	4663.480786	
11.86_422.7362m/z	422.7362422	11.8588	pos							1353.150275	1420.649339	1106.455983	1425.039114	1590.245069	1042.162995	2088.209601	1494.800541	2254.542375	
11.86_441.3293m/z	441.3293237	11.8588	pos							4106.165815	3832.298791	5033.53254	4098.19018	4376.793715	3543.058829	4154.919072	4339.00886	4466.53646	
11.86_441.8309m/z	441.8309165	11.8588	pos							1791.701498	1811.448415	1789.321036	1714.629562	2186.956137	1541.179818	2555.006966	1699.476853	2061.990657	
11.86_446.2844m/z	446.2844181	11.8588	pos							14399.77374	13422.97527	14617.50273	15634.30591	18547.20514	13664.02309	17005.85052	14916.31372	16511.96948	
11.86_536.7812m/z	536.7811993	11.8588	pos							5322.987856	4820.703562	6724.004613	6458.857034	6904.0151	5967.501313	6947.902038	6248.711295	7558.291073	
11.86_592.8127m/z	592.8127091	11.8588	pos							31391.66028	30592.14206	34139.47572	35592.40282	36975.87307	35435.07156	37880.75181	36142.06819	37216.56568	
11.87_222.8624m/z	222.8623637	11.87055	pos							368.5818677	142.5283742	287.6932562	183.1996987	403.6883045	319.708767	404.1249798	259.9487979	476.8720313	
11.87_324.9029m/z	324.9028783	11.87055	pos							2121.376161	954.4859208	1425.916848	1275.646256	2303.889653	1872.592431	2058.528083	1689.320281	2106.837686	
11.87_405.7835m/z	405.7834957	11.87055	pos							3962.09195	3281.793457	3813.666533	4255.225973	4701.1353	3806.618292	4534.128158	3848.297004	5108.36616	
11.87_407.7783m/z	407.7782694	11.87055	pos							169.8414996	174.8413768	359.8968817	200.8303332	370.6276371	752.6593367	464.2903828	246.9661962	547.4253427	
11.87_419.8492m/z	419.8492246	11.87055	pos							1193.432785	859.7943714	1293.825012	1105.340876	1596.779416	1200.972688	1718.761685	1257.807461	1449.772661	
11.87_425.7658m/z	425.765794	11.87055	pos							1085.435303	928.2581059	996.4377419	1483.876698	1253.72302	1524.967595	1269.906506	1167.802228	1109.601043	
11.87_443.8066m/z	443.806636	11.87055	pos							19270.25594	20082.68588	22211.25667	22554.18256	25053.3127	20301.25558	23955.04042	20668.03087	22249.97099	
11.87_446.7865m/z	446.7864857	11.87055	pos							4806.870853	5688.567256	6054.523641	5193.936463	6818.018263	5200.688091	5517.593336	5466.855582	6324.425386	
11.87_482.7626m/z	482.7626158	11.87055	pos							20802.65629	21067.07508	23227.093	26506.40085	28192.37465	25107.10508	27039.65824	24204.52898	26493.65809	
11.88_816.6981m/z	816.6981374	11.88283333	pos							3570.884791	2497.367565	3662.902923	1797.478139	2234.747297	1228.734789	5486.438483	3704.362558	3560.995355	
11.90_220.8654m/z	220.8653555	11.89678333	pos							1312.300452	726.0292808	926.4924232	775.5324755	1579.482301	971.3502237	1357.495882	919.2528486	1281.011925	
11.90_327.9323m/z	327.9323227	11.89678333	pos							2972.838972	2737.247979	3155.844631	3241.293879	3506.956228	3056.349737	4344.944247	3273.475209	3947.253	
11.90_421.7936m/z	421.7936426	11.89678333	pos							8561.254109	7175.49786	7594.524552	7917.702535	9969.805692	7552.178092	10254.06964	8552.704953	9840.323815	
11.90_422.2955m/z	422.2955466	11.89678333	pos							2891.481194	3182.406635	2957.047972	3243.710105	3667.158106	3291.05675	3854.45891	3478.285751	3659.736114	
11.90_424.2713m/z	424.2712982	11.89678333	pos							11673.0054	11475.29759	12570.14173	11961.67314	15714.52211	11477.9174	14623.66209	12452.81205	13409.42351	
11.90_424.7725m/z	424.7724838	11.89678333	pos							5837.850235	6076.745966	7204.687554	6885.436747	8535.535519	6212.559524	7067.726768	6315.464912	7957.191032	
11.90_549.7013m/z	549.7013137	11.89678333	pos							2072.729025	1293.919392	1730.904714	2274.639436	2340.075245	2388.137103	2517.751491	2468.570343	3042.719322	
11.90_802.5630n	825.5533131	11.89678333	pos							18808.41555	13464.77101	18645.89022	18620.29081	21046.4552	17364.54115	24637.72067	19323.72291	20034.84487	
11.91_402.7603m/z	402.7603306	11.9137	pos							1317.195549	1127.701663	1527.34448	1024.092382	1528.016802	1099.560435	1448.052568	1238.94413	1736.254923	
11.91_582.7838m/z	582.7837603	11.9137	pos							4118.380258	3842.266582	4405.925302	5173.268644	4768.352815	4484.659636	5482.576453	4819.355978	5502.026179	
11.93_132.0031m/z	132.003089	11.92588333	pos							1750.734718	1380.181347	1613.766118	1341.800156	1224.759445	1536.431201	1422.17978	1325.638801	1452.268948	
11.93_215.9831m/z	215.9830708	11.92588333	pos							3742.831222	3096.545876	3485.60245	3229.013653	2816.904037	3691.096552	3430.831319	3149.39917	3460.013886	
11.93_305.8429m/z	305.8429435	11.92588333	pos							2080.258938	1083.671235	1723.506264	1576.922226	1857.350323	2131.826927	1119.327584	1398.804439	1532.488975	
11.93_307.2258m/z	307.2257925	11.92588333	pos							357.7042243	579.921209	433.2725666	349.2338012	524.9626123	343.0421445	431.7488988	716.9012642	247.2347207	
11.93_327.8248m/z	327.8247766	11.92588333	pos							4338.058012	4427.264887	4987.329846	5520.429573	5273.574255	4454.649361	5579.57711	4993.144399	5639.367571	
11.93_341.8930m/z	341.8929547	11.92588333	pos							1117.714057	883.3047598	879.8917715	1042.277687	1086.317504	1151.38597	1009.133472	977.0862524	1033.34147	
11.93_464.7984m/z	464.7983839	11.92588333	pos							1120.360095	1443.938026	1245.981677	1981.820195	2180.969005	1560.509725	1521.404521	1245.699178	2063.716141	
11.94_261.1307m/z	261.1306816	11.93648333	pos							1552.246367	1598.821939	1752.805684	1583.602185	1571.060137	1519.90647	1684.885018	1431.226424	1438.688575	
11.94_283.8760m/z	283.8760262	11.93648333	pos							1460.146689	1774.761067	2112.170858	1594.628774	1762.009219	1668.422514	1738.336613	1477.067592	1895.083727	
11.94_838.5555m/z	838.5555343	11.93648333	pos							8858.934416	6138.542422	5558.190907	3608.392693	1618.012168	2282.28721	6111.901012	3927.024145	3442.876989	
11.95_305.8580m/z	305.8580479	11.9467	pos							1133.555693	1403.938463	1185.976416	1169.898123	1037.906776	1154.841682	1233.181029	1037.520302	1244.515429	
11.95_422.7364m/z	422.7363676	11.9467	pos							1806.021846	1595.38474	1731.309581	1612.862364	1230.633502	1422.291375	1712.603259	1675.734209	1579.315433	
11.95_550.7505m/z	550.7504936	11.9467	pos							5002.747678	4475.611726	5052.016228	6033.99316	5387.322398	6038.457573	5645.335365	4187.619006	5555.693217	
11.96_297.0821m/z	297.0820556	11.96068333	pos							57654.48735	800.3621373	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	
11.96_395.8125m/z	395.8124651	11.96068333	pos							3007.849512	2895.999849	3321.115614	3781.657581	2750.067456	3089.446504	3028.237967	3182.950504	3207.854588	

11.96_688.5194m/z	688.5193902	11.96068333	pos
11.97_103.9557m/z	103.9556885	11.97468333	pos
11.97_594.1287n	617.117912	11.97468333	pos
11.97_732.5452m/z	732.545234	11.97468333	pos
12.00_220.8653m/z	220.8653123	12.00096667	pos
12.00_422.7728m/z	422.7728419	12.00096667	pos
12.00_536.7810m/z	536.7810475	12.00096667	pos
12.00_562.7061m/z	562.7060677	12.00096667	pos
12.01_365.8328m/z	365.8327939	12.0133	pos
12.01_518.7394m/z	518.7393774	12.0133	pos
12.01_626.4595n	644.4933433	12.0133	pos
12.03_120.0255m/z	120.0255002	12.02543333	pos
12.03_288.8527m/z	288.8527255	12.02543333	pos
12.04_372.0726n	355.0692837	12.03775	pos
12.04_427.2198m/z	427.2198108	12.03775	pos
12.05_282.2660m/z	282.2660216	12.0496	pos
12.05_422.7362m/z	422.7361908	12.0496	pos
12.05_528.7679m/z	528.767947	12.0496	pos
12.05_538.4074n	561.3965949	12.0496	pos
12.05_836.5400m/z	836.5400447	12.0496	pos
12.05_838.5560m/z	838.5560298	12.0496	pos
12.06_215.9831m/z	215.983063	12.06195	pos
12.06_305.8582m/z	305.858219	12.06195	pos
12.06_309.1304m/z	309.1303904	12.06195	pos
12.06_332.8191m/z	332.8190782	12.06195	pos
12.06_369.2973m/z	369.2972585	12.06195	pos
12.06_419.8492m/z	419.8491869	12.06195	pos
12.08_305.8429m/z	305.8428934	12.07935	pos
12.08_307.8403m/z	307.8402645	12.07935	pos
12.08_324.9030m/z	324.9030042	12.07935	pos
12.08_494.3813n	517.3704924	12.07935	pos
12.08_541.8158m/z	541.8157754	12.07935	pos
12.10_450.3552n	473.3443069	12.09976667	pos
12.10_468.7938m/z	468.793808	12.09976667	pos
12.10_470.7891m/z	470.7890694	12.09976667	pos
12.11_283.8760m/z	283.8760103	12.11036667	pos
12.11_351.8637m/z	351.8636854	12.11036667	pos
12.11_365.8329m/z	365.8328717	12.11036667	pos
12.11_380.3365m/z	380.3364635	12.11036667	pos
12.11_385.2918m/z	385.2918431	12.11036667	pos
12.11_395.8123m/z	395.8122729	12.11036667	pos
12.11_397.8093m/z	397.8093142	12.11036667	pos
12.11_406.3288n	429.3181428	12.11036667	pos
12.11_470.7381m/z	470.7381084	12.11036667	pos
12.12_431.3241m/z	431.3241054	12.1244	pos
12.12_446.8093m/z	446.8092655	12.1244	pos
12.12_453.7711m/z	453.7710992	12.1244	pos
12.12_599.7740m/z	599.7740199	12.1244	pos
12.14_332.8192m/z	332.8191804	12.1367	pos
12.14_343.8510m/z	343.850976	12.1367	pos
12.14_405.7836m/z	405.7835568	12.1367	pos
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12.14_473.8281m/z	473.8281268	12.1367	pos
12.15_402.8018m/z	402.8018325	12.14558333	pos
12.15_550.7504m/z	550.7504028	12.14558333	pos
12.15_592.8126m/z	592.8125693	12.14558333	pos
12.16_281.0501m/z	281.0501332	12.15966667	pos
12.16_305.8583m/z	305.8582665	12.15966667	pos
12.16_524.8254m/z	524.8254232	12.15966667	pos
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12.18_307.8403m/z	307.840323	12.17538333	pos
12.18_327.8248m/z	327.8247652	12.17538333	pos
12.18_371.1008m/z	371.1007737	12.17538333	pos
12.18_456.8380m/z	456.8380145	12.17538333	pos
12.18_463.7996m/z	463.7996345	12.17538333	pos
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12.19_395.8125m/z	395.8124692	12.19128333	pos
12.19_397.8091m/z	397.8090914	12.19128333	pos
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12.19_604.6414m/z	604.6413536	12.19128333	pos
12.21_582.7840m/z	582.7840425	12.20523333	pos
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12.22_299.0613m/z	299.0613034	12.21766667	pos
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12.22_563.3573m/z	563.3573435	12.21766667	pos
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12.23_131.5291m/z	131.5291448	12.2313	pos
12.23_275.2577m/z	275.2577039	12.2313	pos
12.23_315.8716m/z	315.8716167	12.2313	pos
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12.28_388.8505m/z	388.850539	12.27816667	pos
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12.28_563.8592m/z	563.8592331	12.27816667	pos
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12.29_536.8908m/z	536.8907528	12.28886667	pos
12.29_560.8799m/z	560.8798973	12.28886667	pos
12.30_468.7938m/z	468.7938367	12.29785	pos

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12.30_604.6410m/z	604.6409556	12.29785	pos
12.31_305.1566m/z	305.1565694	12.3086	pos
12.31_496.3423n	519.3315105	12.3086	pos
12.31_496.8434n	519.8332139	12.3086	pos
12.31_762.5985m/z	762.5984676	12.3086	pos
12.32_341.8929m/z	341.8929268	12.31761667	pos
12.32_357.1465m/z	357.1465205	12.31761667	pos
12.32_399.3076m/z	399.3075598	12.31761667	pos
12.32_485.7840m/z	485.7840291	12.31761667	pos
12.32_517.3553m/z	517.3552801	12.31761667	pos
12.32_550.7505m/z	550.7505214	12.31761667	pos
12.33_288.8526m/z	288.852564	12.33003333	pos
12.33_324.9030m/z	324.9029674	12.33003333	pos
12.33_405.7832m/z	405.7832436	12.33003333	pos
12.33_436.7811m/z	436.7811386	12.33003333	pos
12.33_600.6987m/z	600.6986718	12.33003333	pos
12.34_472.7341m/z	472.7340632	12.34246667	pos
12.34_494.8407m/z	494.8407274	12.34246667	pos
12.34_838.5568m/z	838.5567751	12.34246667	pos
12.36_354.8437m/z	354.8437088	12.35646667	pos
12.36_474.3292n	497.3184468	12.35646667	pos
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12.36_495.3425m/z	495.3424609	12.35646667	pos
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12.37_395.8124m/z	395.812375	12.37401667	pos
12.37_399.3471m/z	399.347101	12.37401667	pos
12.37_472.8277m/z	472.8277373	12.37401667	pos
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12.39_452.8180n	475.8073004	12.38798333	pos
12.39_966.6935m/z	966.6935444	12.38798333	pos
12.40_379.9160m/z	379.9159663	12.3983	pos
12.40_618.7374m/z	618.7374282	12.3983	pos
12.40_650.7711m/z	650.7711087	12.3983	pos
12.40_922.6675m/z	922.6674638	12.3983	pos
12.41_332.8617m/z	332.8616853	12.41428333	pos
12.41_404.7472m/z	404.7471878	12.41428333	pos
12.41_430.3031n	453.2922625	12.41428333	pos
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12.41_451.3163m/z	451.3163339	12.41428333	pos
12.41_596.7556m/z	596.755567	12.41428333	pos
12.43_245.0993m/z	245.0992635	12.42968333	pos
12.43_340.2086m/z	340.2086392	12.42968333	pos
12.43_409.2661m/z	409.2660859	12.42968333	pos
12.43_409.7676m/z	409.7676163	12.42968333	pos
12.43_450.8146m/z	450.8146098	12.42968333	pos
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12.44_354.8439m/z	354.8438778	12.44213333	pos
12.46_325.9369m/z	325.9369142	12.45588333	pos
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12.46_463.7997m/z	463.7997443	12.45588333	pos
12.46_599.7740m/z	599.7740117	12.45588333	pos
12.47_103.9557m/z	103.955742	12.46661667	pos
12.47_315.8717m/z	315.8716806	12.46661667	pos
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12.47_582.7839m/z	582.7839026	12.46661667	pos
12.47_816.5804n	839.5663768	12.46661667	pos
12.48_200.8626m/z	200.8626192	12.4791	pos
12.48_394.7941m/z	394.7941059	12.4791	pos
12.48_550.7505m/z	550.7505345	12.4791	pos
12.49_220.8653m/z	220.8653257	12.48818333	pos
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12.49_478.7478m/z	478.7478451	12.48818333	pos
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12.50_402.8019m/z	402.8019351	12.50068333	pos
12.50_417.7967m/z	417.796686	12.50068333	pos
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12.51_762.5984m/z	762.598365	12.51148333	pos
12.51_838.5563m/z	838.5562641	12.51148333	pos
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12.52_323.8845m/z	323.8845468	12.52398333	pos
12.52_746.5610m/z	746.5610413	12.52398333	pos
12.53_303.1410m/z	303.1410382	12.53313333	pos
12.53_305.1567m/z	305.1566803	12.53313333	pos
12.53_343.8507m/z	343.8507041	12.53313333	pos
12.53_395.8121m/z	395.8121453	12.53313333	pos
12.53_414.7753m/z	414.7752607	12.53313333	pos
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12.53_528.7681m/z	528.7681137	12.53313333	pos
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12.54_488.8717m/z	488.8717267	12.54226667	pos
12.54_668.1471n	691.136353	12.54226667	pos
12.54_702.5352m/z	702.5351604	12.54226667	pos
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12.55_354.8436m/z	354.8435927	12.55465	pos
12.55_490.8178m/z	490.8177951	12.55465	pos
12.57_149.1071m/z	149.1070924	12.56695	pos
12.57_200.8623m/z	200.8623352	12.56695	pos
12.57_324.9031m/z	324.9031182	12.56695	pos
12.57_326.8984m/z	326.8984259	12.56695	pos
12.58_477.7708m/z	477.7708182	12.57735	pos
12.59_334.8145m/z	334.8144774	12.58981667	pos

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956.2237807	667.511557	1322.047565	1423.089208	1298.055668	1480.356443	1411.989138	1710.239365	1228.124456		
2979.346109	2247.304899	2834.628444	3088.253119	2669.018122	2581.216576	3170.879754	2856.661366	2661.13604		
18644.59741	18691.70136	21034.58215	21390.87501	21373.12929	21187.1454	21565.2523	20123.01021	22811.25146		
10194.56954	8944.42726	10524.74948	10551.86842	10726.21453	11195.79351	10644.06888	9865.913297	11041.11773		
17169.17644	10435.31091	7693.654502	3037.881521	1479.700984	1632.021033	6815.879529	4457.99807	3611.561267		
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2695.535153	2288.335895	2704.123399	2754.962653	2728.28078	2444.902473	2976.612339	2775.987778	2187.880676		
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26118.53312	25717.32708	29971.83525	30052.9783	33580.48065	36139.57763	32237.57408	30369.74152	33564.67848		
1007.295017	1452.953315	1482.42264	1613.996691	1997.563525	1457.312305	1578.931401	1502.349462	1924.410432		
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27123.6498	27490.66896	27561.26105	30064.38496	30621.33828	31070.36718	28760.88004	28097.18095	28344.29788		
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2145.373055	2168.336086	2716.622176	2925.647608	2908.965459	3214.260588	1515.937827	1978.539838	2504.794713		
2753.304612	2416.560029	2754.7037	2659.925355	2609.826644	3102.1378	2300.424598	2153.656524	2519.750273		
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12931.85433	12047.43279	12824.83884	11597.89122	12809.58414	13204.78796	12396.15532	11766.96697	12377.2559		
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8481.021843	7835.829198	8258.399449	8897.936801	8506.922925	10218.38558	9616.864551	7967.91215	8376.502244		
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2345.02567	1515.231563	2134.36345	1720.391679	1794.245709	2441.37604	2388.28736	2048.93315	2266.660436		
3596.174817	2145.93616	3733.19758	2672.394984	2711.222954	3932.146261	3431.529752	3439.666038	3710.531133		
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2939.712416	3613.976665	2954.715254	3369.339145	4047.566251	3224.570031	4416.245953	3370.718656	2779.919654		
4202.022748	3944.613906	2747.727737	3622.864549	4502.422914	3764.880314	4069.901527	3685.640259	3333.266463		
52808.63631	53198.38112	58229.28095	61127.95345	63922.77693	64541.50794	64645.4033	58853.2815	66776.32356		
1029.752107	1069.107252	1061.999105	529.5631115	798.9253706	696.4008682	698.2602963	908.3101025	597.6676992		
20262.00264	18663.23597	20004.62877	21851.60506	23761.00115	23834.00521	22415.62905	20853.27941	23096.39782		
1700.886931	1643.770653	1262.074279	1485.029463	1878.433308	1517.624739	2187.274667	1748.666487	1410.91166		
2401.075629	2054.992175	2107.081043	1808.541009	2128.151833	1980.822999	2406.439647	2284.368031	1975.295532		
424.9822608	3374931.346	528.5841466	173.3936829	0.914478402	0.001403199	115.1851339	330.5327704	307.5508447		
18541.13217	16221.66111	15873.32381	16520.10087	15646.54911	14353.75081	20015.67336	17319.20862	15881.50673		
2544.895136	3564.741869	2209.446014	2367.764435	3116.936526	2424.412308	2953.791767	2720.03088	1701.095219		
2399.028049	2441.292355	2220.728375	2183.770931	2701.248555	2073.021536	3224.392744	2456.917074	1846.686485		
1466.11809	1232.857743	1003.13368	1293.099754	1730.016316	1483.533118	1194.575283	1297.488914	1336.893679		
390.600047	263.6512077	150.9333556	120.2859632	151.1352451	107.4472565	190.4066119	193.2203276	145.3161012		
761.3169958	712.8814866	504.6152826	678.3930321	757.8093551	839.2802801	632.7059999	723.73651	849.7245342		
2200.425329	1893.295505	1496.772176	1773.364515	2329.225104	2295.959041	2308.036422	1939.12035	2064.823898		
483.080753	373.2590541	189.4927418	341.8390113	430.5033926	458.2882817	394.5956445	400.0225949	478.2740822		
4497.787062	4496.993435	3740.924362	4741.426772	5800.241246	6073.775312	5093.710211	5712.148936	5931.623996		
815.0005162	600.8775808	551.2624807	921.186563	884.8055961	1039.939402	852.5587092	733.3336182	1175.201959		

12.59_352.8009m/z	352.8009478	12.58981667	pos	3177.013845	3221.371832	3492.771518	3903.895696	4335.065322	4318.24647	3569.310605	4098.487528	4191.322764		
12.59_379.9157m/z	379.9157365	12.58981667	pos	5441.125488	7531.71726	4750.562579	5951.675782	6989.993134	7635.070843	7404.195971	6564.252744	6543.70674		
12.59_567.6670m/z	567.6670208	12.58981667	pos	211.6155579	104.2934931	165.9001859	357.7419874	575.2002962	686.2232107	75.75697579	451.5438996	729.4261095		
12.59_606.5527m/z	606.5526697	12.58981667	pos	1370.354176	2190.0626	1393.208255	1357.105296	1711.070908	1736.031382	1716.846851	1668.000609	1865.704324		
12.59_640.4751n	663.4643419	12.58981667	pos	67817.05011	63159.63198	61951.80399	61206.71282	63040.31685	66483.58339	68521.07559	66907.04724	62151.68331		
12.60_332.8190m/z	332.8189608	12.59883333	pos	1080.068626	1357.905327	1255.735853	1596.189302	1685.835304	2226.595241	1502.505671	1453.134316	1866.748504		
12.60_400.8065m/z	400.8064987	12.59883333	pos	4794.264295	5565.966834	4898.07821	5944.983732	6641.27557	6182.793124	6211.769795	6117.96912	6087.198379		
12.60_550.7504m/z	550.7503752	12.59883333	pos	1852.2484	2698.52167	1602.317307	2423.489214	2729.961916	3833.241139	2204.488934	2302.564134	2771.614527		
12.60_596.4490n	619.438227	12.59883333	pos	85680.39796	81168.272	76522.24842	77116.30825	81642.60768	82820.15167	83525.96767	80938.16753	73927.24742		
12.60_604.6414m/z	604.6413651	12.59883333	pos	6446.88743	6632.075068	6858.981111	8136.846026	8962.779161	9457.717051	7736.529298	8171.777672	7770.490945		
12.62_422.8812m/z	422.8811883	12.62173333	pos	6099.602589	5717.984096	6038.554448	6780.07601	6758.427241	7259.829509	6479.623041	6319.775919	7595.818395		
12.62_429.3181m/z	429.31811	12.62173333	pos	2129.12491	3579.971522	2585.658366	2458.450421	2462.809107	4462.096911	3662.926276	2272.067493	2533.353256		
12.64_325.9371m/z	325.93708	12.64406667	pos	1305.381841	1845.583859	1594.93524	1395.716779	1673.851367	2460.631511	2140.393567	1514.084811	1640.817008		
12.64_395.8121m/z	395.8121389	12.64406667	pos	1865.516589	2209.673628	2301.80126	2419.309685	2806.46187	2643.723887	3015.830747	2354.925037	2118.866557		
12.64_423.3867m/z	423.3867185	12.64406667	pos	1416.088003	1605.539046	1362.256952	1118.471353	1438.353513	1941.302655	1543.232245	1207.062695	1532.284515		
12.64_472.7793m/z	472.7793288	12.64406667	pos	2267.224528	2708.438162	2596.525519	3719.360047	3651.478176	3381.01072	3705.752428	3585.773496	3161.427826		
12.64_552.4230n	575.4121564	12.64406667	pos	120151.8063	112495.897	108259.7117	108801.9119	114698.0675	118313.4613	118232.294	112969.7032	110610.9062		
12.67_219.8580n	242.8472026	12.66695	pos	256030.7356	253809.525	262290.0036	279806.788	292173.4864	296458.4109	285904.3912	274561.005	292879.7833		
12.67_454.7692m/z	454.7692191	12.66695	pos	3022.111368	3529.232292	3639.327373	4288.965807	4164.216858	4170.798285	4322.282483	3406.731378	4699.12232		
12.67_508.3969n	531.3860268	12.66695	pos	171328.6126	159928.4599	155851.5357	163129.5676	166124.7057	174892.7844	174457.1098	164584.7206	173452.5127		
12.68_200.8625m/z	200.8625178	12.68108333	pos	732.3649066	545.3059443	710.4473288	916.0711367	958.6969776	619.3480688	1017.243125	747.3799341	803.7860515		
12.68_299.9375m/z	299.9375308	12.68108333	pos	782.0627807	723.7648956	894.3890347	840.0287338	1074.914586	996.2350845	1005.973561	906.7122557	938.4026393		
12.68_427.7502m/z	427.7501782	12.68108333	pos	160.5738512	207.2519936	441.7938386	364.6186819	431.6625726	326.7068849	363.6519271	344.847505	334.7642259		
12.68_473.3443m/z	473.3442649	12.68108333	pos	2275.185214	1517.502763	2062.395043	2242.235186	2195.738438	2118.1671	2044.014505	2442.979732	2836.127828		
12.68_473.8280m/z	473.8280463	12.68108333	pos	10303.68559	11448.24287	8678.006742	11104.76697	13148.44087	12607.94662	12862.75635	11790.90997	13055.44546		
12.68_514.7967m/z	514.7966732	12.68108333	pos	21140.91761	21979.58885	22819.80999	25003.11958	24611.9721	24664.63775	25425.7045	22885.078	25686.03196		
12.68_592.8123m/z	592.8123005	12.68108333	pos	3183.434551	2372.041092	3157.268402	3696.980923	4175.333479	3338.823098	4176.021701	3119.215934	4078.868739		
12.70_446.7128m/z	446.7127853	12.70028333	pos	2921.053241	2878.003365	2861.463196	3946.746461	4338.493414	4643.234613	3968.295209	3683.077242	3945.653053		
12.70_464.3706n	487.35984	12.70028333	pos	256888.7317	239102.0841	240097.1849	244831.6714	248411.2252	261265.1313	261961.6206	250345.8446	257604.9104		
12.70_504.7679m/z	504.767899	12.70028333	pos	13889.71512	15361.83059	15951.51386	18425.5716	19246.86853	19784.66564	18799.20485	16252.20359	18956.70246		
12.70_540.7212m/z	540.7212138	12.70028333	pos	1144.727538	934.566492	1143.047614	1339.232505	1545.017518	857.9789198	1021.432099	1200.775955	1500.089447		
12.70_788.5429m/z	788.5429212	12.70028333	pos	6878.948592	4092.711339	4434.557576	3698.788708	2832.555137	1427.781487	5271.363155	3728.318939	3859.327897		
12.71_288.8524m/z	288.8524323	12.711	pos	2163.291595	1849.843896	1958.640304	2483.319871	2178.889704	2175.117569	2144.514954	2239.500864	2280.231752		
12.71_290.8496m/z	290.8495971	12.711	pos	625.7801147	525.74505	615.6704219	788.0875445	940.2409003	732.5635613	676.092741	748.3798547	748.37227		
12.71_369.2973m/z	369.2972977	12.711	pos	3652.927311	3436.874818	3174.403165	4193.798629	3657.953338	2951.133857	3292.235127	3284.795953	3476.794642		
12.71_420.3445n	443.3336351	12.711	pos	528104.768	501140.7759	501797.149	510845.9405	521405.4698	527176.0329	544334.8312	514221.9908	535620.6258		
12.72_244.9598m/z	244.9597867	12.72343333	pos	1558.702341	1692.072366	1654.155468	1850.807534	1773.823502	1330.557532	1382.497197	1752.071398	1681.639169		
12.72_376.3183n	399.3074969	12.72343333	pos	624873.5124	585430.7086	594673.053	605228.2635	617712.07	614591.3728	646175.0661	611376.5505	626296.4556		
12.72_377.3256m/z	377.3255715	12.72343333	pos	19118.0037	17070.36589	18073.61918	18909.44176	17860.38834	18439.22888	20077.16208	19488.78701	17984.38149		
12.72_401.3134m/z	401.3134337	12.72343333	pos	2630.275333	2763.142172	2400.016382	3184.159924	2755.852956	2289.489435	2477.74435	3010.129082	2659.597909		
12.72_422.3833m/z	422.3833148	12.72343333	pos	33741.98919	29824.37762	31434.74872	33603.36918	31268.41552	31923.71522	34530.92139	32222.50216	33038.98578		
12.72_466.4097m/z	466.4097306	12.72343333	pos	5455.974612	4626.153474	4843.65597	5976.173096	5071.958084	4159.693533	4306.038064	5101.978847	4815.243622		
12.74_305.1566m/z	305.156598	12.73915	pos	2287.493226	2028.609126	1813.668388	2499.097997	2141.337293	1680.843947	1700.606457	2034.100492	1927.651463		
12.74_343.8509m/z	343.8509243	12.73915	pos	4223.592869	5053.584131	4977.201424	5813.361714	5714.017221	5036.312323	5119.848247	5372.51501	4988.71175		
12.74_440.3843m/z	440.3843035	12.73915	pos	1371.571764	1227.696538	1313.025705	1246.868314	1269.954604	1478.100078	1446.250632	1482.250637	1350.420989		
12.74_527.7192m/z	527.7192156	12.73915	pos	10908.43115	10837.69928	10577.0747	12917.21153	14317.24954	14235.88425	13069.22433	12554.69648	13478.9929		
12.75_477.7706m/z	477.7705782	12.74965	pos	2282.874247	2179.576925	1961.811632	3402.590296	2613.367842	1736.123693	2087.215197	2252.03265	1973.255988		
12.76_273.1668m/z	273.166847	12.76383333	pos	1239.194728	859.7906485	1193.142972	1178.131681	922.2967553	915.8098507	885.9330847	1102.085569	859.5316877		
12.76_327.8247m/z	327.8247042	12.76383333	pos	17468.16945	16798.08511	18236.31493	17041.78848	18527.36664	19087.73688	18681.34632	16705.88605	19051.27847		
12.76_366.8330m/z	366.8329676	12.76383333	pos	1916.908848	2372.749506	2537.674154	2198.491634	2320.924195	2946.574486	2462.495162	2453.313919	2358.290653		
12.77_315.8715m/z	315.8714665	12.7728	pos	2121.207743	1607.36094	2078.152023	1849.09051	1534.953236	1812.956489	1458.505435	1878.762697	1381.983646		
12.77_566.8878m/z	566.8878005	12.7728	pos	11824.41074	11487.18278	12275.89144	11946.3523	13107.78892	14257.1019	12521.535	12719.1974	12640.41628		
12.77_568.3889m/z	568.3888736	12.7728	pos	995.3176537	1041.81468	527.7138325	108.9761853	852.4658614	982.6377486	350.32426	711.476738	670.909738		
12.79_332.8193m/z	332.819254	12.78523333	pos	1357.435815	1138.681707	1215.749414	1270.524807	1136.107145	1688.495214	1365.242549	1130.706846	1393.083006		
12.79_423.3867m/z	423.3866608	12.78523333	pos	3103.450411	2521.857282	3098.147575	2602.674807	2903.935072	3540.312266	3818.993164	3216.965159	2975.647737		
12.79_464.7240m/z	464.7239858	12.78436667	pos	5760.631628	5463.00309	6300.011365	7192.801871	7950.792145	8506.277573	5944.413919	7541.468448	7910.306013		
12.79_473.8279m/z	473.8279423	12.78523333	pos	6071.616156	5946.554883	6362.767944	5805.291838	6346.619776	8221.60753	6593.740755	5618.219349	5997.818134		
12.79_482.7627m/z	482.762705	12.78523333	pos	8072.708314	8349.341361	9794.956273	9385.210276	9954.049119	11000.75449	8649.776098	9237.726147	11249.31142		
12.79_531.7869m/z	531.7868791	12.79436667	pos	35689.64493	35414.59168	37828.69167	42742.27887	44717.70704	45370.61671	41973.44114	39781.59351	45411.33882		
12.79_548.3521m/z	548.3520528	12.79436667	pos	5072.248649	3385.380834	4610.443043	3937.527403	4932.115998	5075.133165	5912.083604	4682.913849	4651.28688		
12.79_567.6675m/z	567.6674569	12.78523333	pos	502.5146377	571.8496368	885.1204698	584.864487	746.0012653	985.4549448	860.8582012	701.1891019	1104.881049		
12.80_103.9557m/z	103.9556931	12.80346667	pos	3344.742542	3018.971575	3565.516011	2879.417786	2969.143317	3137.579579	2822.662583	2875.000115	3457.678166		
12.80_352.8970m/z	352.8970434	12.80346667	pos	4045.628545	3073.650479	4076.249113	2315.386423	3339.951585	4302.959335	3132.172312	2732.20985	3507.738783		
12.80_397.8672m/z	397.8671689	12.80346667	pos	1085.162963	999.147494	965.8123684	943.5737285	1118.899349	1420.288276	1163.491903	1018.77266	921.2528112		
12.80_494.7608m/z	494.7608065	12.80346667	pos	2752.658168	2353.547231	3298.200269	2264.011694	3324.852006	3690.502239	2398.348897	2620.521655	3282.544862		
12.80_545.7580m/z	545.7580986	12.80346667	pos	2491.20691	2302.61355	2681.209336	2250.911411	3492.07302	3541.659713	2485.608698	2538.060303	3106.950894		
12.80_545.8745m/z	545.874526	12.80346667	pos	6330.892406	5719.216041	5350.921795	5396.604286	5684.022213	6096.912389	6190.901124	6423.834362	6211.6976		
12.80_546.3763m/z	546.3762757	12.80346667	pos	3126.367391	3049.893365	2878.937705	2544.634599	2545.993378	3008.342874	3318.202384	3178.301537	2860.861297		
12.80_546.6387m/z	546.6386671	12.80346667	pos	20109.8202	22394.21887	23705.74081	30985.51922	32203.24203	34167.96883	27744.39468	27979.55382	30763.99066		
12.80_585.6778m/z	585.6777835	12.80346667	pos	1264.810351	1177.477098	1928.562847	1314.457142	2085.616668	2463.407324	1292.472698	1649.770897	2170.700311		
12.82_343.8507m/z	343.8507198	12.82411667	pos	1461.502187	1816.024616	2205.372059	948.3365512	2749.049444	2706.780548	1827.148069	1319.125415	2290.822826		
12.82_352.8010m/z	352.8009956	12.82411667	pos	2450.359345	2480.478073	3291.077172	2407.749619	2776.039288	3694.043669	2673.139486	2592.450741	3589.283798		
12.82_454.7693m/z	454.7692571	12.82411667	pos	5380.442213	5273.719947	4773.400871	4557.745438	6428.335196	6670.294219	5626.861685	5450.259491	6004.056905		
12.82_463.7995m/z	463.7995099	12.82411667	pos	26067.39889	26042.19775	24750.97569	30071.90741	31401.16671	31693.50212	30176.2458	28019.41283	30116.73261		
12.82_521.8854m/z	521.8854255	12.82411667	pos	1454.720592	1393.30323	1329.785153	1318.70011	982.0533056	1577.739249	1511.915279	1692.595342	1691.985477		
12.82_524.3632m/z	524.363187	12.82411667	pos	4602.498985	4265.74311	4617.602255	4448.182705	4518.165493	4872.661278	4188.380606	4643.729445	4888.837067		
12.82_548.8538m/z	548.8537033	12.82411667	pos	1758.424861	2128.413393	2355.122385	1799.280946	2014.05265	1970.95644	2242.760778	2509.943789	2264.976398		
12.82_554.6934m/z	554.6934082	12.82411667	pos	1150.651218	1249.283797	1801.698734	799.1894367	1998.426777	2337.54284	1320.325622	1499.629639	1671.448907		
12.85_200.8625m/z	200.8625236	12.84508333	pos	1659.740155	1380.450929	1623.582469	1371.981623	1743.227981	1977.904031	1963.11769	1661.79405	1877.934269		
12.85_215.9831m/z	215.9831111	12.84508333	pos	1886.372946	1493.033277	1845.410991	1444.710347	2015.080421	1854.060133	1738.953877	1667.412877	1834.146979		
12.85_400.8065m/z	400.8065304	12.84508333	pos	5024.244889	4247.989533	4973.123334	5447.914911	5928.231276	6221.803935	5526.910501	5413.040949	6466.008095		
12.85_472.7341m/z	472.7340886	12.84508333	pos	1894.780847	1992.148616	2318.384038	1499.195995	1953.816483	2568.300889	2302.030302	2071.086012	2115.049056		
12.85_514.7967m/z	514.7966847	12.84508333	pos	7915.820135	6873.747152	7637.101552	7369.028357	9127.252293	10104.10911	8245.638356	7823.673435	8664.990676		
12.85_523.8616m/z	523.8616409	12.84508333	pos	10166.60972	9351.611701	10734.97837	8927.540035	9584.896213	10436.54495	11088.00925	9462.554143	9567.220718		
12.86_217.9790m/z	217.9790226	12.861	pos	1396.193288	1173.594428	1526.914215	1156.36498	1336.280858	1428.376731	1306.874338	1246.031982	1388.280441		
12.86_406.2056n	429.1948627	12.861	pos	19455.13459	17931.13804	19659.90384	16773.09512	18467.61261	21648.12281	20894.39805	17463.05578	17542.03567		
12.86_502.3503m/z	502.3503413	12.861	pos	7830.99404	7092.176524	6538.001464	6687.703851	6327.05519	6641.368674	7545.294678	7532.353868	7334.04444		
12.86_522.6815m/z	522.6815182	12.861	pos	958.7722926	1313.906678	2069.03027	1061.221624	1967.220196	2291.929121	1344.835949	1702.092039	1612.349001		
12.86_532.7109m/z	532.7109045	12.861	pos	74864.20423	77138.60084	80825.09429	98786.05728	104111.6087	102637.9672	90550.49076	91205.26879	99563.18508		
12.86_592.8123m/z	592.8122593	12.861	pos	3062.526903	3065.467444	4570.830247	2847.984723	4270.823997	5876.489308	4336.503618	3372.582575	5830.905832		
12.88_284.2854m/z	284.2853774	12.87801667	pos	4600.883434	3554.196202	3560.637676	3413.777975	3429.414577	3608.453756	4498.382202	4699.166932	4249.995532		
12.88_498.9002m/z	498.900232	12.87801667	pos	3149.904964	3011.409614	2757.900894	3836.832563	3003.079753	3220.14237	4305.369533	3818.805387	4496.307743		
12.88_499.3710m/z	499.370958	12.87801667	pos	4689.39855	4075.091561	4536.068982	3883.309348	4158.791573	3832.232355	4507.814888	4447.792995	4178.02636		
12.88_499.8724m/z	499.8723558	12.87801667	pos	2327.515804	1539.063028	1750.158323	1896.78352	1816.038089	2005.89007	2080.883542	1981.270805	1821.239126		
12.89_395.8121m/z	395.8120888	12.8938	pos	1986.183388	1590.735186	1620.742499	2211.680691	2417.876061	2285.394545	2925.890095	2759.265219	2381.681869		
12.89_450.7523m/z	450.7523372	12.8938	pos	79752.8488	83012.31214	88733.63865	96924.82806	106165.2605	104606.8357	95117.89427	93236.90148	103971.6183		
12.91_294.9385m/z	294.9385321	12.90603333	pos	219328.4053	211076.6437	217497.4943	225695.8731	235163.3621	233587.2073	231667.1811	220544.3395	230957.8242		
12.91_298.8814m/z	298.8814386	12.90603333	pos	202250.9675	200522.2543	206266.3193	223105.0203	231922.2333	230947.8929	225469.472	215713.323	229485.2291		
12.91_344.8511m/z	344.8511437	12.90603333	pos	220.5097566	229.3163653	271.7897044	385.2944086	384.7293018	319.0958559	426.0598109	568.6478845	317.0506713		
12.91_365.8328m/z	365.8327919	12.90603333	pos	6237.410346	5948.480467	6849.054155	7188.435969	7214.402962	7865.32064	7559.483457	7955.214638	9869.14803		
12.91_397.8089m/z	397.8089377	12.90603333	pos	822.6472561	748.7764719	700.8646116	796.0714706	952.2430598	896.2286985	1127.82964	967.890175	848.2864744		
12.91_422.8308m/z	422.8308448	12.90603333	pos	2306.783373	2193.682513	2142.723177	2570.004885	2619.586502	2862.044642	2833.05827	2822.046143	3031.646933		
12.91_459.8257n	482.8146659	12.90603333	pos	5941.358602	5263.401091	5542.261263	5331.538006	5338.296831	6767.583934	6407.039011	6210.436241	6141.064744		
12.91_477.3575m/z	477.3575481	12.90603333	pos	2336.505269	1986.346089	1769.003012	2387.930805	1877.392647	2004.185077	2977.988494	2711.700919	2223.682199		
12.91_477.7710m/z	477.7710403	12.90603333	pos	7962.31984	8599.96045	8876.018379	8281.526361	11079.50251	11698.9868	8662.748155	10054.58537	11234.82477		
12.91_480.3372m/z	480.3372133	12.90603333	pos	3753.100642	2907.97203	2832.567209	3943.232354	3452.916742	3488.316091	4471.545652	3823.57214	3882.561398		
12.91_482.3131m/z	482.3131167	12.90603333	pos	15836.37002	15343.85411	14564.24308	13935.01258	16066.79364	16372.84124	16517.25831	14761.49737	16127.13525		

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13.33_220.8653m/z	220.8652863	13.33273333	pos							15639.14317	14799.17607	14585.91609	15181.57521	17015.17879	16856.27358	15966.71093	15808.2359	17004.00739	
13.33_346.3077n	369.2969824	13.33273333	pos							1074494.804	1073817.557	1048056.843	1082271.593	1142841.094	1143849.193	1167890.366	1118048.16	1146796.906	
13.33_446.7130m/z	446.7129802	13.33273333	pos							1900.031496	1518.21225	1130.556659	1791.364944	1790.206604	1850.316995	1646.815536	1755.671382	2083.627674	
13.34_273.1667m/z	273.1667401	13.34165	pos							911.4505666	951.0643158	765.4538926	958.492578	835.6395027	905.2066743	644.5433668	886.7873613	675.0926663	
13.34_371.3034m/z	371.303432	13.34165	pos							13821.55859	12928.60564	12611.69615	14165.14192	13845.03301	14784.92931	14468.75909	14004.24095	14126.57396	
13.36_328.3206n/z	328.3206122	13.36138333	pos							576.5032821	428.8230893	565.0935287	391.6207079	267.1518655	221.354073	560.8719008	243.2287791	488.8526985	
13.36_352.8010m/z	352.8010317	13.36138333	pos							1807.193614	1027.035826	932.426601	1137.178479	1264.345537	1823.938434	1618.174915	1468.129129	1983.734135	
13.36_354.8435m/z	354.8435233	13.36138333	pos							21750.62919	23267.63647	22842.66505	25918.20972	28106.37921	26118.05282	26819.29361	26667.19676	26575.57089	
13.36_531.3858m/z	531.3858208	13.36138333	pos							3040.462568	2937.973782	2599.871262	2984.98346	2775.344773	2240.8493	2562.741586	3071.088407	2615.122386	
13.36_935.5895m/z	935.5895282	13.36138333	pos							1664.910033	2079.955836	1899.757237	236.6850444	26.88379251	14.51481208	2695.795658	827.8387326	1388.270467	
13.37_250.8815m/z	250.8815224	13.37201667	pos							4469.234558	4633.417703	4794.160945	5288.189175	5352.254866	5247.044975	5225.175843	4801.346076	4942.552678	
13.37_327.8247m/z	327.8246934	13.37201667	pos							20742.47194	21857.04396	20407.01612	23585.41536	24654.60615	24220.80923	23026.28765	22363.95415	23372.27404	
13.37_788.5426m/z	788.5426084	13.37201667	pos							9552.730628	10288.55851	7663.131048	3602.835475	3022.402596	1975.228444	6921.516477	8348.747749	5476.869246	
13.37_861.9149m/z	861.9148625	13.37201667	pos							1757.278567	3768.989601	1818.334387	1784.774923	3208.122473	1714.482124	1639.664786	2704.397844	2290.596379	
13.39_681.8124m/z	681.8124211	13.38981667	pos							2036.604354	2005.035045	1194.689103	99.23175661	585.8835745	0.001403199	1219.670563	508.38167	639.157987	
13.39_698.1958n	721.1832333	13.38981667	pos							6491.678618	696159.9538	26156.55738	1089.576687	508.4769885	799.351444	1940.019569	1290.541196	535.3486045	
13.40_454.7668m/z	454.768779	13.40058333	pos							7683.958107	8847.305418	9060.282815	10648.37511	12506.44755	12137.75349	10079.40065	10239.18547	10834.13907	
13.40_531.3857m/z	531.3856884	13.40058333	pos							3798.201185	4647.292134	4821.06748	3777.01803	5462.47401	3474.296785	5049.839698	4776.815141	5167.482097	
13.40_549.7011m/z	549.7011471	13.40058333	pos							51200.01893	52938.84469	57007.10465	72271.38475	73059.19389	73339.35648	64416.97437	66107.11022	71148.18409	
13.41_146.9754m/z	146.9753808	13.41138333	pos							15.02059862	19.90062602	11.69876212	0.001403199	0.001403199	0.001403199	8.120830796	0.001403199	5.934050422	
13.41_310.8345m/z	310.8344512	13.41138333	pos							1278.344393	2362.05518	1760.213279	1482.486076	2040.849582	1523.76175	2120.989843	1909.957836	2471.148209	
13.41_359.7754n	342.7721013	13.41138333	pos							81655.69359	83139.83213	87412.74633	99178.87588	103814.5218	106785.0095	98325.17351	94027.21402	100991.2684	
13.41_425.7662m/z	425.7661916	13.41138333	pos							1077.122218	1428.256735	1315.415524	1427.105408	1639.274671	1263.900707	1839.272158	1082.245666	1948.638189	
13.41_477.7711m/z	477.7710894	13.41138333	pos							1639.197996	2406.803487	1835.498632	1633.184318	2505.145733	1804.099259	2102.877139	2102.13386	2620.684068	
13.42_206.0665m/z	206.0665256	13.42045	pos							556.2742643	502.3534276	656.3433129	401.0698192	551.9442511	359.3432405	663.9987919	553.4821009	618.1731652	
13.42_244.9449m/z	244.9449478	13.42045	pos							101.661138	254.207477	212.299289	179.0608329	261.0039776	331.8651921	285.9135012	164.0694954	220.4963955	
13.42_473.3443m/z	473.3443153	13.42045	pos							3139.074868	4200.831939	4346.11007	3019.487205	4621.805137	2865.660304	4294.019675	3942.07272	3662.504369	
13.42_725.8383m/z	725.8382743	13.42045	pos							1066.927545	1370.719414	1279.951185	0.001403199	0.001403199	0.001403199	732.5932151	388.7665829	0.001403199	
13.43_288.8525m/z	288.8525367	13.43471667	pos							925.3118525	871.8678983	1332.441296	941.7391832	1218.130847	950.4827558	1419.321221	1035.223267	1198.897255	
13.43_464.7239m/z	464.7239402	13.43471667	pos							1943.556842	2489.99537	2111.718454	1810.568669	2332.664937	1996.841295	2606.333965	2310.628328	3000.190317	
13.43_487.3599m/z	487.3599011	13.43471667	pos							9214.406661	10546.17131	11864.13731	9656.921148	10800.92566	9357.718321	10987.53763	10597.74647	10385.08945	
13.43_670.2406m/z	670.2405554	13.43471667	pos							19789.7678	34896.08243	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	58.87137162	
13.45_624.1762n	647.164744	13.44906667	pos							600222.8289	88.7293993	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	
13.45_686.5556m/z	686.5555839	13.44906667	pos							3964.825611	3950.615789	5006.924323	6691.801995	7407.958733	6788.267902	4987.695617	6130.684864	7303.293178	
13.46_103.9557m/z	103.9556985	13.46155	pos							1845.728064	2060.229243	2560.95057	1867.275921	2463.043106	1857.713735	2589.253305	2185.041932	2246.520171	
13.46_585.6779m/z	585.6779159	13.46155	pos							3625.614519	5254.203457	4636.942924	6090.117219	6506.558844	7895.690693	6703.516605	6047.423573	7271.147501	
13.46_746.5658m/z	746.5657934	13.46155	pos							7671.703981	8337.341191	7679.857258	5410.849404	6804.988816	6239.232649	5777.512504	6191.34337	7340.962378	
13.48_244.8443m/z	244.844306	13.47723333	pos							763.971027	1208.948623	1795.334474	1305.294578	1746.803683	1464.212623	1673.442608	1371.697682	1002.479205	
13.48_383.2764m/z	383.2764233	13.47723333	pos							1012.898329	986.041265	1491.193997	1385.93205	1589.83334	1208.121899	1670.880286	1279.655864	1010.284173	
13.48_395.8121m/z	395.8120581	13.47723333	pos							2411.590329	2680.751435	3724.97611	3306.486461	3465.312175	3339.346998	3414.500927	3315.844495	3317.579414	
13.48_612.6968m/z	612.69678	13.47723333	pos							3337.494503	4185.555657	4496.220755	4415.04885	5734.839575	4803.873674	4947.455723	4803.235822	5749.610353	
13.48_862.2514m/z	862.2513799	13.47723333	pos							15251.81907	11893.89028	14850.42747	14789.4021	39593.39679	13660.98966	16568.94141	17602.5175	17883.30966	
13.49_178.8806m/z	178.880637	13.49236667	pos							13903.41722	13473.48645	14320.77252	15261.63951	16803.75269	16402.46497	15813.80113	15715.24234	16117.38456	
13.49_261.1304m/z	261.1304491	13.49236667	pos							142585.0939	137812.517	136154.2092	139073.659	146390.6069	145401.4638	149163.1796	138485.949	143333.3902	
13.49_366.8339m/z	366.8329993	13.49236667	pos							2259.468769	2585.322322	2343.478543	2771.378507	2687.751628	2744.675877	2992.016992	2581.176707	2635.760449	
13.49_384.7388m/z	384.7388435	13.49236667	pos							1847.487889	2565.596128	3682.673229	3845.087308	3922.864428	3710.077816	3332.331382	3670.3332	3898.703141	
13.49_859.0865m/z	859.0865276	13.49236667	pos							3686.730519	2066.729051	3573.093788	2302.675389	2529.501634	3268.490352	2062.943965	2119.713771	2935.655387	
13.50_162.9067m/z	162.9067227	13.50328333	pos							286223.174	295298.2125	312862.8142	340581.0556	344847.2679	359115.4249	336463.6936	323540.3854	340448.8799	
13.50_711.1626m/z	711.1625625	13.50328333	pos							3141.181007	2774.568243	1816.981018	0.001403199	0.001403199	0.001403199	1395.492545	1346.087424	360.8261852	
13.50_850.0607m/z	850.0607196	13.50328333	pos							976.8895106	803.6479917	803.0022625	703.4113855	413.9362185	382.2692546	676.5200727	810.5579625	1038.536133	
13.50_861.9149m/z	861.9148861	13.50328333	pos							29885.22014	37605.22715	30793.40396	31740.8145	34987.401	31184.45514	34282.44149	34272.23256	38950.90192	
13.51_288.8526m/z	288.8526463	13.51415	pos							630.2734964	1132.999045	1354.970703	1219.374595	1259.433	1601.494986	1198.162617	1524.49321	1796.852005	
13.53_216.9224m/z	216.9224189	13.525	pos							1379.212684	1829.593154	1604.80924	1816.905756	1336.701291	1787.779374	1204.381963	1858.632202	1935.850517	
13.53_541.1202m/z	541.1202252	13.525	pos							0.001403199	76.59783508	9764.745022	78.23425179	0.001403199	0.001403199	113.4892229	78.73003763	0.001403199	
13.54_1068.7045m/z	1068.70455	13.5373	pos							5159.170465	6335.225118	3633.722113	4347.059194	4169.549449	4154.158369	4087.717538	4382.922233	5214.974405	
13.54_1083.3782m/z	1083.378211	13.5373	pos							3302.593031	3362.882295	3637.110034	2291.711241	2562.666578	1737.439252	1919.106148	2947.137539	3417.657657	
13.54_200.8626m/z	200.8626058	13.5373	pos							323.4151691	520.4007802	482.3555863	397.7836104	413.170545	679.5490137	379.9149478	501.2154526	631.1165726	
13.54_315.8716m/z	315.8716223	13.5373	pos							2144.722797	2748.146422	3225.039449	3238.578837	3376.82398	4431.90898	2604.547225	3400.884642	4173.800914	
13.54_399.8492m/z	399.8491944	13.5373	pos							324.1780728	188.5000424	476.158158	2.614152194	51.92564316	55.07343361	90.10708303	126.4360666	2.164512923	
13.54_494.7612m/z	494.7611773	13.5373	pos							3510.028843	4077.488391	5016.654586	4542.171259	5738.51533	6042.777589	4961.177943	4560.638717	5599.70169	
13.54_876.5908m/z	876.5908353	13.5373	pos							12065.09664	12749.4362	12406.00748	11627.04599	13891.47164	11210.60374	14962.14613	14864.19743	14507.17167	
13.55_190.0972m/z	190.0972144	13.54818333	pos							979.0972105	1343.32059	1428.762093	1247.317725	1197.816457	1480.785057	1352.035995	1291.660618	1272.365267	
13.55_594.1285n	617.117674	13.54818333	pos							7633266.389	28286.73294	3611.060881	857.8581527	278.3240396	134.5767689	1009.09134	291.398922	48902.07628	
13.55_746.6013m/z	746.601307	13.54818333	pos							3835.921572	3426.667032	1627.161119	312.8086343	155.9591891	122.0746722	1314.557001	728.4315799	748.8728947	
13.56_288.9106m/z	288.9105819	13.5607	pos							15749.39779	18683.80364	12479.2446	15718.00122	15866.37478	13654.65036	16216.55825	13281.04365	15069.99967	
13.56_390.8200m/z	390.8200979	13.5607	pos							1319.757406	1672.573749	1452.696956	1660.024595	1401.401106	1957.868524	1559.880657	1553.439767	1987.277103	
13.56_397.2152m/z	397.2152384	13.5607	pos							567.1498027	923.2769998	533.7605392	428.6800573	713.2707058	781.7606294	614.2014689	721.9496982	868.3068425	
13.56_425.2139m/z	425.2139462	13.5607	pos							8173.930769	9500.165248	8513.2152	7747.943441	6707.780685	9543.191272	8476.348739	8135.944328	8605.736114	
13.56_864.7108m/z	864.7108207	13.5607	pos							11646.80571	2908.423695	3541.259934	1849.806775	1652.715209	3274.293575	9382.112638	8049.604645	2300.009613	
13.57_487.3598m/z	487.359779	13.56991667	pos							10423.08768	10863.46436	9466.895717	9872.529494	9206.577422	11018.33404	11579.04557	9793.767284	10802.29527	
13.57_612.6967m/z	612.6967018	13.56991667	pos							1791.148011	3526.378644	3136.978709	4563.84946	3548.125389	4632.20748	2869.431738	4047.965812	4126.302978	
13.58_172.1118m/z	172.1118442	13.58256667	pos							600.2592068	654.8779642	676.8009665	723.5546852	632.539161	720.8916454	641.7912033	604.2535206	716.5868281	
13.60_103.9557m/z	103.9557198	13.59691667	pos							1863.168081	2075.236554	1816.43555	1790.579204	1697.085908	2079.351916	2102.331481	1820.467964	1937.080741	
13.60_231.8941m/z	231.8941364	13.59691667	pos							387.1345483	479.6192321	499.3391382	619.266239	511.2340713	722.149735	581.7638977	602.8283329	677.3537078	
13.60_297.0819m/z	297.0818945	13.59691667	pos							11170.47298	330.645012	39.05370617	33.28590574	60.7094492	26.06465094	60.70194887	31.69136429	84.65188655	
13.60_371.1006m/z	371.1005952	13.59691667	pos							20817.42383	67101.19787	9859.57399	6686.571116	6435.741469	6974.038794	15968.03469	7050.042126	6103.485496	
13.60_522.1364m/z	522.1363879	13.59691667	pos							269.7585001	83.01575434	100.0995643	0.001403199	162.2988795	133.2827967	0.001403199	65.64511106	65.27757026	
13.60_536.1413n	559.1305127	13.59691667	pos							159436.0949	150500.0411	113888.9491	142348.9835	137130.9023	146903.9762	154941.7796	141544.6606	132946.8187	
13.60_582.2062m/z	582.206238	13.59691667	pos							2349.016874	2934.742271	2008.872071	2516.689887	2880.167772	2945.489645	2426.160689	2829.50742	2743.455845	
13.60_877.2616m/z	877.2616058	13.59691667	pos							2140.087105	3013.178287	2233.693846	2957.114016	2097.381045	1932.786299	3832.888373	2717.977775	2076.702488	
13.61_220.8653m/z	220.8652971	13.60948333	pos							1407.581116	1712.102011	1509.335429	2024.162095	1519.003681	1562.818459	1783.493191	1720.143859	1539.263184	
13.61_222.8624m/z	222.8623932	13.60948333	pos							479.364864	461.1730975	457.5811699	667.8339673	497.0050446	446.7808019	471.0827382	476.4778435	453.1429462	
13.61_310.8346m/z	310.8345762	13.60948333	pos							842.4368736	1012.816803	950.4147485	1467.224668	1430.307199	1251.335346	1219.484552	1221.28194	1185.16813	
13.61_405.8409m/z	405.8409033	13.60948333	pos							1313.025227	1476.783088	1322.247652	1809.531627	1294.300616	1739.007371	1572.052688	1340.564365	1677.702601	
13.61_501.3754m/z	501.3754134	13.60948333	pos							5427.531474	4899.402736	3990.917006	5823.615901	4226.364967	4145.765384	6107.836561	4610.36932	3902.557281	
13.63_148.9932m/z	148.993158	13.62965	pos							114380.8085	110944.3866	108995.6076	114099.5796	118785.1131	115879.2088	122028.7325	109506.3373	116379.9749	
13.63_861.5766m/z	861.5766064	13.62965	pos							17821.28609	20027.98617	17952.48973	13728.90407	15499.00784	15906.20733	19358.22985	16714.16615	18907.18062	
13.64_332.8615m/z	332.8615483	13.64235	pos							158088.5228	161743.5491	157980.1879	180734.5391	181087.5533	188204.8996	180670.4584	172127.9068	185483.7831	
13.64_681.8121m/z	681.8121132	13.64235	pos							2816.857107	3593.24999	1633.37626	1000.619258	1088.499255	465.7922598	2289.920111	2847.16436	2408.089501	
13.66_471.7721n	454.7688573	13.6585	pos							7328.914416	7655.108809	7603.443671	11007.09528	10448.31116	10078.27112	10139.99422	9627.088782	9476.210108	
13.66_526.7121n	509.7087983	13.6585	pos							161765.262	173452.3045	176490.014	216792.6525	234533.8309	227073.5592	206132.93	200664.6023	220550.5553	
13.66_563.6416n	546.638353	13.6585	pos							91978.67708	104889.8604	104512.7226	141323.7195	147487.7243	141281.425	129115.0936	128150.9113	139429.3953	
13.67_305.1566m/z	305.1565925	13.67386667	pos							12081.83558	12241.11771	12437.6762	13831.11881	13621.68915	13891.44476	13133.00838	13147.25835	12618.84678	
13.67_369.7912m/z	369.79115	13.67386667	pos							121942.7158	130772.3154	127220.2112	157447.5132	164696.1881	164547.3194	148848.474	142893.568	157394.1423	
13.67_412.8020m/z	412.8020281	13.67386667	pos							585.3578995	561.5917197	610.0359948	960.5544392	903.9430528	1115.06026	854.7788005	767.1359642	701.6816866	
13.67_472.7793m/z	472.7792984	13.67386667	pos							86707.67817	92655.04684	89191.50962	108920.4284	112907.1105	111374.4747	102678.0645	98408.96261	107422.3348	
13.67_612.6965m/z	612.6964507	13.67386667	pos							6752.443176	6968.840023	7218.289195	10073.84368	11113.44248	9387.30645	9301.687527	8773.276038	10195.82233	
13.67_765.1557m/z	765.1556641	13.67386667	pos							307456.5127	2584.27703	5903.067958	198638.4977	6088.347261	1057.540653	4066932.469	59887.5863	2819.457755	
13.69_148.0866m/z	148.0866412	13.68831667	pos							16643.60677	16229.69645	16135.71806	16368.18011	17161.2587	17191.63905	17479.87564	16793.57959	17356.6335	
13.69_247.8842m/z	247.884168	13.68831667	pos							132501.0795	139428.5094	161550.7131	171404.9467	180190.5982	183148.1744	178205.2477	168447.7655	184467.1834	
13.69_299.9375m/z	299.937512	13.68831667	pos							589.0576005	636.5624611	533.9264678	696.3303687	741.9961275	611.1266903	658.2666986	664.4242126	593.0230604	
13.69_594.6865m/z	594.6865448	13.68831667	pos							3088.881169	3933.610487	4073.569071	6308.68568	5272.852495	5890.076989	4955.393093	5192.637036	4789.310938	
13.70_172.1119m/z	172.1118739	13.69921667	pos							271.0294404	248.249421	229.0030483	409.3746696	313.105802	278.6662418	405.5319181	325.7837665	293.2389131	
13.70_501.3752m/z	501.3752269	13.69921667	pos							3379.554199	3812.545163	3133.92532	5165.260027	4445.919721	4599.751709	4343.280785	4370.75899	3365.346772	
13.70_610.1831m/z	610.1830858	13.69921667	pos							4181.425007	5837.810698	5924.435527	27565.12715	15579.45417	10822.34127	6806.397238	6074.780541	373200.1876	
13.71_384.7387m/z	384.7387324	13.7103	pos							3665.711304	4942.175155	4687.292424	6525.767728	6067.945246	6345.522698	5383.802248	5632.722976	6306.236559	
13.71_487.3598m/z	487.3597829	13.7103	pos							7768.159771	9261.246485	8682.275943	7087.11069	8981.805463	7223.251684	8259.826973	8692.584542	9794.112125	

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14.33_516.3658m/z	516.3657944	14.33463333	pos	523.321112	543.7448831	297.3297257	412.7346055	446.6913175	327.3436426	383.3770879	584.5902486	412.275128
14.33_842.0985m/z	842.0984515	14.33463333	pos	48439.76001	49319.04071	45170.28688	45142.82702	47943.26944	46995.76369	55367.13338	45094.2481	48423.01956
14.33_842.5997m/z	842.5996845	14.33463333	pos	45799.77531	48043.03713	43856.96756	47218.29125	49229.45584	45696.83031	49454.28296	47706.56194	47859.2231
14.33_860.2635m/z	860.2634808	14.33463333	pos	25304.50684	28686.62814	24921.69334	27046.62862	26957.65159	23322.77223	23960.97055	24786.4044	28622.53508
14.33_866.8631m/z	866.8631285	14.33463333	pos	21002.48691	26182.22556	25990.15704	28565.26577	34449.27738	28282.8994	29009.98407	27358.02202	27201.89605
14.33_878.6428m/z	878.6427723	14.33463333	pos	46311.02747	85674.64579	97785.07824	67667.50608	121551.4445	158573.6028	90122.76296	78436.70247	78067.99406
14.33_879.1451m/z	879.1451113	14.33463333	pos	31911.44422	49563.20638	56549.61417	43427.89416	74986.50645	94042.81017	50519.35294	45895.39731	50687.46152
14.33_918.9652m/z	918.9651637	14.33463333	pos	10956.16518	14354.1087	10836.03709	13124.65055	14346.14989	11257.42837	9879.63785	10868.76277	11108.98318
14.33_921.6617n	944.6819467	14.33463333	pos	510324.4241	471448.4547	575717.254	774207.9344	594207.0872	378784.7883	800098.0268	932738.1036	1134184.916
14.33_957.6893m/z	957.6893475	14.33463333	pos	25213.06766	32244.57086	37586.25672	33073.01375	30035.02903	29933.46377	40569.10482	41376.638	43838.22662
14.33_988.2029n	989.2101951	14.33463333	pos	1052182.204	1156909.86	828589.6387	800484.7285	550552.4089	178884.9002	525258.7871	374725.8215	719520.3485
14.34_1072.3058m/z	1072.305791	14.34413333	pos	126715.4942	220967.4507	3847787.534	2609.998765	8247.863251	3415.695941	224898.7436	28409.90734	2001.815288
14.34_232.1193m/z	232.1192687	14.34413333	pos	672.3644006	752.671997	603.9155203	668.9465735	584.1070102	535.0835611	744.598007	665.2797931	1375.029907
14.34_841.8478m/z	841.8477845	14.34413333	pos	41858.98664	43734.21417	38949.33738	39390.81114	40801.81136	37474.52243	41575.20826	38923.01239	41014.67098
14.34_858.0985m/z	858.098519	14.34413333	pos	60713.05516	72119.28598	64348.45523	69471.57011	77352.02874	73188.78274	74601.21547	67016.31692	70492.50318
14.34_870.8692m/z	870.8691628	14.34413333	pos	66618.07153	84460.46872	77256.67032	84183.85894	96862.8827	90611.71632	91203.04722	87442.95273	85353.4028
14.34_871.1193m/z	871.1193409	14.34413333	pos	91984.91608	102330.3445	101100.926	109788.745	118803.3844	112757.3042	111952.7069	98032.24656	110987.6271
14.34_901.1580m/z	901.1579959	14.34413333	pos	141336.9222	135039.2803	111015.7891	207687.5549	240469.9444	280796.0392	118587.2503	104910.3913	143199.8413
14.34_964.7195m/z	964.7194727	14.34413333	pos	138096.491	291730.7225	275977.2944	81851.63999	245020.2241	274858.6617	363792.3433	302165.3919	76522.54133
14.34_966.6951m/z	966.6951219	14.34413333	pos	297299.8627	573659.0747	553267.9952	164251.6528	479181.8079	574312.9733	733912.4188	632192.5716	180947.7957
14.34_967.1969m/z	967.1969345	14.34413333	pos	241346.1827	470232.0676	450001.8375	133972.4164	393858.7162	472081.6296	592030.7871	515922.3573	145600.8173
14.34_980.2753m/z	980.2752958	14.34413333	pos	30108.92723	39102.64836	37529.61927	58717.54538	66474.67728	51082.11357	60830.06992	68711.83572	72172.61937
14.36_108.0809m/z	108.0809479	14.357	pos	1492.128624	1303.664216	1204.62249	1277.537356	1223.902612	1252.769188	1304.4407	1230.581479	1392.695988
14.36_244.9598m/z	244.959795	14.357	pos	714.3683666	764.749136	887.074987	948.0837776	806.2334852	608.4688539	730.470954	943.8722612	704.8877382
14.36_496.3285m/z	496.3284606	14.357	pos	872.2928695	1329.074103	969.8259076	736.9228001	1144.391161	795.7446816	777.8902284	1037.051413	1077.825175
14.37_871.6021n	872.609339	14.3685	pos	75897.43113	89504.19247	85447.63912	96376.33564	100958.5935	103711.7231	101171.6693	86700.81659	97223.08608
14.39_324.8062m/z	324.8061593	14.3867	pos	1884.841034	2026.025989	1783.554826	2505.004683	2601.388155	2071.456055	1860.306251	2195.674718	2066.663456
14.39_474.3155m/z	474.3154514	14.3867	pos	597.4073293	687.1582702	548.2630808	472.6603795	532.7916703	538.9196626	558.1508106	510.404663	552.8975115
14.41_501.3753m/z	501.3752931	14.40608333	pos	7769.33718	6888.72497	6169.854602	7382.910535	6845.04755	6939.843822	6431.907215	7644.158763	9520.997086
14.43_116.1070m/z	116.1070432	14.42566667	pos	1970.245839	1746.109628	1640.282935	1952.371689	1887.976468	1898.12265	1619.290726	1803.186233	2059.558662
14.44_136.1119m/z	136.1118708	14.43715	pos	668.3966048	625.7463097	818.3513595	763.7190581	811.5635779	937.9865624	712.5761266	749.0050997	623.9493986
14.44_886.7847m/z	886.7847259	14.43715	pos	6238.589318	1109.238077	1863.429219	2882.926301	4619.532144	4211.398559	7441.406871	5161.585322	2405.347523
14.44_920.1917m/z	920.1917161	14.43715	pos	116153.3715	123389.938	107706.9915	277254.5185	263377.5724	62638.09617	119110.453	210939.4437	250497.1025
14.45_942.7064m/z	942.7064087	14.45033333	pos	127345.6512	113946.3946	169951.33	132051.4334	184586.1829	124222.7532	269850.7768	252547.1495	320208.7285
14.46_1045.2358n	1046.243035	14.46188333	pos	29037.14763	46171.37719	38790.8799	57397.87411	62731.21445	53143.3183	57967.95425	50329.06877	56462.55581
14.46_790.5906m/z	790.590598	14.46188333	pos	63823.16881	72340.05645	64121.42644	25185.98571	26863.0508	25852.33843	65478.64447	54915.79168	38787.50179
14.46_833.3690n	856.3581734	14.46188333	pos	153561.376	167392.4793	166466.0019	179685.8824	192264.7862	190507.908	186596.3635	172200.0733	185507.5915
14.46_851.6196n	869.6326804	14.46188333	pos	93635.99213	98350.11961	86295.94385	113890.2308	114848.4578	105881.6966	102630.2196	99664.82097	116210.4208
14.46_857.8475m/z	857.8475038	14.46188333	pos	87404.5641	100887.7794	91633.52436	99244.07	109045.3046	100909.8333	101701.8358	96222.17149	102509.8947
14.46_898.1784m/z	898.1784471	14.46188333	pos	80157.03446	77517.94308	61882.76175	122637.7055	140134.5868	163548.002	74193.04481	61223.84613	88931.3797
14.46_960.7321n	983.7529091	14.46188333	pos	86587.39582	112051.7804	129951.8154	76421.26176	91659.24842	50722.03067	104566.5824	50594.82348	28834.70966
14.46_985.7259n	986.7331461	14.46188333	pos	733241.4495	822104.1251	567772.1494	535600.1499	348648.498	102553.7473	346713.0556	239569.8983	483395.0098
14.47_858.7527m/z	858.7527211	14.4724	pos	24453.44706	8825.878103	9168.332941	10814.26833	13552.6474	13559.68013	24188.33904	19345.31158	11688.48369
14.47_900.6560m/z	900.6560056	14.4724	pos	175356.2898	174076.354	138561.1834	279919.5324	316027.1407	366110.7159	158110.6497	134029.6096	186250.7529
14.47_939.7265m/z	939.7264736	14.4724	pos	10533.34731	12576.37326	21501.88955	14573.31501	13076.410135	15513.41425	41710.74979	37971.37501	50017.99899
14.48_852.1020m/z	852.1019966	14.48083333	pos	6348.738589	6521.590844	5935.373031	7439.494805	8523.332228	7981.028344	5973.623787	6705.452345	5145.870342
14.49_305.1566m/z	305.1565628	14.48943333	pos	4734.084731	5067.807492	4995.346889	5529.113814	6895.794663	6024.242619	5478.425025	5346.946235	5028.888731
14.49_487.3598m/z	487.359829	14.48943333	pos	23274.31577	22360.212	22227.86799	23739.71427	25464.42686	23496.65807	24731.84738	22902.08168	23757.58674
14.50_1001.7151m/z	1001.715099	14.49786667	pos	20990.18907	26547.2838	26790.32776	36211.89435	40280.90993	33020.88969	29287.17971	29190.62179	40869.08887
14.50_866.6115m/z	866.6115049	14.49786667	pos	10864.94995	15008.54814	14085.33272	14826.68191	17752.23914	17069.88273	16193.94013	13907.58954	15599.91746
14.50_867.1137m/z	867.1136602	14.49786667	pos	7938.748784	13310.97112	13727.28922	16772.703	15221.79429	14737.0112	14583.40471	15249.48909	14524.58098
14.51_791.0927m/z	791.0926527	14.50626667	pos	6334.201917	11220.4537	11461.15167	4580.087676	4255.799225	5126.283793	11109.89479	8978.87012	6524.996223
14.52_920.6937m/z	920.693666	14.51608333	pos	59272.14558	64314.95733	57694.39254	151140.3741	142407.8729	27084.19468	70162.65526	117196.8448	135460.7222
14.53_116.1071m/z	116.1070534	14.52588333	pos	614.7055515	613.2003559	787.9347051	699.5892928	762.3365324	885.5034821	767.9852709	632.7786736	696.4375139
14.53_193.0849n	176.0816267	14.52588333	pos	1153.913155	1112.363132	1063.032392	1148.450898	1436.709052	1281.83494	1321.269413	1141.396723	1277.048744
14.53_273.1667m/z	273.1667094	14.52588333	pos	1322.770852	1178.190509	1168.399579	1258.538994	1376.626134	1399.15461	1357.405083	1200.688715	1337.494007
14.53_898.6805m/z	898.6804775	14.52588333	pos	26283.7876	29547.29336	22933.02669	46666.99995	54149.45476	62175.74815	29106.59251	25398.16849	35709.0856
14.54_1001.2585n	1024.230067	14.53985	pos	54089.85178	67584.81374	75503.03111	60809.3945	71734.80757	48803.9325	59379.71717	28702.87912	36593.88341
14.54_1046.7473m/z	1046.747255	14.53985	pos	14781.30828	19288.79922	11893.1895	28750.61466	30684.82942	26122.90683	19000.18001	23461.01543	28713.39431
14.55_876.1660m/z	876.1659764	14.54965	pos	19718.61601	47519.69245	47964.32098	29821.68583	54876.6202	65807.36575	46245.86955	32104.93259	36469.587
14.57_865.3729m/z	865.3728838	14.57093333	pos	12771.12561	16659.68951	15736.69865	20706.41818	21925.27351	21985.7443	20049.82568	20325.01395	20706.6448
14.60_1029.2496n	1030.256911	14.60023333	pos	485538.4692	186330.013	254174.7448	37252.00653	4583.574466	8679.043274	509558.6681	455511.4196	205980.4265
14.60_1051.7636n	1052.770828	14.60023333	pos	100762.7798	184529.5958	277936.1586	6732.464666	10753.79655	10841.90004	281824.3018	105746.1845	20051.64254
14.60_108.0809m/z	108.0809226	14.60023333	pos	5008.0157	4832.549564	5243.054898	5357.353319	5605.842669	5501.032807	5658.954478	5361.20643	5462.940698
14.60_1161.9584m/z	1161.958415	14.60023333	pos	212619.3944	158348.8476	77562.25472	170106.6555	225845.5829	270955.728	62247.82678	77572.66812	136878.7759
14.60_707.1673m/z	707.1673422	14.60023333	pos	13997.94458	638.8167714	233.962581	0.001403199	0.001403199	0.001403199	385.57413	631.0142083	64.35972992
14.60_861.6133m/z	861.6133485	14.60023333	pos	16927.71785	15642.52304	16950.40782	18629.38325	17897.10563	18557.88316	18986.30949	17112.16371	15585.58433
14.60_902.7334n	925.7235812	14.60023333	pos	270866.6961	297948.6364	263851.6421	168015.5109	233262.0088	420713.3327	247734.8579	206558.3247	204600.1645
14.61_852.3525m/z	852.3524554	14.60706667	pos	11242.76583	15472.81821	17640.19138	18571.18696	19198.96638	16897.97032	16633.23488	17423.65016	17370.21173
14.62_1006.2680m/z	1006.267966	14.61855	pos	37615.87069	57082.25315	14171.92125	23948.21912	4224.190131	23810.92468	6077.205171	22711.74913	47079.32373
14.62_610.1598n	633.1489136	14.61855	pos	71985.24858	66721.44396	68781.21	60078.27665	65410.05581	69030.06565	66407.7902	60086.86854	64594.23849
14.62_855.1202m/z	855.1202198	14.61855	pos	35761.94228	43561.30605	38370.23222	51161.0081	53451.62535	51158.04842	58538.99417	52603.7086	52353.32424
14.63_1005.7662m/z	1005.766221	14.62908333	pos	62368.57482	85664.3748	16041.42953	30549.61892	3538.250408	126.3739013	4243.852117	26890.95187	67654.40628
14.63_1009.7134n	1010.720708	14.62908333	pos	1216009.627	953518.3307	395678.3954	461435.5859	162340.489	36660.85907	481336.0168	814163.0867	911725.2139
14.63_213.1132m/z	213.1131512	14.62908333	pos	1590.348265	1907.446793	2450.858093	2827.66523	2337.36094	2394.971796	2384.052366	2631.68438	3046.485532
14.63_577.1255m/z	577.1254831	14.62908333	pos	2081.500837	491.8012897	2005.882575	542.8438836	601.8032866	487.8312131	520.6024642	379.3404644	565.5968124
14.63_593.1566m/z	593.156587	14.62908333	pos	81841.03614	32882.51967	71993.17106	13036.06166	11248.41977	15189.07861	24690.1414	16395.27364	20901.08371
14.63_656.2249m/z	656.2248626	14.62908333	pos	1018.093734	1220.738107	1460.757447	1261.126337	1567.226335	1708.403859	1476.46986	1392.287516	1427.405225
14.63_842.3494m/z	842.3494266	14.62908333	pos	36369.00914	42332.46921	40682.07842	38581.08035	38329.94405	37206.77744	42539.2392	37458.00791	40961.82176
14.63_940.2288m/z	940.2287958	14.62908333	pos	4565.295454	5510.286356	8920.880258	6240.612757	1247.276802	6505.982647	15045.9189	13957.99571	21779.94044
14.64_1030.7589m/z	1030.758913	14.63885	pos	302176.1959	90391.77028	54328.18239	34445.5111	4481.856927	2481.319235	186247.63	245807.5165	130740.9514
14.64_1032.2289n	1033.236178	14.63885	pos	566708.7489	227060.5788	311414.2642	59417.99078	12097.0817	15784.28987	615880.5445	542468.2615	257508.4613
14.64_1099.2751m/z	1099.275073	14.63885	pos	85098.76904	103243.138	43036.89612	2893.194968	6174.457458	161.7914223	3666.615826	459.3000259	1224.873811
14.64_941.1974n	964.2172156	14.63885	pos	328147.6039	527093.527	590262.8493	261726.3675	362352.5587	507107.138	820031.0626	723604.7971	515049.0754
14.64_951.7606m/z	951.7605732	14.63885	pos	65598.49136	60418.99211	82038.59324	373539.8393	458370.814	445439.2932	126582.1152	97463.75038	222099.2356
14.64_962.2421m/z	962.2420516	14.63885	pos	16695.04982	38915.39243	39773.59083	15263.57672	42515.07796	59929.03144	58313.71851	54220.78902	18861.00174
14.65_1053.7386n	1054.745896	14.64865	pos	216446.2299	383439.5912	587792.4376	20398.40316	39512.59576	30628.93013	608767.8975	244562.1502	55041.29233
14.65_1068.7588m/z	1068.758815	14.64865	pos	5195.358334	12570.08642	11866.65598	11267.91311	12256.2649	14119.99628	16468.06999	12658.62597	11642.68441
14.65_273.1667m/z	273.1667387	14.64865	pos	249.5584795	443.6840045	604.5751333	668.0276705	578.2894636	480.5885505	550.3561144	725.9949962	687.634385
14.65_385.2917m/z	385.2917171	14.64865	pos	1528.802778	2451.858581	2964.299045	3240.833166	2447.006484	2316.568495	2485.751504	2871.868713	3543.186185
14.65_429.3179m/z	429.3179425	14.64865	pos	2917.135673	3967.070614	4858.069468	5798.332562	4715.232009	4494.890222	4948.994617	4986.633336	5868.283081
14.66_136.1118m/z	136.1118277	14.65708333	pos	212.3625598	359.6279912	519.2708355	617.9011935	476.9920279	468.5807619	486.0084074	591.9600925	630.7157028
14.67_197.1534m/z	197.153392	14.67403333	pos	147.242285	662.8303676	557.511476	630.2910027	651.2933923	586.5834308	645.2358472	639.3028256	755.6948052
14.67_259.1148m/z	259.1148112	14.6656	pos	363.732489	668.258487	1077.680828	1362.370584	1131.622829	1021.583716	1086.718104	1138.784507	1532.401086
14.67_531.3859m/z	531.385889	14.6656	pos	1089.852518	1734.455623	2401.355925	2575.525444	2669.969324	1476.896695	2099.073081	2309.994497	2687.428179
14.67_921.1040m/z	921.1039608	14.6656	pos	66117.10388	132.6226824	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199
14.67_946.8024m/z	946.8023962	14.6656	pos	5885.829444	11263.50967	9871.378587	58832.72448	73008.83263	70779.23263	20884.43488	29506.31871	42408.62303
14.68_866.1615m/z	866.1614533	14.68246667	pos	31964.75714	1418.772459	1919.565045	1102.686951	2903.333935	2702.345038	943.2674817	1197.22949	1494.274601
14.69_790.2455m/z	790.2455381	14.69226667	pos	82103.62866	788.6160227	865.0803654	1397.647274	710.3740184	398.0295554	1396.212742	3964.841031	252.0564324
14.69_801.2271m/z	801.227059	14.69226667	pos	42684.03487	2577.101807	2111.13693	189394.6727	8809.992063	2346.695098	2597.202205	1943.381477	3436.981618
14.70_232.1189m/z	232.1188796	14.70206667	pos	602.2464927	673.9378569	752.5375228	815.8347375	883.5366498	845.5560528	869.4391059	753.7568257	997.732007
14.70_297.0818m/z	297.0818346	14.70206667	pos	67915.10769	1857.384894	3999.326368	1684.285103	1037.320037	1093.668633	1045.539689	1870.514984	1866.516927
14.70_322.0770m/z	322.0770477	14.70206667	pos	34638.17612	2066.073113	2663.372808	1015.629395	720.5879746	788.8177773	879.5837556	1303.343494	1081.714292
14.70_372.0724m/z	355.0691353	14.70206667	pos	155328.3244	6763.058761	9970.940718	4424.172395	3777.913405	3033.959594	6959.14817	5759.204811	4970.919231
14.70_429.0881m/z	429.0880912	14.70206667	pos	91910.66909	6558.08616	8752.863779	2611.779548	7625.343493	1630.249715	2419.29891	3245.668723	2272.082425
14.70_447.0987m/z	447.0987428	14.70206667	pos	27970.9247	3272.897482	1726.444075	530.5562081	4672.175518	504.9512135	669.9518585	455.4225071	379.0550071
14.70_462.1226n	445.1192697	14.70206667	pos	37530.901	12068.69026	73250.48569	22288.31794	17313.62044	15550.68889	14392.77305	27057.54935	27792.95449

14.70_503.1065m/z	503.1065254	14.70206667	pos																
14.70_519.1381m/z	519.1380515	14.70206667	pos																
14.70_725.1623m/z	725.1622676	14.70206667	pos																
14.70_758.1967n	781.1859479	14.70206667	pos																
14.70_776.2308m/z	776.2307549	14.70206667	pos																
14.70_800.2307m/z	800.2307349	14.70206667	pos																
14.70_803.1664m/z	803.1663581	14.70206667	pos																
14.70_804.2615m/z	804.2614671	14.70206667	pos																
14.70_995.7864m/z	995.7863593	14.70206667	pos																
14.71_457.3493m/z	457.3493072	14.71186667	pos																
14.72_596.1662m/z	596.1661902	14.72411667	pos																
14.73_537.5345m/z	537.5345166	14.73391667	pos																
14.74_669.1555m/z	669.1554795	14.74373333	pos																
14.74_671.1445n	694.1339952	14.74373333	pos																
14.74_710.1812m/z	710.181245	14.74373333	pos																
14.78_273.1667m/z	273.1666771	14.77848333	pos																
14.79_1022.2506m/z	1022.250648	14.79195	pos																
14.79_1043.2594n	1044.266648	14.79195	pos																
14.79_998.7285n	999.7357423	14.79195	pos																
14.82_181.1219m/z	181.1218993	14.8167	pos																
14.82_305.1565m/z	305.1565027	14.8167	pos																
14.82_443.3336m/z	443.3335834	14.8167	pos																
14.83_1128.8019m/z	1128.801924	14.82528333	pos																
14.83_1147.8239m/z	1147.823857	14.82528333	pos																
14.83_116.1070m/z	116.1070267	14.82528333	pos																
14.83_133.0759m/z	133.0758591	14.82528333	pos																
14.83_190.0972m/z	190.0971715	14.82528333	pos																
14.83_258.2059m/z	258.2059383	14.82528333	pos																
14.83_911.1741n	912.1813533	14.82528333	pos																
14.84_1065.7765m/z	1065.776544	14.83506667	pos																
14.84_1149.8045m/z	1149.804522	14.83506667	pos																
14.84_457.3493m/z	457.3492517	14.83506667	pos																
14.84_842.5999m/z	842.5998637	14.83506667	pos																
14.85_136.1118m/z	136.1118063	14.85371667	pos																
14.85_501.3753m/z	501.3753374	14.85371667	pos																
14.86_140.1067m/z	140.1067372	14.86423333	pos																
14.86_189.1635m/z	189.1634632	14.86423333	pos																
14.86_239.1483m/z	239.1482755	14.86423333	pos																
14.86_385.2916m/z	385.2915596	14.86423333	pos																
14.86_956.2093m/z	956.2092895	14.86423333	pos																
14.87_1096.7976m/z	1096.797552	14.87405	pos																
14.87_168.5999m/z	168.5999283	14.87405	pos																
14.87_175.1479m/z	175.1478727	14.87405	pos																
14.87_195.1257n	213.159341	14.87405	pos																
14.87_207.1237m/z	207.1237288	14.87405	pos																
14.87_208.1270m/z	208.1270035	14.87405	pos																
14.87_413.3228m/z	413.3227823	14.87405	pos																
14.87_910.6731n	933.6940715	14.87405	pos																
14.89_271.2744m/z	271.2744	14.88798333	pos																
14.89_393.2888m/z	393.2888274	14.88798333	pos																
14.89_487.3597m/z	487.3597209	14.88798333	pos																
14.89_977.2174n	1000.2392	14.88798333	pos																
14.90_727.1404m/z	727.1403511	14.89778333	pos																
14.91_180.1510n	181.1582925	14.9076	pos																
14.91_443.3334m/z	443.3334152	14.9076	pos																
14.93_152.0816m/z	152.0815896	14.927	pos																
14.93_545.4016m/z	545.4015539	14.927	pos																
14.94_194.0920m/z	194.0920205	14.93678333	pos																
14.94_200.1642m/z	200.1642299	14.93678333	pos																
14.94_209.1896m/z	209.1896367	14.93678333	pos																
14.94_275.2365m/z	275.2364853	14.93678333	pos																
14.95_215.1250m/z	215.1249974	14.95311667	pos																
14.95_612.1975m/z	612.1975273	14.95311667	pos																
14.95_954.7015n	977.7207986	14.95311667	pos																
14.96_1037.2679m/z	1037.267879	14.95995	pos																
14.98_1134.8146m/z	1134.81459	14.97523333	pos																
14.98_162.0910m/z	162.0909945	14.97523333	pos																
14.98_219.1853m/z	219.1852555	14.97523333	pos																
14.99_223.2052m/z	223.2052139	14.98843333	pos																
15.00_563.1641m/z	563.1641024	14.99705	pos																
15.01_415.0357m/z	415.0356893	15.00546667	pos																
15.02_203.1426m/z	203.1426058	15.02476667	pos																
15.05_281.0499m/z	281.0499354	15.0502	pos																
15.05_385.2918m/z	385.2917595	15.0502	pos																
15.05_878.2805m/z	878.2805355	15.0502	pos																
15.06_239.1482m/z	239.1482253	15.05856667	pos																
15.06_308.0250m/z	308.0249556	15.05856667	pos																
15.06_355.0692m/z	355.0691874	15.05856667	pos																
15.06_382.0436m/z	382.0435554	15.05856667	pos																
15.06_429.0881m/z	429.0880797	15.05856667	pos																
15.06_457.3496m/z	457.3496331	15.05856667	pos																
15.06_462.1226n	445.1192994	15.05856667	pos																
15.06_503.1066m/z	503.1066068	15.05856667	pos																
15.06_519.1380m/z	519.1380228	15.05856667	pos																
15.06_577.1252m/z	577.1252214	15.05856667	pos																
15.06_610.1599n	593.156595	15.05856667	pos																
15.06_799.1809m/z	799.1808879	15.05856667	pos																
15.06_815.2120m/z	815.2120047	15.05856667	pos																
15.06_849.2414n	850.2487799	15.05856667	pos																
15.06_855.2039m/z	855.203937	15.05856667	pos																
15.06_864.2640m/z	864.2639669	15.05856667	pos																
15.06_871.1778m/z	871.1777856	15.05856667	pos																
15.06_874.2489m/z	874.2489149	15.05856667	pos																
15.06_893.2544m/z	893.2543667	15.05856667	pos																
15.07_816.1841n	834.2178954	15.06696667	pos																
15.07_929.7800m/z	929.7800263	15.06696667	pos																
15.08_399.3074m/z	399.3073744	15.08395	pos																
15.08_765.1553m/z	765.1552569	15.08395	pos																
15.10_784.1996m/z	784.1995909	15.10426667	pos																
15.11_443.3337m/z	443.3337298	15.11406667	pos																
15.12_373.0801m/z	373.0800682	15.12383333	pos																
15.14_1122.7973m/z	1122.79729	15.1375	pos																
15.14_116.1071m/z	116.107087	15.14433333	pos																
15.14_140.1201n	158.1536825	15.1375	pos																
15.14_278.2475m/z	278.2474954	15.1375	pos																
15.14_521.1178m/z	521.1177887	15.1375	pos																
15.14_973.8047m/z	973.8047382	15.14433333	pos																

194379.7365	4213.321819	4837.867423	2903.246628	794.4008719	1212.219845	996.0280311	2336.272771	2377.427641											
989602.2134	31949.50369	125530.6089	42532.58094	28102.17883	39210.78546	25089.45383	49024.18658	47162.86243											
320280.3885	1877.998045	858.7683758	1204.272992	0.001403199	128.3075962	587.8447179	691.8115225	242.4622679											
12612841.99	214976.1374	95615.58512	207459.1548	60086.88075	49118.59702	60618.52899	86410.50944	92144.62931											
4726586.77	138369.9087	38903.551	18765.73286	22311.24751	20740.4196	35446.50339	22213.36641	21356.0971											
17879.6817	0.001403199	0.001403199	0.001403199	4029.458999	0.001403199	47.80439345	87.98268103	73.03807409	128.1913284										
52271.48881	289.5099156	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199										
560160.4235	5213.905205	1140.022431	1332.896682	702.1888359	357.7786507	435.9322068	763.5988835	1097.827039											
315258.1154	90712.07485	48708.02247	11194.96631	5123.479814	1538.622897	197014.6856	270999.5616	121591.9553											
11060.67324	12558.78496	10576.9256	9802.026988	12419.93194	10004.28966	10724.29431	11417.04711	9538.403089											
944.9652384	138.8237333	1496.580197	180.8561351	85.60090616	53.02290374	23957.2151	157.3814448	95.09660535											
27108.56767	27327.8165	31319.70856	30202.03315	32367.34205	34077.16242	32551.34475	29759.99637	30951.26347											
69783.91893	753.8024053	3940.179337	125.3608153	1.19465202	118.2351181	606.7592931	1058.31103	508.7752903											
39216.43319	899.3534175	122.9381103	54.86647169	60.65527925	0.001403199	65.79838319	243.1144363	106.1817617											
32360.35802	1310.232723	812.768875	63.3346166	0.001403199	0.001403199	284.6930507	271.3392802	99.54999544											
630.9326702	687.6005372	879.358475	536.9519408	833.3491644	635.9810005	792.8028	787.3201032	533.3541863											
37340.79932	17177.96739	13310.9514	10242.10465	8276.040109	6897.367956	24021.33203	27793.45802	18978.88708											
50728.22845	50732.37435	72697.789	33785.3176	39094.52334	36191.13481	82624.62603	58830.1068	41500.45536											
169335.5794	143657.3299	97522.48606	112174.7419	90211.92559	75819.0051	112502.0185	125529.88	144665.0695											
2219.506059	1822.547945	2014.559608	2108.568181	2133.191774	2111.428989	2221.671925	2145.046632	2218.585935											
7097.253224	8452.642527	8715.710646	8572.230699	9724.346595	8594.358506	8908.61014	8883.563807	9107.389757											
6071.942436	9180.99034	8893.269578	6970.111943	9814.849432	7379.126544	8526.176646	8440.096055	6873.073023											
3101.366515	8008.660921	7651.669383	7794.563538	10656.50874	7183.137829	7908.488017	7801.501559	8976.219682											
19866.61366	19457.84904	26395.96872	30278.32655	28752.78017	31483.28951	26246.90597	26931.37432	25814.99143											
4293.354753	3836.063492	4051.203881	4294.966276	4723.892868	4630.293102	4606.176997	4382.844208	4245.68464											
3349.013232	3266.307988	3473.712048	3592.349329	3942.250418	3844.639989	4031.473647	3930.97258	4017.716222											
24348.8021	23013.61654	23473.09185	24086.40547	25881.9352	24737.38876	26103.89399	24540.81347	25548.26063											
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7814.99515	4212.828408	6310.942409	6810.09748	9374.960915	7741.834303	7075.151261	6721.888184	6942.294126											
897.6505146	774.1876522	897.728192	963.3909184	1028.289	972.030887	1039.495483	912.1727746	1099.940993											
2983.095969	3085.811986	3166.093802	3605.942244	3082.141056	3653.376497	3479.482753	3448.440032	4821.994336											
7146.216741	7057.214726	7117.227482	7333.246183	7689.808271	7354.135123	7759.540574	7261.079091	7537.315259											
4625.01533	4523.545816	4409.134132	4451.807576	4969.469083	4795.37944	4773.890631	4368.116323	4760.119057											
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2074.639985	1886.909495	2157.415096	2368.134747	2086.521984	2743.596841	2296.782443	2463.722323	3632.750971											
25658.43283	32876.47111	39689.95368	20327.49024	37926.09926	31537.03119	49988.87299	35374.85239	22151.31878											
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218.8372213	327.2800916	295.1707878	326.8437966	249.3293904	291.5521101	292.909681	243.7341452	397.7725002											
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798541.4633	772098.2371	770476.3255	794345.1139	840345.2971	822396.7917	848632.8615	796437.3717	834839.2231											
62831.43073	60341.96219	60802.77463	61185.14831	64468.45671	61768.3521	65494.96829	61105.47527	64071.19204											
2700.696698	2652.158182	2346.740018	2544.51434	2166.013028	3793.005731	3777.261744	3178.218056	4964.339793											
47102.83326	41827.78381	58113.37915	79786.76009	62369.90781	43118.50421	68504.56249	83378.89482	108739.3361											
16097.97576	14229.43514	14409.7096	15764.39718	16555.27413	17356.39442	16057.09892	15574.01626	15848.64114											
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13136.25445	12926.00203	12620.33358	13780.4969	14944.02706	13474.41703	14750.18189	14093.23998	14444.10264											
135711.8348	139307.9407	118417.9989	126149.4707	100372.5335	77732.82713	88206.33702	79723.76419	109930.3294											
33805.77519	1544.24285	1664.200007	115.5385168	223.9862657	71.20232847	973.3616074	721.1311722	215.4333623											
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2291.637637	1978.29902	2052.369566	2449.740195	2121.153011	2420.707004	2591.366928	2357.852746	2420.535419											
2344.492484	1757.560524	1894.677111	1884.574798	2122.955241	1934.068078	2183.721718	2031.141709	2161.12462											
3240.493351	2886.028693	3373.529892	3714.326509	3912.795687	3853.659326	3594.863198	3552.889003	3714.671358											
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7132.85592	0.551323836	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	357.9835866											
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39794.12644	42530.75764	46661.43855	56046.24077	61178.64936	52032.27902	49410.47732	51953.85021	51992.81084											
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26972.28724	138895.5782	170226.0388	34699.70428	26154.44753	14912.87339	57809.0759	32485.96981	22274.02468											
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1458.631276	1845.867357	1705.067631	1676.739345	1719.083342	2052.156291	1693.525892	1711.129862	1728.251172											
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15.15_279.0930m/z	279.0929611	15.15476667	pos
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15.16_1184.0030m/z	1184.002955	15.1646	pos
15.16_885.7522m/z	885.7521581	15.1646	pos
15.17_1185.3052m/z	1185.305206	15.17301667	pos
15.18_487.3598m/z	487.3598248	15.18143333	pos
15.20_610.1829m/z	610.1829266	15.19843333	pos
15.21_278.2474m/z	278.2474355	15.209	pos
15.23_1123.4652m/z	1123.465161	15.22598333	pos
15.23_116.107m/z	116.1070888	15.23281667	pos
15.25_239.1484m/z	239.1484103	15.24968333	pos
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15.25_638.2141m/z	638.2141026	15.24968333	pos
15.26_948.2674m/z	948.2673743	15.25653333	pos
15.28_651.1438m/z	651.1437846	15.2846	pos
15.29_248.0583m/z	248.0583116	15.29438333	pos
15.29_463.1296m/z	463.1296344	15.29438333	pos
15.29_519.1382m/z	519.1382491	15.29438333	pos
15.29_565.5662m/z	565.5662387	15.29438333	pos
15.29_667.1751m/z	667.1751492	15.29438333	pos
15.29_873.1992m/z	873.1992445	15.29438333	pos
15.29_906.2338n	889.2304694	15.29438333	pos
15.29_952.3010m/z	952.3010096	15.29438333	pos
15.29_966.2691n	967.2705285	15.29438333	pos
15.35_487.3598m/z	487.3598269	15.34891667	pos
15.36_443.3336m/z	443.3336366	15.36415	pos
15.41_487.3598m/z	487.3598494	15.41201667	pos
15.50_203.1424m/z	203.1424165	15.50008333	pos
15.50_963.2490m/z	963.2489686	15.50008333	pos
15.51_100.0587m/z	100.0587387	15.50691667	pos
15.51_108.0554m/z	108.055421	15.50691667	pos
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15.51_124.0470m/z	124.04702	15.50691667	pos
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15.51_130.0861m/z	130.0861015	15.50691667	pos
15.51_132.0554m/z	132.055357	15.50691667	pos
15.51_139.0969m/z	139.096866	15.5125	pos
15.51_146.0708m/z	146.0708143	15.50691667	pos
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15.51_180.0757m/z	180.0757309	15.5125	pos
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15.51_204.1237m/z	204.1236759	15.50691667	pos
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15.52_112.0628m/z	112.0628283	15.51933333	pos
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15.52_142.0605m/z	142.0605408	15.51933333	pos
15.52_164.1006m/z	164.1005902	15.51933333	pos
15.52_167.0883n	168.0955426	15.51933333	pos
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15.52_180.0955m/z	180.0954917	15.51933333	pos
15.52_180.1005n	163.0972037	15.51933333	pos
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2.00_172.9895m/z	172.9894832	2.004416667	pos
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2.00_221.0907m/z	221.0907228	2.004416667	pos
2.00_268.0738m/z	268.0737882	2.004416667	pos
2.03_111.5369m/z	111.5368735	2.026633333	pos
2.03_119.0254m/z	119.025359	2.026633333	pos
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2.03_157.9737m/z	157.9736569	2.026633333	pos
2.03_163.0340m/z	163.0339548	2.026633333	pos
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2.03_213.0081m/z	213.0081206	2.026633333	pos
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2.03_398.0163m/z	398.0162815	2.026633333	pos
2.05_143.0301m/z	143.0301086	2.048466667	pos
2.05_154.5380m/z	154.537986	2.048466667	pos
2.05_155.0398m/z	155.0397915	2.048466667	pos
2.05_161.0707m/z	161.0707421	2.048466667	pos
2.05_163.5431m/z	163.5431125	2.048466667	pos
2.05_185.0475n	224.011349	2.048466667	pos
2.05_403.2319m/z	403.2319463	2.048466667	pos
2.07_110.0169m/z	110.016904	2.069933333	pos
2.07_112.9718m/z	112.9718337	2.069933333	pos
2.07_156.1017m/z	156.1017021	2.069933333	pos
2.07_159.0763m/z	159.0762796	2.069933333	pos
2.07_179.4929m/z	179.4929448	2.069933333	pos
2.07_190.0032m/z	190.003235	2.069933333	pos
2.07_220.4287m/z	220.4287498	2.069933333	pos
2.07_229.0947n	247.1284779	2.069933333	pos
2.07_312.0135m/z	312.0134899	2.069933333	pos
2.09_114.9609m/z	114.9608979	2.0913	pos
2.09_154.9849m/z	154.9848717	2.0913	pos
2.09_160.1330m/z	160.1329653	2.0913	pos
2.09_183.1015m/z	183.1014991	2.0913	pos
2.09_243.0236m/z	243.0236447	2.0913	pos
2.11_112.9560m/z	112.9559698	2.113216667	pos
2.11_146.0631m/z	146.0631441	2.113216667	pos
2.11_183.1125m/z	183.1125217	2.113216667	pos
2.11_183.9626m/z	183.9625674	2.113216667	pos
2.11_211.0200m/z	211.0199917	2.113216667	pos
2.11_235.9596m/z	235.9595625	2.113216667	pos
2.11_266.9806m/z	266.9806655	2.113216667	pos
2.11_322.0386m/z	322.0385541	2.113216667	pos
2.14_119.0254m/z	119.0254122	2.1354	pos
2.14_129.9513m/z	129.9512619	2.1354	pos
2.14_172.1210n	195.1101256	2.1354	pos
2.14_243.0538n	244.0610609	2.1354	pos
2.14_334.8711m/z	334.8710534	2.1354	pos

29804.8886	25491.2666	29553.34977	38706.55584	35905.68892	32392.08851	22910.57724	26613.59968	33743.93011	
1770.440539	1476.753403	1213.728554	1348.38341	1461.22477	1425.496741	1520.172401	1732.175004	2083.980312	
199258.1439	132322.7845	78794.946	191491.2901	252579.0369	263737.9582	64640.13079	90468.41057	156390.4226	
44943.17195	62446.19987	84464.83048	62830.78316	78367.31179	67510.49314	81814.21655	60867.46319	50661.67418	
25885.63641	40052.16909	36381.62188	3000.702872	2296.069239	1788.867173	22958.70857	17350.34136	5290.718196	
85.57807464	170.9615804	180.0989114	216262.8414	59995.47695	7313.737107	107920.0043	412731.5434	430128.9357	
2970.205412	2506.066613	2390.532911	2861.768155	2412.206163	3547.757518	2771.701523	3171.159483	3195.097079	
149.3046333	776.0741207	224.1165535	195.9549134	201.3580574	69.6711659	133.1384903	553677.0768	3089.524925	
2565.437955	3169.463601	3067.873943	3259.929296	3960.814197	3185.264615	2542.234234	2900.9161	3050.681125	
11995.49454	9507.172016	9935.066035	17300.75301	13734.42187	14417.2071	9860.330548	11951.10239	15194.57911	
295.6542106	364.4172446	318.2985796	376.0590593	473.1945467	390.710433	281.8817624	357.5299287	378.3112941	
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927.950451	114.9616152	0.001403199	28.73573232	0.001403199	0.001403199	0.001403199	225222.316	88.13371583	
0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.351293939	8442.660606	203.5697654	83.27756982	
491.5590982	97.63922161	426.0886159	161.3245095	1229.687418	152.5944558	39709.01814	881.7829552	556.8450529	
513.7765428	626.3172477	409.6582244	1013.498478	618.1309107	378.8046803	4130.676635	491.5959416	281.2735615	
21.98376034	3039.583234	287.4104212	1286.265005	1602.274658	190.7127699	58700.99915	1404.321727	790.1248272	
39175.04729	49237.51829	32151.78573	41799.93439	87920.27378	45017.86786	751922.7941	53421.8718	52162.09741	
1617.844509	1571.053084	1705.780116	1588.085021	1810.782182	1172.311827	1394.809268	1559.996354	1756.92869	
31499.46482	29320.52911	81738.47387	17020.41207	21458.92611	13439.954	262561.9204	35164.52576	26918.94707	
0.001403199	7844.192588	386.4393395	130.1700009	0.001403199	173.1560584	85271.16688	0.001403199	59.89900452	
44930.994	1182.55554	14356.98805	33029.7774	27731.8645	34213.47733	4449390.372	103169.8634	52847.86384	
70.09278919	0.001403199	0.001403199	0.001403199	0.001403199	9.51595745	146702.9081	0.001403199	23.09449644	
2629.119596	1682.777579	1847.872618	4844.26398	4779.382697	6608.61574	183405.7731	6821.298254	7223.979494	
1818.370774	1936.067845	2657.893012	2152.124749	1964.437809	1787.289286	2101.868076	2079.384412	1231.005315	
1827.648042	1309.38571	1720.594407	1769.303476	1841.14202	1441.267012	1816.942241	1815.076964	800.9920812	
1074.175573	1318.898153	1445.266381	1638.129801	1838.366001	1756.731138	1467.061547	1533.678843	2027.333316	
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1422.916137	1817.152272	1190.707003	8810.41724	330176.57	19902.0191	9898.574829	14042.21964	12304.13339	
108.0756891	0.001403199	16.56214316	44.86304559	133.4780435	199.618441	137.9417391	0.001403199	0.001403199	
166.8025477	142.6046814	18.38263956	258.3742389	362.0049977	287.336199	413.7774569	0.001403199	0.001403199	
1833.430789	2430.210385	181.979485	3371.130645	6574.77752	8484.188304	8442.678444	16.34378339	7.010357898	
95.46981932	194.2042923	57.86811084	391.7695206	659.4531879	661.8614969	784.2765393	0.001403199	1.902015417	
687.6205281	400.1630176	88.78241682	615.1574437	1289.663158	1499.973745	1620.101596	10.22465575	0.001403199	
164.9550797	79.38809335	17.7577289	142.6886048	277.2870744	480.914281	631.4518081	22.40318751	10.37240569	
96.70078713	149.5489136	0.001403199	246.7869055	393.4220964	600.5824861	568.1677436	0.001403199	0.001403199	
0.001403199	55.11614494	0.001403199	63.54639279	26.85107283	62.98718483	130.0372918	0.001403199	0.001403199	
101.6797765	157.4846867	0.001403199	225.0545954	264.2685448	264.1100695	417.1183408	0.001403199	0.001403199	
1032.459107	635.3080026	79.30385554	1059.963487	2667.721681	2528.544236	2532.028425	5.948340178	0.001403199	
1538.305088	1182.060461	175.960407	1154.874601	2439.757569	3732.575565	3544.944584	18.00836313	0.001403199	
691.7509666	672.1368087	99.62151897	830.7731862	1802.301753	2604.714216	2330.696288	17.77451038	0.001403199	
258.1679095	217.4126097	13.98778606	256.6772809	228.9206513	826.1934296	928.6069423	0.001403199	0.001403199	
772.3380626	591.2053789	103.4966352	819.5691765	2000.370634	1875.747488	1789.582725	13.91135001	0.001403199	
427.8088481	17.16719279	37.95780665	5.525033154	72.7992871	88.25425637	541.0955429	0.001403199	0.001403199	
243.1435005	271.9006669	26.64829879	251.8581459	799.4609498	691.9580181	963.3567805	0.001403199	0.001403199	
332.4579258	18.51659614	0.001403199	150.195793	1173.442425	262.521542	0.001403199	3.911988872	0.001403199	
2223299.972	1948642.29	1825299.982	2204040.147	2852656.764	3012814.729	2808365.847	1835465.601	1925114.859	
446.9823823	198.4899704	75.84304596	430.4908422	998.9497975	1147.790805	1308.28121	0.001403199	0.001403199	
351.1541727	85.81640993	48.30637329	249.3688339	555.5562086	710.6663008	525.2112166	0.001403199	0.001403199	
18946.9406	7479.51195	2858.78182	13754.1598	33402.67279	42139.17429	36877.06976	13.84311518	3.193313546	
1009.153868	580.2019375	139.5293823	928.9951565	2247.482161	2792.189623	2551.877262	0.001403199	0.001403199	
336.2466093	177.7496894	54.77000861	268.907484	583.2538544	923.5788316	865.638814	0.001403199	0.001403199	
2347.893601	1382.395261	312.0446031	1883.56834	5174.973704	6299.257699	6239.365318	13.89059401	0.001403199	
1430.099275	792.4827973	170.2356564	1417.233672	3270.262199	3057.068033	4267.448799	0.001403199	0.001403199	
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33579.39031	21695.41032	4475.896991	31031.42802	76225.20363	94912.20528	94592.48532	215.6025467	8.103413115	
3272.505213	3234.857692	3408.54472	1354.25699	1392.97075	1304.020699	1717.974181	1956.881221	1700.246398	
694.7869419	669.0504318	901.636462	327.2785763	384.0932035	269.5964339	1326.22717	1324.170362	1495.182629	
24157.941	25775.85248	25621.81772	10041.51395	10609.681731	10088.01416	12601.9563	13697.3706	13040.62714	
231.1872708	102.4146467	298.4378083	156.3691444	118.1594667	424.4642862	244.5286553	549.350132	650.5936958	
1440.590925	1402.713847	1608.46814	380.8581605	590.7375287	735.1440253	772.2121516	822.8573506	713.915073	
69.49191039	95.22116346	164.7671276	238.0925173	171.1343535	164.9560128	139.2103815	140.3353973	188.2217928	
137.0785399	238.301257	173.3255278	210.5426189	168.2646092	225.1823659	219.5694158	245.4358567	185.2780054	
44.24416992	92.85167709	167.4490431	177.1092055	301.5990911	300.344525	139.8562985	221.0032567	295.2683678	
273.0270948	159.5934697	214.8613183	165.6261593	117.3190012	158.9619811	170.579559	213.7561379	243.2136178	
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732.8286498	927.7419608	1027.930735	72.28020679	83.17980303	64.93999076	1622.024654	1783.700292	1862.700045	
775.2876504	837.9228681	763.0454881	419.5678498	578.1599764	545.2907376	867.9736347	847.6437503	919.615561	
116.3294412	144.9284004	138.1051496	0.001403199	0.001403199	0.001403199	273.9107547	397.1744998	310.5912578	
547.6387186	677.0005592	804.9240371	646.6784473	651.5955374	632.9019217	1230.233086	1242.223739	1194.076021	
6065.803329	6882.18473	6430.332264	135.3193224	8.366245486	225.2829664	5812.050997	5426.442871	4774.981815	
1089.895602	725.6210352	1100.327074	585.9521305	639.0270875	547.3069342	927.7470869	1051.231779	928.9454846	
2172.397177	2342.434052	2544.000318	1804.73741	1338.103189	1405.424668	1862.695786	2222.704463	2001.156406	
203.090576	151.4369355	202.8003432	88.81129345	75.58308565	234.7576265	95.50491094	225.0202319	275.5631048	
176.8824917	131.0796721	86.09088325	20.72967472	65.4060487	60.70100235	137.3665569	45.76186619	50.97631964	
120.6296887	122.8990714	222.4170168	73.16989139	104.8818769	68.45236952	120.3397737	64.94989967	166.3374864	
26005.9027	23104.53418	21671.70853	20509.56837	20339.51072	19466.29154	22185.30503	21408.19269	20532.06835	
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6.723754665	0.001403199	0.001403199	0.001403199	13.78018882	7.910954718	0.001403199	0.001403199	25.01987724	
157.4915854	125.1130108	186.4561024	147.5426855	184.5001956	153.3810172	151.9778196	146.9131313	156.0648977	
3266.450587	3116.019615	3532.079769	1748.782278	1761.995412	1785.585802	2322.236382	2326.902346	2443.326074	
701.8024713	499.2125685	555.1293892	400.7703889	364.9806075	462.5146321	532.8445767	543.3728115	547.9525664	
438.466885	234.2259196	275.735825	344.3809572	393.6820021	522.4690706	248.9649612	230.3928041	404.4474457	
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82165.00423	87082.65383	91871.19888	116103.2058	107231.4108	106466.5375	94231.20995	110231.2249	103731.0134	
2079.40161	1347.057745	2215.584277	933.6934454	872.3619024	1420.905473	1551.452954	1966.924708	1931.088245	
385.1382103	232.4483422	303.4495172	315.45561	384.5186415	355.2529467	317.9868653	348.8339732	381.6039795	
157.3042749	162.1462773	234.3060436	92.69997809	19.93471638	84.06034409	448.7873914	159.3696747	33.9756709	
1343.571943	1037.470692	1096.003126	503.4604958	549.7454515	475.0024175	603.2207991	550.6046587	504.1891067	
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3265.739765	2851.324261	3154.905668	2862.196034	2726.108542	2731.834713	2653.056174	2966.65429	2674.436793	
280.0048715	180.6372375	285.7469364	257.2057024	275.3820873	255.9239156	264.777103	280.4313793	288.5228075	
117.4719976	25.38172713	88.23260744	62.30474381	160.5500159	95.96780663	109.1489819	58.24327901	44.77902702	
189.0170457	183.3720087	162.9872227	114.1159286	101.3824374	209.2875883	81.04522915	74.03337288	34.27789628	
242.2896193	111.2225743	198.7524051	305.8822979	347.8820945	166.450198	442.0849517	229.8243713	158.3099196	
1853.991926	1569.81128	1730.239005	2615.897102	2473.296689	2147.059804	2301.116603	2514.663679	2350.513096	
257.6275148	87.6053517	297.1275463	193.935107	131.9619572	253.5254756	90.50537557	157.4745266	124.7650442	
1161.164831	946.9570002	1084.09782	1735.541213	1826.738773	1586.696383	1351.717712	1567.294851	1195.708557	
501.9357123	768.1050495	540.7794265	1751.859447	1457.965713	1346.629624	1197.489397	1510.309292	1142.526787	
196.8442167	177.0067639	288.3319993	154.3875518	186.0057984	233.4696073	214.8128317	221.1989702	172.1736976	
511.6753227	317.8455489	466.8359429	447.6398475	380.7189158	497.4758863	348.5396711	495.1130468	409.4899206	
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24211.75747	24699.7136	25939.8291	13698.48814	12387.60454	13059.11314	17295.8306	20566.35491	19130.41531	
1267.447721	845.9119209	1421.253054	1168.68868	1441.018536	1403.602044	1339.404267	1383.625061	1378.375383	

2.16_169.9973m/z	169.9973156	2.157266667	pos																		
2.16_173.9772m/z	173.9771907	2.157266667	pos																		
2.16_273.9752m/z	273.9752234	2.157266667	pos																		
2.18_130.1226m/z	130.1225539	2.178633333	pos																		
2.18_137.0789m/z	137.0788641	2.178633333	pos																		
2.18_140.9510m/z	140.9510473	2.178633333	pos																		
2.18_147.0630m/z	147.0630339	2.178633333	pos																		
2.18_230.9457m/z	230.9457431	2.178633333	pos																		
2.20_111.9845m/z	111.9845	2.200433333	pos																		
2.20_174.9925m/z	174.992523	2.200433333	pos																		
2.20_213.9826m/z	213.9826337	2.200433333	pos																		
2.20_366.9135m/z	366.9135116	2.200433333	pos																		
2.20_372.8813m/z	372.881264	2.200433333	pos																		
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2.22_203.9585m/z	203.9584798	2.220616667	pos																		
2.22_405.0093m/z	405.0092669	2.220616667	pos																		
2.22_440.8684m/z	440.8684422	2.220616667	pos																		
2.24_127.0501m/z	127.0501025	2.240783333	pos																		
2.24_142.0649m/z	142.0649188	2.240783333	pos																		
2.24_157.0970m/z	157.0969926	2.240783333	pos																		
2.24_209.5894m/z	209.5894252	2.240783333	pos																		
2.24_224.9327m/z	224.9326781	2.240783333	pos																		
2.24_278.8962m/z	278.8962518	2.240783333	pos																		
2.24_325.0525m/z	325.0525331	2.240783333	pos																		
2.26_119.0686m/z	119.0685857	2.260566667	pos																		
2.26_173.9774m/z	173.9773532	2.260566667	pos																		
2.26_188.0678m/z	188.0677641	2.260566667	pos																		
2.26_265.0034n	266.0106435	2.260566667	pos																		
2.26_300.8799m/z	300.8799496	2.260566667	pos																		
2.26_477.9725m/z	477.9725289	2.260566667	pos																		
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2.28_104.0622m/z	104.0621796	2.28185	pos																		
2.28_110.0170m/z	110.0170195	2.28185	pos																		
2.28_119.0729m/z	119.0729397	2.28185	pos																		
2.28_121.0841m/z	121.0841191	2.28185	pos																		
2.28_161.0838n	144.0805535	2.28185	pos																		
2.28_166.0803m/z	166.0803207	2.28185	pos																		
2.28_248.9013m/z	248.9013152	2.28185	pos																		
2.28_298.8781m/z	298.8781155	2.28185	pos																		
2.30_112.0507m/z	112.0506998	2.303833333	pos																		
2.30_137.0959m/z	137.0959106	2.303833333	pos																		
2.30_139.9984m/z	139.9984242	2.303833333	pos																		
2.30_344.9316m/z	344.931629	2.303833333	pos																		
2.32_157.9737m/z	157.9736628	2.32085	pos																		
2.32_163.0387m/z	163.0387225	2.32085	pos																		
2.32_204.0864m/z	204.0863881	2.32085	pos																		
2.34_131.9297m/z	131.9296737	2.342433333	pos																		
2.34_237.9793m/z	237.9793061	2.342433333	pos																		
2.34_282.9101m/z	282.9100911	2.342433333	pos																		
2.34_287.9796m/z	287.9795815	2.342433333	pos																		
2.34_299.0085m/z	299.0084886	2.342433333	pos																		
2.36_101.0600m/z	101.0599799	2.360916667	pos																		
2.36_119.0253m/z	119.0252926	2.360916667	pos																		
2.36_129.9788m/z	129.9788288	2.360916667	pos																		
2.36_163.0340m/z	163.0339533	2.360916667	pos																		
2.36_172.0059m/z	172.0049795	2.360916667	pos																		
2.36_202.4902m/z	202.4902492	2.360916667	pos																		
2.36_220.9614m/z	220.9614422	2.360916667	pos																		
2.36_239.1485m/z	239.1484729	2.360916667	pos																		
2.36_288.1435m/z	288.1435418	2.360916667	pos																		
2.36_326.9729m/z	326.9728877	2.360916667	pos																		
2.38_169.9974m/z	169.9973562	2.382883333	pos																		
2.38_300.0508m/z	300.0507783	2.382883333	pos																		
2.40_161.9732m/z	161.9732023	2.403116667	pos																		
2.40_211.0034m/z	211.0034238	2.403116667	pos																		
2.42_333.8731m/z	333.8730869	2.421616667	pos																		
2.44_128.0423m/z	128.0422937	2.43685	pos																		
2.44_203.1427m/z	203.1427475	2.43685	pos																		
2.44_234.9469m/z	234.9468839	2.43685	pos																		
2.45_176.9590m/z	176.9590431	2.450033333	pos																		
2.45_197.0006m/z	197.0005661	2.450033333	pos																		
2.47_116.9720m/z	116.9719649	2.465483333	pos																		
2.47_161.0183m/z	161.0183443	2.465483333	pos																		
2.47_190.1071m/z	190.1070782	2.465483333	pos																		
2.47_201.0730m/z	201.073008	2.465483333	pos																		
2.48_111.5369m/z	111.5369327	2.484216667	pos																		
2.48_139.9984m/z	139.9984254	2.484216667	pos																		
2.48_157.9737m/z	157.9736833	2.484216667	pos																		
2.48_185.0779m/z	185.0779069	2.484216667	pos																		
2.50_224.9328m/z	224.9327508	2.499733333	pos																		
2.50_403.2321m/z	403.232146	2.499733333	pos																		
2.51_112.0507m/z	112.0506793	2.513183333	pos																		
2.51_131.9297m/z	131.9296999	2.513183333	pos																		
2.51_203.9585m/z	203.9584944	2.513183333	pos																		
2.54_178.9903m/z	178.9903222	2.53565	pos																		
2.54_181.1222m/z	181.1221572	2.53565	pos																		
2.54_189.9589m/z	189.9588709	2.53565	pos																		
2.54_285.0957n	286.102966	2.53565	pos																		
2.54_333.8731m/z	333.8731099	2.53565	pos																		
2.54_372.8812m/z	372.8811803	2.53565	pos																		
2.56_207.0989m/z	207.0988606	2.555983333	pos																		
2.56_221.0719n	244.0611255	2.555983333	pos																		
2.58_113.0347m/z	113.0346951	2.578	pos																		
2.58_140.9511m/z	140.9510637	2.578	pos																		
2.58_144.0370m/z	144.0370464	2.578	pos																		
2.58_163.1172m/z	163.1172061	2.578	pos																		
2.58_190.9668m/z	190.9668055	2.578	pos																		
2.58_236.9066m/z	236.9065586	2.578	pos																		
2.58_440.8685m/z	440.8685101	2.578	pos																		
2.60_116.9720m/z	116.9719811	2.597883333	pos																		
2.60_117.0548m/z	117.0547691	2.597883333	pos																		
2.60_167.1064m/z	167.106444	2.597883333	pos																		
2.60_176.9591m/z	176.9590612	2.597883333	pos																		
2.60_240.1800m/z	240.1800244	2.597883333	pos																		
2.60_252.9750m/z	252.9749626	2.597883333	pos																		
2.60_303.9569m/z	303.9569038	2.597883333	pos																		
2.61_188.1152m/z	188.1152082	2.6129	pos																		

2379.322145	1812.170805	2572.70278	2148.700212	2102.079001	2118.52096	2288.573501	2339.401947	2296.387451													
284.7387643	174.6151226	287.8462229	248.2389313	274.7128631	275.6661921	261.90527	226.9977937	313.4928224													
1856.246298	1422.763339	2139.227031	66.12227553	53.7328241	0.001403199	1343.972787	1304.303013	1218.190315													
477.7636393	375.9998532	467.2337244	323.9873779	325.8853815	380.5644065	799.9959057	945.516903	865.6052913													
40.33870465	42.49039501	105.9482976	69.38528094	109.3049906	55.71712985	77.47739363	67.90802479	54.42429452													
1532.421666	1091.263823	1437.011004	1247.37338	1274.829463	1354.887265	1287.750538	1358.651227	1306.588152													
16.60450775	19.66644406	23.45020945	0.001403199	18.84625115	9.031084011	4.428460339	80.26468217	82.80691649													
6200.134994	4565.211012	5107.482969	4891.636107	4603.660056	5263.361616	5196.378056	5047.206808	5120.844271													
1858.539365	1418.681441	1736.736516	1586.84688	1712.779807	1689.982004	1514.273831	1558.02269	1631.204717													
0.001403199	0.001403199	0.001403199	22.02826039	26.93580061	44.34170344	30.22393005	0.001403199	0.001403199													
87090.35719	80753.47971	75435.01729	74361.92331	76837.9229	74445.4542	86030.86447	76637.05205	78316.83276													
2887.227287	3180.181837	4453.843057	0.001403199	0.001403199	0.001403199	1510.381391	2290.935883	1892.709507													
5146.709974	3994.74854	4415.76935	4401.726532	4153.829469	4786.050181	3879.608228	4816.212585	4708.837964													
212.7836495	198.6964589	181.1562468	100.6482464	76.81339717	237.2241711	208.7950414	212.6021102	172.1034834													
330.5622703	293.3844209	354.0682862	402.9735099	348.8856397	428.4308218	524.6931858	392.0008279	608.7803376													
2910.260972	2878.341603	2792.553541	0.001403199	0.001403199	150.8086006	1793.124465	2649.154877	1777.804503													
3159.349932	3022.98231	2246.832084	2742.421614	2337.175166	2622.220113	2228.342407	3193.231354	2881.991915													
7253.169	7450.817605	7172.75961	7839.917418	8627.810408	9109.809027	8341.896468	8057.668273	9080.941448													
147.0569641	94.92021174	135.2626812	153.6097239	69.31065386	94.32429663	33.52714062	125.5489097	140.998342													
87.56235028	109.114696	33.30453506	93.13595141	60.65476015	103.2723687	38.14893548	137.8874833	147.4589442													
159.9107129	59.40915162	94.8610474	143.8689425	112.374125	96.86854734	206.1621719	0.001403199	117.7776485													
6724.822205	5663.490737	5427.229182	5639.020335	6189.420614	6232.852853	6072.764762	6311.659424	6732.519331													
286.9292485	208.9557896	209.2643801	137.9334	206.9709075	440.8710296	482.4852085	297.9643606	360.2684691													
5077.839106	5761.53393	5456.276879	2903.356855	2693.065409	2311.741388	3888.538803	5460.213545	4810.123714													
36.26910772	68.54073775	45.1848807	94.39032872	69.47588166	83.8926679	64.80770813	103.5766754	103.8566955													
245.1488517	214.1392959	221.8425421	117.3322419	120.7176698	285.2972588	271.7934736	243.8323928	221.7082485													
1005.119922	704.9080834	625.6095778	689.4231871	845.4800527	767.6544371	757.3887666	846.2502205	839.4587598													
3277.379169	3620.782368	2918.16885	4315.319735	3847.705436	4586.339862	3574.591795	4155.956769	3654.638183													
180.8627756	371.8350994	208.0133915	318.2665811	87.5822531	107.6313673	344.7396237	310.6416651	376.0058545													
2299.660722	2521.672539	1710.893706	0.001403199	0.001403199	171.5235092	2009.72147	2134.504467	2452.495995													
75232.96092	79961.2085	78509.18314	107430.0396	100596.2766	103308.2032	94203.01008	100723.7936	94215.09052													
0.001403199	0.001403199	0.001403199	30.9248708	0.001403199	0.001403199	11.16594971	13.89366334	14.92054849													
0.001403199	0.001403199	0.001403199	10.90219749	0.001403199	0.001403199	26.14564029	11.56992483	10.39220026													
106.8184533	103.5362915	138.824104	149.466726	100.9332764	174.8600854	154.3217556	154.0026027	128.6501163													
6288.390738	6803.290175	6853.793761	9033.501739	8806.057148	9155.208282	8240.945217	8747.98103	8183.261309													
5714.746962	4442.126641	3856.48397	2839.598141	2677.585014	2652.969147	3938.695169	3328.349556	3275.248825													
163.4458965	236.467311	158.7829736	26.75943107	222.966701	260.7287673	231.3891963	246.0296793	104.0164687													
1113.567485	898.1838717	797.8387145	798.3364986	1100.871088	1234.379653	1235.430329	1024.195887	1029.075099													
604.5448401	542.3925337	392.8553597	369.9705354	527.1039603	571.9425431	670.8525385	571.5864601	569.6696081													
62.67761582	69.20671379	33.18654832	17.54631909	56.05502598	73.69684006	56.41930468	56.05264378	79.48360806													
2628.988532	2435.279247	1811.774012	1999.053631	2046.361614	2429.952016	2540.183624	2299.838647	2394.847482													
22.35525476	87.91423228	0.001403199	0.001403199	21.51306266	38.53046895	22.48746295	48.21299282	42.72164566													
8241.191007	8547.21936	7941.303534	244.8457265	406.6588931	379.4009787	6378.652387	6822.330515	5931.681927													
1310.207653	1352.602817	903.2416597	1274.333204	1357.083486	1262.031286	1359.094298	1181.577118	1715.50581													
2795.722941	2478.865251	2212.399881	1950.045737	2182.959417	2590.441165	2592.84344	2436.436692	2223.911761													
1207.574054	906.6688135	954.2244958	874.5469068	1217.806935	1138.784058	1194.603524	1119.33437	1190.555435													
2683.428652	2567.364666	1941.046774	2060.186088	2611.591387	2437.443205	2572.306757	2547.931981	2491.412027													
2020.625207	1960.391502	1990.810165	1006.507829	983.6900137	861.2812349	574.3641395	807.5647601	629.1148244													
1601.299785	1889.682099	1083.983061	1358.323472	1373.690714	1105.053859	1492.349775	1509.884201	1323.606627													
1637.794621	1986.884482	1128.124856	1718.183569	2016.482761	1969.894528	1836.563212	1814.741207	2110.190511													
1790.309561	1910.740412	1624.523562	2583.625929	2408.679937	2638.080541	1796.630957	2343.586281	1915.440494													
1090.087774	1068.702771	951.6258754	1132.091498	1131.177819	1220.783679	1301.129781	1284.406892	1276.119952													
295.7725641	302.0565681	215.87509	255.1108873	243.0364242	230.490464	316.7840809	243.060786	195.5194238													
3218.455537	3067.937488	2798.716603	3420.551201	3658.219924	3862.067229	4168.651729	3647.023644	3873.445802													
6589.302397	7522.504728	7085.208315	10332.78773	10800.35774	11571.9711	8648.410377	9556.493115	8463.173321													
1407.513626	1713.666127	1122.714811	1730.980183	1652.620644	1876.233556	1679.665222	1598.926086	1454.923048													
0.001403199	40.51061835	35.53517591	32.49842942	145.8614129	0.001403199	0.001403199	182.4079885	23.61423547													
1878.967166	2200.256706	1177.880419	1868.535434	2016.380586	2149.565547	1974.989959	2076.791243	1915.223409													
1699.516568	2073.072518	1177.113302	1531.67741	1525.38495	1442.927243	1648.991578	1556.622162	1532.870222													
232.2862752	384.1828433	428.3618735	834.2720016	880.3817687	976.4276096	640.6336725	537.5124283	698.8110824													
608.1009488	629.6730925	699.1572236	0.001403199	0.001403199	0.001403199	2598.284447	3211.483977	2887.982895													
4019.784474	3997.654028	3275.707556	3091.42813	4160.482748	4631.560561	4473.48108	4128.010414	4357.656729													
3140.688927	3428.494832	3002.063241	1290.530502	1412.092988	1261.374592	1202.759488	1359.3695	1181.363267													
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470.9072536	729.9897585	377.5702873	420.2423736	480.7739955	612.5124078	636.8422796	634.4207198	621.3053596													
2634.826844	2766.5154	2113.232227	2743.718995	2900.894965	2702.423114	3082.324234	2776.839362	2838.32645													
172.4378726	57.41587187	144.7760803	89.35550557	27.72931542	68.00986277	111.7889178	13.15833664	109.5348408													
428.474765	350.290102	230.2758312	451.1439163	433.9095095	458.2965172	529.6016249	442.580205	451.6553005													
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424.4980869	460.1318966	451.9930362	607.3402718	667.4762319	730.7691503	676.0882132	616.8329233	619.2300937													
569.0582934	606.2859775	682.9846849	864.9272814	839.266134	997.1080063	936.3621615	850.7564628	857.1991333													
981.6460215	1038.142588	867.6603779	1127.335444	1064.953367	1255.304635	1314.600769	1154.475799	1101.736426													
708.9418674	917.7588715	1137.690694	1483.632063	1488.912387	1579.011252	1237.69473	1491.384798	1372.019409													
244.7102052	284.1997275	231.3239815	317.7066867	340.0990787	252.9603221	311.8665298	424.6634294	380.8812298													
548.1466585	509.3669265	641.9722053	863.1761677	752.4955683	1026.735244	1221.559028	855.0061255	880.1511061													
45.463301	34.79376762	49.17003483	124.6420836	117.1184015	137.4324218	67.11082299	76.35089397	88.50375734													
57.70903896	35.94235156	58.1894346	23.29665518	56.45268996	115.9059098	79.78789097	62.00085681	76.97243809													
1994.809823	1680.060374	1889.805736	2211.078688	2439.250852	2719.247799	2678.21904	2199.265973	2464.634818													
1785.287367	1696.936877	1674.796932	1588.357603	2148.577217	2608.694508	2074.682817	2199.673672	2473.721706													
2042.060854	1360.57311	1522.140833	2202.926863	1993.774065	2631.463934	2466.223034	1940.435841	2666.595384													
1708.572492	1677.746179	1295.223158	2116.122635	2255.587555	2110.140835	3657.492264	2087.82513	2294.710578													
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1927.618863	1557.150942	1864.667964	2005.924135	2173.081458	2003.450509	2353.216208	1807.019306	2242.150307													
152.7590337	194.2345408	112.8586997	178.0266678	206.7945883	205.1798875	199.1935658	171.8669488	268.3869622													
2472.401941	2334.583428	2353.912512	2455.174081	2545.786582	2286.143631	2839.401762	2214.961961	2839.151866													
1281.238331	888.5751111	1136.993646	1013.658433	988.5249288	1260.970659	1442.181874	1109.323994	1229.053584													
435.5513698	329.9342547	405.3823696	440.9461183	395.3553547	429.1604121	489.5121719	397.2911052	530.3780642													
21714.1317	23222.46326	21860.695	27544.45183	29167.64363	32206.02634	23471.99089	25554.8483	25051.07048													
2129.105468	1744.459967	2063.89958	2266.769089	2249.907809	2432.235308	2578.028938	2126.200427	2788.04178													
21987.0749	21099.47623	20267.49335	20515.25615	24623.35844	23395.86827	24226.1567	20193.25817	23074.97689													
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4015.57827	3841.242668	4224.193534	9250.427603	9175.859047	10120.52463	10058.08571	11332.83022	11991.13501													
819.7545929	695.1528627	919.6377756	731.557365	717.5700257	751.4416253	605.1767071	715.8138962	695.6572846													
949.277132	795.6708468	914.4177184	770.198559	885.5960142	983.0026188	644.1467069	773.4450913	957.3248528													
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332.1704044	277.4930971	207.1617881	14.056316	11.19247905	24.1404604	122.7879437	16.93071556	0.001403199													
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28429.03634	28337.40936	28337.57878	30892.15792	34636.24884	34969.11548	34554.2484	30398.59578	33059.03355													
8145.572202	8291.014164	6781.303143	8160.848675	8191.076703	9309.382555	7785.819644	7401.239236	9182.038106													
397.9868405	405.2513417	439.1100389	455.2742466	468.1408356	213.2850142	350.3703009	433.1887604	549.2856189													
514.3054572	423.9454962	474.6540518	548.8496398	572.7176575	633.7183399	580.7557937	521.7876896	639.4420197													
2054.79432	2147.060897	2044.55312	2049.528583	2149.765922	1983.645321	2525.541392	2394.070473	2657.561147													
391.1200438	401.9260398	392.8649401	405.3894322	385.6548536	430.7456285	343.2381587	423.7127454	405.8598057													
771.6526297	698.6526076	847.826528	624.0173341	744.2457753	421.7559816	447.0749345	630.0151329	788.1200083													
6617.83543	7319.691665	7770.251257	2947.728771	2874.866791	2551.143417	3091.109099	3931.827511	3504.805239													
1236.683564	1866.073821	1828.836043	581.7855218	549.3304421	588.993991	738.7138097	1005.420307	944.7972768													
241.667345	285.2605954	297.3311577	257.3433997	298.5932755	327.1418168	63.47189386	168.2717552	165.6411787													

2.61_278.8962m/z	278.896245	2.6129	pos							1323.465927	1416.611936	1085.487585	1451.657717	1579.340243	1644.379825	1679.370425	1479.565218	1347.423057	
2.61_278.9906m/z	278.9906334	2.6129	pos							2133.824675	2306.787635	2409.637133	0.001403199	44.70739729	0.001403199	2802.988895	3530.53183	3382.975039	
2.63_164.9203m/z	164.9202903	2.627966667	pos							1313.355187	1274.319369	1308.902091	1447.817461	1757.404028	835.4986706	1169.859717	1559.165771	1766.19916	
2.64_131.9297m/z	131.9296633	2.6413	pos							1282.710747	1262.488949	1147.052237	1214.106671	1227.30054	856.3938967	988.9786877	1131.975311	1478.274304	
2.64_143.9626m/z	143.962591	2.6413	pos							22.98523919	28.80802249	90.96632955	75.46367231	80.11608277	34.69972639	110.9301439	42.83014488	63.20502278	
2.64_183.1015m/z	183.1015454	2.6413	pos							6419.116982	6265.796022	6186.049711	6147.414487	6035.836816	6329.061115	7239.001015	6427.770594	6359.396119	
2.64_224.9327m/z	224.9326648	2.6413	pos							3778.738334	3702.679419	3519.914546	3356.598089	4072.544845	3599.760972	3766.716492	3416.907494	3779.281232	
2.64_371.1008m/z	371.1008461	2.6413	pos							1900.659255	1455.217711	1548.776583	1282.075328	1616.520519	1369.408658	1669.611273	1437.291967	1586.419617	
2.66_110.0171m/z	110.017073	2.655183333	pos							17.93095313	69.87935241	33.86976567	22.47158821	34.92383956	19.86873641	22.71822338	5.579953194	45.00065853	
2.66_154.9849m/z	154.9848543	2.655183333	pos							133.7023498	280.5379077	246.7171973	45.30643193	86.37071118	0.001403199	159.8450861	46.66632843	44.34931237	
2.66_173.1171m/z	173.1171475	2.655183333	pos							5533.478577	5096.952253	4802.017708	4616.880291	4861.478805	4968.101758	5421.912558	4952.521597	5125.130312	
2.66_193.0831m/z	193.0831325	2.655183333	pos							1315.945302	1274.871042	1136.050162	1270.024482	1340.280174	1358.871414	1514.63598	1257.511853	1645.229995	
2.66_203.9586m/z	203.9585547	2.655183333	pos							304.8753198	222.7615371	303.7865065	270.5180675	195.0772784	140.650628	195.4042007	209.3273767	348.7473582	
2.68_298.8781m/z	298.8781454	2.677116667	pos							867.691706	875.245194	671.7321846	682.8902661	1054.635054	916.7106397	1032.503899	824.2663279	859.0083094	
2.68_440.8685m/z	440.8685394	2.677116667	pos							3350.1187	3898.363269	3156.161369	3417.442285	4061.477573	2564.705152	4417.636605	3345.82573	3971.394011	
2.70_113.9605m/z	113.9604525	2.669483333	pos							1055.440462	1042.790378	1001.598196	1353.600013	1393.10461	1346.271076	1014.958762	1149.769225	1338.985663	
2.70_148.0391m/z	148.0391198	2.669483333	pos							684.0736206	764.5788428	725.5206963	734.5324202	1016.308631	971.1610428	1095.336896	780.6924423	869.480125	
2.70_186.0810m/z	186.0810095	2.669483333	pos							78.85868922	185.7800597	185.8425214	340.4231166	391.0876857	302.2219105	278.5706966	237.1052179	359.7388509	
2.70_205.1544m/z	205.154439	2.669483333	pos							1221.576052	1458.949739	1412.031197	1278.955011	1566.095112	1390.848769	1838.620361	1477.619072	1772.003518	
2.70_207.0987m/z	207.0987372	2.669483333	pos							1022.512701	1204.303326	868.3442162	600.2288857	1018.330619	700.8375435	822.1374031	852.5449757	948.7304243	
2.70_224.0114m/z	224.0113848	2.669483333	pos							29688.22438	27371.98095	25818.86875	24848.73456	27283.24745	25362.28333	30004.39128	26156.72029	28187.0086	
2.70_225.9911m/z	225.9911252	2.669483333	pos							141.770482	153.9118893	171.6613522	110.9490813	147.7102774	129.5857297	172.3489154	168.637084	274.9246302	
2.70_250.0698n	273.0589906	2.669483333	pos							19136.26826	23838.21833	21869.03534	22549.99391	22699.88911	24610.93349	21935.74156	23130.53265	22059.73632	
2.72_119.5229m/z	119.5229241	2.721583333	pos							173.9889914	336.7064286	300.9389039	477.885876	762.7160081	622.2770352	464.5143481	412.893756	380.9970333	
2.72_137.0513m/z	137.0512601	2.721583333	pos							36.02760558	82.14869021	76.24037974	64.63522496	66.12470761	47.55103642	78.79414088	55.74560939	98.19609526	
2.72_138.0490m/z	138.0490389	2.721583333	pos							0.001403199	78.88424245	140.7045217	130.3577258	126.9167012	119.4348846	84.83190462	131.137661	120.7972688	
2.72_169.9974m/z	169.9973835	2.721583333	pos							3272.961175	4078.38391	3593.614893	3534.194697	4420.141531	3859.296646	4516.070731	3476.795105	3890.163852	
2.72_181.0713n	182.0785933	2.721583333	pos							35350.44847	44438.51124	41782.12835	37604.54244	44442.35922	41857.24502	50103.27897	48215.44044	49454.12699	
2.74_128.0423m/z	128.0422778	2.743533333	pos							91.16696355	78.76782683	90.95979702	23.34504523	35.74562075	34.72295512	118.7679609	72.619277	91.94620815	
2.74_169.0860m/z	169.0860291	2.743533333	pos							1744.106747	2048.864763	1621.809428	1888.02242	1767.410395	2031.70747	1881.258092	1796.388412	1839.921539	
2.74_217.0153m/z	217.0153057	2.743533333	pos							64.14458135	37.83426249	72.34159478	104.0911456	137.4194912	144.4230667	100.3146083	193.1426134	37.72121607	
2.76_112.0507m/z	112.0506712	2.755716667	pos							82.25154712	108.0180225	93.05889084	111.5725136	109.6779181	127.0361867	105.4543428	110.7674875	93.42447013	
2.76_155.0445m/z	155.0445127	2.755716667	pos							421.2889404	546.8354655	540.9001933	433.5338896	497.5177601	498.1881257	626.78437	336.4679596	407.5220785	
2.76_166.0836m/z	166.0835159	2.755716667	pos							116.8775507	184.9145748	171.1142363	181.5382219	343.5219744	226.4057173	200.0894607	145.7791561	233.2922881	
2.76_173.9846m/z	173.9845857	2.755716667	pos							423.1209556	360.0063745	370.5915398	252.4741587	419.6922603	423.0901642	327.1181116	312.2048817	379.5856365	
2.76_184.9608m/z	184.9607664	2.755716667	pos							79.18397271	87.71955972	79.98815273	100.1381571	29.31933575	184.7913436	106.7633204	38.13364029	96.42444677	
2.76_215.0887m/z	215.0886567	2.755716667	pos							1576.035465	1604.864472	1500.293389	1572.06878	1665.675447	1495.21119	2074.370397	1604.466867	1687.567553	
2.76_221.1534m/z	221.1533851	2.755716667	pos							1176.030777	1281.781959	1430.279745	1252.293798	1381.754742	1507.218151	1806.639118	1357.793282	1342.994219	
2.78_111.5369m/z	111.5368743	2.775583333	pos							52.74837443	79.1955104	78.89535621	198.8133257	175.9414583	195.552537	85.42989993	87.87677756	170.7383763	
2.78_143.9626m/z	143.9625991	2.775583333	pos							24.46015965	25.47036787	29.66043804	24.14934012	59.92774353	92.2035654	32.46906684	70.9182806	66.61873686	
2.78_195.0995m/z	195.0995181	2.775583333	pos							847.7526286	916.0326989	950.2906866	940.8579205	819.5397567	842.5811679	941.6163491	1072.506288	829.9145977	
2.79_129.9539m/z	129.953892	2.79025	pos							484.8774781	485.3576908	400.8123652	436.5161182	366.3065437	472.5391405	499.0666185	509.9839629	406.6790406	
2.79_164.9203m/z	164.9202691	2.79025	pos							2207.547569	2540.340415	2169.170632	3220.654656	2931.188944	3206.202623	3060.685717	2642.736108	2617.032076	
2.79_218.9938m/z	218.9938012	2.79025	pos							240.5956995	231.6229543	352.4194447	747.0452135	520.2716179	493.4877121	371.4531663	327.4059699	432.5865263	
2.79_333.8731m/z	333.8730672	2.79025	pos							5134.545802	5060.930936	4202.928437	5031.167	5186.243565	4692.681565	5063.325714	4839.864491	4891.611298	
2.80_163.0388m/z	163.0387935	2.804116667	pos							2760.159576	2278.660183	2042.459965	2552.041838	2562.12409	2522.25248	2771.724152	2455.753742	2291.351783	
2.80_204.9666m/z	204.9665559	2.804116667	pos							420.9251597	423.5817238	476.759157	582.741966	473.7283124	559.0758299	562.51704	493.9834375	444.9029582	
2.80_238.0681m/z	238.0681212	2.804116667	pos							1127.22418	1421.384001	1364.015375	1364.509766	1126.951348	1265.623217	1865.211601	1844.101448	2039.359249	
2.80_440.8684m/z	440.8684387	2.804116667	pos							4120.57257	4370.474213	4348.053442	6410.08525	4883.075305	6912.228834	6269.887368	5125.359825	4989.955882	
2.82_163.0340m/z	163.033995	2.821016667	pos							1125.951495	1078.127742	1273.685911	2666.186039	1903.007399	1870.873684	1340.802777	1725.638149	1407.273552	
2.82_181.9772m/z	181.9771725	2.821016667	pos							8657.791482	8360.995265	7804.807471	7827.722941	8438.177638	8253.338363	9088.907439	8243.797476	8064.50367	
2.82_282.9101m/z	282.9100564	2.821016667	pos							4151.629076	3953.898392	3571.067115	3651.507443	3694.713719	3318.402573	3982.160876	3505.5139	3310.054911	
2.84_168.0765m/z	168.0765438	2.839933333	pos							95.61570038	162.7632134	134.4204296	161.6611862	162.2516969	203.1495432	239.6382044	185.3061314	149.6808132	
2.84_183.9626m/z	183.9625862	2.839933333	pos							401.9339785	346.270082	374.373782	421.399958	308.353212	408.8815256	388.2801764	382.5589652	328.2966643	
2.84_184.1096n	202.1434288	2.839933333	pos							1847.195842	1492.852365	1424.375815	1404.47771	1235.471531	1482.469086	1457.402084	1552.81296	1346.635993	
2.84_294.8648m/z	294.8648067	2.839933333	pos							1893.84671	1440.602329	1328.86847	1831.646039	1779.414424	1450.085464	1902.544229	1686.622985	1605.244676	
2.85_113.0347m/z	113.0346942	2.851983333	pos							1302.569586	1021.330555	1115.305986	1245.297198	1102.267228	1244.445003	1144.894914	1223.67962	1042.070777	
2.85_155.0444m/z	155.0444092	2.851983333	pos							204.7120357	207.0076466	181.6550079	300.6093989	178.8486511	313.454689	210.7605635	337.9822707	254.8393022	
2.85_198.0701m/z	198.070123	2.851983333	pos							1330.129658	1221.072735	1491.489721	2154.149701	1563.629985	1363.962274	1251.312062	1672.869323	1569.716701	
2.85_212.0908n	195.0875321	2.851983333	pos							2802.058677	2646.879426	3213.876555	3294.427796	3424.527268	3581.566991	3445.810661	3967.438785	3468.265058	
2.85_224.9327m/z	224.9326788	2.851983333	pos							1691.816456	1131.399021	1463.809244	1379.363297	1236.611315	1549.782882	1353.180143	1650.317032	1246.193659	
2.87_169.9974m/z	169.9974238	2.86595	pos							2110.830353	1480.995185	1885.138011	1910.888373	1520.603158	1949.023577	1625.414924	1807.76842	1569.491195	
2.87_212.6170m/z	212.6170414	2.86595	pos							0.001403199	0.001403199	24.42856308	0.001403199	0.001403199	0.001403199	43.06608287	76.39436722	26.61483661	
2.87_267.6245m/z	267.6244972	2.86595	pos							2126.653894	2150.078636	2373.45152	2436.930689	2201.522876	1796.146026	1668.569602	2568.516559	2318.782978	
2.87_296.9914m/z	296.9913934	2.86595	pos							1232.599634	945.4363077	1381.392632	1401.193381	1145.005312	1588.704706	909.4230915	1796.658157	1074.234466	
2.88_181.1219m/z	181.1219011	2.87815	pos							913.7420642	779.8133705	832.2886454	720.7781132	609.454397	669.6718753	749.5070958	814.9031755	702.4905468	
2.88_197.1170m/z	197.1169974	2.87815	pos							1056.880124	894.5303124	1020.980427	1121.76018	999.9154478	1083.785472	865.1904034	987.5917419	783.8928411	
2.88_203.9710m/z	203.9710109	2.87815	pos							351.4896162	326.3008223	405.341932	533.1296146	418.8023131	469.3445844	529.8280631	485.2716379	465.8984364	
2.88_212.1152m/z	212.1152044	2.87815	pos							679.9364283	665.0724911	835.5222366	506.7672321	530.031863	573.4734225	655.1726639	933.9678611	837.447081	
2.88_215.0887m/z	215.0886569	2.87815	pos							1939.057626	1641.942956	1544.613473	1653.388039	1509.738909	1791.470107	1714.989186	2295.912696	1772.277595	
2.88_230.9458m/z	230.9457544	2.87815	pos							4752.141852	4027.278387	4070.628431	4437.109608	4466.543549	4940.235372	4319.428155	4613.407885	4665.791147	
2.89_115.9621m/z	115.9621099	2.8904	pos							137.8432829	37.82194086	39.4251534	55.47059554	35.6692154	45.94756964	8.97555274	23.13719716	0.001403199	
2.89_116.0528m/z	116.0527856	2.8904	pos							1054.331907	1084.821735	1042.087728	1054.672666	1102.697438	1215.859895	1168.29034	1167.158895	966.209749	
2.90_128.0423m/z	128.0422836	2.904316667	pos							115.0379808	54.8518766	0.001403199	52.73632006	0.001403199	49.26611137	0.001403199	0.001403199	45.43291329	
2.90_154.9848m/z	154.984848	2.904316667	pos							99.86102009	51.87911232	222.2603558	0.001403199	43.01800258	88.35680014	249.9276402	109.9318498	35.88361034	
2.90_193.1309m/z	193.1308723	2.904316667	pos							1056.14641	923.1753744	1172.328663	1032.852336	1177.728138	1116.861999	1089.356226	1165.176115	1037.733829	
2.92_129.9788m/z	129.9788443	2.9178	pos							2644.560213	2594.878208	2981.152737	2863.292881	3546.137003	3480.227805	3243.524391	3180.71235	3211.230418	
2.92_140.9511m/z	140.9510979	2.9178	pos							460.019432	456.4535534	413.8325609	486.248707	628.830228	564.239919	467.9717798	570.1469639	603.1329815	
2.92_202.9705m/z	202.9704772	2.9178	pos							95.20961055	77.66055166	66.94593389	27.95521754	124.9495938	36.55921592	76.3397247	30.26672363	0.001403199	
2.93_131.9297m/z	131.9296726	2.928333333	pos							2446.802368	2228.480334	2614.924078	2475.016075	2503.67115	2494.211995	2419.676869	2700.821819	2546.637121	
2.94_101.0600m/z	101.0599685	2.942283333	pos							319.8882934	276.0670525	320.9428498	352.8150382	398.161325	316.4857391	303.9642588	439.8520097	410.8767157	
2.94_331.9152m/z	331.9151688	2.942283333	pos							581.8899125	307.2525009	589.0880417	601.1975227	775.3743109	840.4751762	700.4681497	656.1699377	671.3851934	
2.95_116.9720m/z	116.9720157	2.950733333	pos							404.8705207	264.0034952	270.6053809	341.3885256	355.1243499	547.6291472	391.6317077	556.6006241	507.5585595	
2.95_143.9626m/z	143.9626327	2.950733333	pos							22.8581689	0.001403199	22.75298423	22.9976587	43.71706223	0.001403199	18.02024509	0.001403199	28.52238594	
2.95_164.9203m/z	164.920257	2.950733333	pos							1710.184241	1671.366333	1807.030417	2580.582713	2822.985664	3223.257479	2568.441868	2509.015422	2757.413548	
2.95_171.0479m/z	171.0478878	2.950733333	pos							25.71421921	30.23533675	47.43569737	25.16936885	43.86041788	25.6102699	34.18777946	0.001403199	20.19320098	
2.95_177.0820n	200.0712976	2.950733333	pos							11800.4032	14115.81487	14999.94415	4126.80699	4612.088547	4749.302538	7320.903742	7991.748408	7501.57121	
2.95_224.9327m/z	224.9326643	2.950733333	pos							1592.370185	1567.148315	1478.391144	2000.705382	2232.289748	2636.191921	2169.715487	2067.072548	2664.594079	
2.95_310.8504m/z	310.8504152	2.950733333	pos							224.2974915	174.9610282	228.5223923	418.9159418	410.7836853	777.4567591	429.8356395	490.7750769	341.3676191	
2.95_333.8732m/z	333.8731532	2.950733333	pos							4301.511395	4538.697658	5307.751293	5222.611161	6281.967514	5675.390614	5386.507332	5483.366732	5358.18886	
2.96_157.9737m/z	157.9737168	2.9608	pos							1238.604529	1063.127299	1114.133178	1098.219707	1713.30378	1644.713514	1449.735648	1569.238383	1517.565976	
2.96_183.0802m/z	183.0801946	2.9608	pos							379.9443367	499.7562069	679.1513548	735.7934898	709.0144258	726.305512	801.9657208	599.6030895	568.7951773	
2.96_207.0988m/z	207.0987644	2.9608	pos							659.1406701	511.1297152	686.5993244	700.75647	598.6041198	548.4889039	1009.941113	717.2131133	636.233899	
2.97_139.9983m/z	139.9983299	2.971383333	pos							0.001403199	0.001403199	18.40976037	0.001403199	15.10313438	0.001403199	19.6953234	34.85864496	40.66487657	
2.97_165.0545m/z	165.0544596	2.971383333	pos							1600.492725	1637.844346	1930.668391	1670.045888	2025.887872	1846.505486	1977.556119	1770.78003	2075.88247	
2.97_372.8812m/z	372.881174	2.971383333	pos							15693.10166	14990.65414	14932.24295	18458.80203	19056.39538	18674.90809	20591.68612	16782.08293	18369.02598	
2.99_124.0474m/z	124.0474086	2.98815	pos							142.1197843	67.91314019	81.84654267	92.78572132	121.486706	76.89628959	105.8764309	79.33917475	120.9631684	
2.99_203.9585m/z	203.9585212	2.98815	pos							464.1150541	482.0874952	527.9952133	422.1784298	693.4903213	643.8342728	699.8543989	623.7176403	619.673473	
3.01_111.9845m/z	111.9845286	3.01015	pos							609.924201	742.6430022	949.5563995	694.2449112	825.9574917	1169.028889	995.4738847	734.8864212	748.8357067	
3.01_305.8987m/z	305.8986897	3.01015	pos							19740.29827	18379.98301	17518.17777	22018.15784	23371.67199	23409.84476	23397.55432	20003.08575	20314.62606	
3.03_158.5369m/z	158.5368855	3.027516667	pos							0.001403199	48.27489991	77.51909796	136.0633226	152.6919523	123.2232031	89.89680926	85.38855325	115.7953121	
3.03_220.9766m/z	220.976599	3.027516667	pos							2067.638403	2498.465917	3072.011288	173.072765	56.85685198	171.0828175	1905.262754	1923.867956	2080.329894	
3.03_236.0002m/z	236.0001578	3.027516667	pos							14944.77655	16401.18887	18076.65758	4865.661163	4612.917177	4866.37377	13871.05128	14170.31514	13983.15049	
3.03_266.9791m/z	266.9791422	3.027516667	pos							483.1918166	606.4793646	846.7971301	605.6646275	529.9502096	381.2945799	526.8006335	563.2577354	529.7423864	
3.03_332.9601n	315.9568165	3.027516667	pos							6482.388664	7744.505738	8707.20187	336.6752171	212.0155778	368.2551044	6611.375445	6256.79815	6522.041229	
3.03_332.9621m/z	332.9621095	3.027516667	pos							2313.248179	3689.403502	4360.667553	202.3438782	258.6378622	121.9975915	3400.845319	2983.290237	3000.500588	
3.03_356.9832m/z	356.98323	3.027516667	pos							11595.50483	13825.54858	14359.95097	891.1298036	533.3122224	693.4943434	10022.32097	10558.05946	11157.59455	

| | | |

3.35_282.9101m/z	282.910051	3.34955	pos
3.35_284.9098m/z	284.9097829	3.34955	pos
3.35_328.9148m/z	328.9148185	3.34955	pos
3.35_372.8813m/z	372.8812859	3.34955	pos
3.36_199.1326m/z	199.1326379	3.363133333	pos
3.36_230.9458m/z	230.9457908	3.363133333	pos
3.36_274.1644m/z	274.1643778	3.363133333	pos
3.36_386.1195m/z	386.1194941	3.363133333	pos
3.38_149.9402m/z	149.9401672	3.378983333	pos
3.38_308.9647m/z	308.9646944	3.378983333	pos
3.40_142.9666m/z	142.9666189	3.396566667	pos
3.40_165.0909m/z	165.0908848	3.396566667	pos
3.40_204.0977m/z	204.0976894	3.396566667	pos
3.41_111.5369m/z	111.536924	3.414066667	pos
3.41_133.0647m/z	133.0646819	3.414066667	pos
3.41_143.9589m/z	143.9588944	3.414066667	pos
3.41_146.1174m/z	146.1173747	3.414066667	pos
3.41_170.4692m/z	170.4691691	3.414066667	pos
3.41_195.0994m/z	195.0993512	3.414066667	pos
3.41_261.1302m/z	261.1302292	3.414066667	pos
3.41_287.8882m/z	287.8882066	3.414066667	pos
3.41_326.0609n	327.0681998	3.414066667	pos
3.43_114.9610m/z	114.9609618	3.431116667	pos
3.43_166.5199m/z	166.5198895	3.431116667	pos
3.43_217.0349n	218.0421275	3.431116667	pos
3.43_234.9562m/z	234.9562042	3.431116667	pos
3.43_295.9848m/z	295.9848425	3.431116667	pos
3.45_132.1018m/z	132.1017802	3.446883333	pos
3.45_166.0862m/z	166.0862249	3.446883333	pos
3.45_318.1907m/z	318.1907016	3.446883333	pos
3.47_138.9858m/z	138.9857776	3.468983333	pos
3.47_144.0370m/z	144.0370489	3.468983333	pos
3.47_282.9101m/z	282.9101134	3.468983333	pos
3.48_138.9952m/z	138.9951521	3.48465	pos
3.48_165.0545m/z	165.054489	3.48465	pos
3.48_188.0664m/z	188.0664478	3.48465	pos
3.48_207.0989m/z	207.0989235	3.48465	pos
3.48_236.9065m/z	236.9065352	3.48465	pos
3.50_181.9772m/z	181.9772074	3.503883333	pos
3.50_270.9557m/z	270.955735	3.503883333	pos
3.50_440.8687m/z	440.8686509	3.503883333	pos
3.52_215.0888m/z	215.0888473	3.520533333	pos
3.52_239.1486m/z	239.1486275	3.520533333	pos
3.52_248.9013m/z	248.9013291	3.520533333	pos
3.52_344.9317m/z	344.9316779	3.520533333	pos
3.52_372.8812m/z	372.8812123	3.520533333	pos
3.52_724.3321m/z	724.3321108	3.520533333	pos
3.52_724.6664m/z	724.6663776	3.520533333	pos
3.52_724.9998m/z	724.9998219	3.520533333	pos
3.53_133.9746m/z	133.9745649	3.530816667	pos
3.53_159.0763m/z	159.076278	3.530816667	pos
3.53_203.0819n	221.115756	3.530816667	pos
3.53_211.0944m/z	211.0943511	3.530816667	pos
3.53_215.1274m/z	215.1273878	3.530816667	pos
3.53_224.0776m/z	224.0775501	3.530816667	pos
3.53_229.1431m/z	229.1431423	3.530816667	pos
3.54_131.9670m/z	131.9669514	3.5398	pos
3.54_191.1064m/z	191.1064446	3.5398	pos
3.54_199.0941m/z	199.094108	3.5398	pos
3.54_261.1304m/z	261.1304144	3.5398	pos
3.54_294.8648m/z	294.8648065	3.5398	pos
3.55_156.9939m/z	156.9939498	3.552233333	pos
3.55_204.9666m/z	204.9665966	3.552233333	pos
3.55_230.0610n	248.0947994	3.552233333	pos
3.55_403.2323m/z	403.232317	3.552233333	pos
3.55_661.8009m/z	661.8009431	3.552233333	pos
3.55_662.3027m/z	662.3027304	3.552233333	pos
3.57_287.8886m/z	287.8885699	3.568016667	pos
3.57_626.2829m/z	626.2828618	3.568016667	pos
3.57_626.7846m/z	626.7846161	3.568016667	pos
3.58_153.0544m/z	153.0544433	3.582033333	pos
3.58_202.1435m/z	202.143467	3.582033333	pos
3.58_217.9982m/z	217.9981652	3.582033333	pos
3.58_220.1541m/z	220.1540746	3.582033333	pos
3.58_633.8009m/z	633.8009135	3.582033333	pos
3.60_113.9605m/z	113.9604618	3.604716667	pos
3.60_114.5584m/z	114.5583542	3.596	pos
3.60_114.9716m/z	114.9715555	3.596	pos
3.60_142.1106n	125.1072848	3.604716667	pos
3.60_164.9203m/z	164.9202673	3.596	pos
3.60_169.0857m/z	169.0857367	3.596	pos
3.60_169.9974m/z	169.9973838	3.604716667	pos
3.60_185.1214m/z	185.1214086	3.604716667	pos
3.60_230.1860m/z	230.1860041	3.604716667	pos
3.60_243.9774m/z	243.977403	3.604716667	pos
3.60_634.3017m/z	634.3016881	3.596	pos
3.60_726.8325m/z	726.832518	3.596	pos
3.60_727.3336m/z	727.3336016	3.596	pos
3.63_170.9607m/z	170.9606912	3.626683333	pos
3.63_220.0944n	243.0835506	3.626683333	pos
3.63_224.0114m/z	224.0113596	3.626683333	pos
3.63_224.9325m/z	224.9325244	3.626683333	pos
3.63_344.9317m/z	344.9317339	3.626683333	pos
3.63_372.8812m/z	372.8811656	3.626683333	pos
3.65_133.9745m/z	133.9745081	3.648783333	pos
3.65_135.1167m/z	135.1166909	3.648783333	pos
3.65_213.1482m/z	213.1481632	3.648783333	pos
3.65_240.0651m/z	240.065075	3.648783333	pos
3.67_179.5501m/z	179.5500575	3.671416667	pos
3.67_204.1227m/z	204.1227461	3.671416667	pos
3.67_242.0106m/z	242.0105758	3.671416667	pos
3.67_292.9698m/z	292.9697701	3.671416667	pos
3.67_299.0603n	338.0176877	3.671416667	pos
3.67_327.1549m/z	327.1549417	3.671416667	pos
3.69_111.9845m/z	111.9845174	3.6941	pos
3.69_142.9616m/z	142.9616248	3.6941	pos
3.69_142.9666m/z	142.9666314	3.6941	pos
2473.998242	2282.883695	1942.373014	2034.131929	1862.956317	1840.091315	2120.960819	1565.573829	1664.503287
350.656438	227.4288717	205.7492386	442.2721564	340.5915181	313.3921058	315.3763748	262.7596564	213.8438097
3084.278121	2411.729664	2382.46805	2772.502063	2973.679672	2735.4273	2836.530418	2435.652081	2228.089806
4152.471518	3668.37	3476.332064	4780.531	4669.61504	4444.158862	4390.524646	3396.31708	3513.064921
1354.213759	1137.182516	1204.75475	1172.228317	1356.966918	1174.426585	1299.601417	1013.093193	1179.448245
7399.953083	6296.216573	5668.702922	6984.990362	7275.875669	7673.764325	6978.202472	5826.147605	6634.942925
1257.890997	1240.836984	1367.860254	1798.382956	2259.551529	2122.823033	1689.625447	1602.786476	1779.285313
1203.341311	1228.353274	1159.290286	1447.659845	1339.022684	1516.138178	1185.703857	1508.291551	1137.964786
2905.528526	2117.108525	2196.422817	2566.113588	2702.903451	2433.637063	2625.16718	2098.013195	2395.987308
13815.80976	14200.57489	14140.0136	15731.16807	16660.3941	16779.64898	11777.39314	12186.66807	12666.38001
766.8982624	780.0304451	623.8690417	711.6493828	799.4832213	730.1642016	841.065139	770.4078665	806.0771451
1907.031699	1614.68601	1542.061572	1878.855086	1808.478557	1832.432903	1999.487693	1636.413668	1599.238753
1474.695111	1741.365293	1438.552634	846.8078929	985.1431506	948.0319823	792.1156183	916.843026	831.9163186
12.88377306	26.43196339	21.01146609	92.16206179	88.96513696	101.6153148	74.49948213	78.35554981	90.11446229
986.6188508	716.5719334	657.8982858	454.2981653	528.8437293	414.448436	576.2203264	555.3935758	669.3223592
777.4014817	792.7175154	726.8396303	769.2186546	784.6926078	738.041847	889.549243	805.3341574	825.6014125
877.0470841	659.7930582	739.7203011	782.7401212	902.9579537	734.645502	883.4991074	687.7364804	839.5975762
112.4429708	127.5253589	117.4640974	140.897793	168.0346437	187.4954015	79.69583263	104.3110237	182.4113731
738.4973722	507.3747215	437.8269352	518.9362884	451.1312609	503.0151571	413.9939738	533.2762951	563.0543389
1713.635075	1020.962346	703.8836608	995.9525807	1236.386255	950.8940825	1199.46631	897.3650311	847.5374264
2184.151396	1254.926305	1321.178404	1524.620832	1907.49657	1416.908807	1609.917118	1200.448638	1748.711798
79336.81372	66967.35961	63547.1284	25813.69284	27412.12853	28516.79517	31158.99855	31919.86133	31220.88938
138.9277035	88.38226712	89.80332545	124.0670997	139.0015997	112.9492017	198.9317606	138.0884351	143.8043444
1051.632694	848.7080394	950.1967556	445.0178061	354.1616328	469.3841439	567.3619675	724.9092108	738.1225509
84715.19564	66045.09977	67103.25925	34107.21513	33875.62233	35286.4575	54493.3631	53937.74436	54915.52153
849.6579784	807.710968	671.3798871	1365.917473	1430.151539	1428.753733	858.8263846	775.9294757	1116.350427
6216.196308	4901.259503	5004.815727	2374.316146	2465.85683	2444.002776	3982.660251	3979.299804	4037.813264
2048.487619	1891.307348	1803.484586	1481.062766	1905.532169	1572.283029	2079.342271	1704.476783	1720.916179
240.8033804	146.4041497	153.8606348	136.4441014	142.1292954	162.4365283	182.1836792	178.6934963	93.10890805
5460.720068	4447.785686	4419.716168	6987.269791	6794.695055	6704.2432	4363.115709	4056.827667	4434.28327
217.0247649	261.5960741	256.2463197	232.5212336	275.5122886	341.2275362	284.596912	277.5998475	261.990588
141.7805923	79.41337214	96.33838436	110.8882241	77.34492153	105.9372845	58.25201865	112.9021379	83.95058619
3401.929113	3169.520752	2638.859149	2229.701078	2337.991915	2380.988067	2988.144879	2425.776753	2867.004987
3207.609239	2992.493793	3000.620509	2465.843576	2991.991958	2964.870029	3320.895402	2967.819533	3291.839993
538.9097721	412.0450222	443.6277398	557.0307838	517.4589486	401.185991	502.7378225	465.59182	543.0644319
976.6448945	655.6364352	905.3237489	812.7042772	748.3388291	821.7893963	811.5524147	510.848864	717.7667267
3207.758892	2676.107642	2423.927525	2311.264665	2353.262624	2217.298149	3039.869009	2448.84271	2790.637272
3188.873015	4002.756081	3490.920853	3711.028616	4093.03769	4338.04587	4774.702736	3512.422965	4277.583435
1945.858153	1932.104523	1621.723327	1612.004709	1900.547909	2035.002023	2143.924112	1707.822836	1729.064408
249.9308704	349.5462846	422.5971622	0.001403199	0.001403199	62.44198593	5411.981345	5457.097099	5644.802855
1887.051059	2032.899536	2706.429836	2727.61025	3497.690865	3359.39704	4111.815637	2866.286899	3042.763834
6046.64528	5779.043448	5328.099561	5406.750391	5579.580948	5386.703171	6067.558786	5337.968378	5262.936606
1348.293428	1187.32185	1600.18944	1312.14069	1389.917202	1420.219286	1727.552512	1507.406322	1557.075831
873.2339316	903.3777542	832.1198778	796.3076615	868.3460423	1067.386843	1163.193638	939.0744219	1076.84854
1985.246861	1731.98224	2234.324789	85.48990104	110.9623519	66.16382521	1670.463592	1606.206229	1698.870011
1965.110948	2106.272144	2451.400506	2206.626443	3288.878278	2973.790225	3920.89405	2566.387322	3032.310996
342.1925851	1007.762551	972.6690525	402.3293078	717.7833687	952.1954653	0.001403199	138.7902145	178.5069769
167.4216479	700.3023012	708.2902093	767.2530577	699.2790972	566.6990682	0.001403199	165.9425507	297.1581496
252.2151059	717.1705638	410.8000829	194.7808121	271.7997106	530.1254494	0.001403199	159.2505264	0.001403199
467.453288	415.3105453	328.6196562	246.9468488	352.2168209	327.5647981	443.190947	378.7912023	277.9549768
298.9604311	603.4811624	416.652141	422.8906874	419.1840457	306.3958665	581.3324359	458.4050242	462.0060586
707.3510337	810.9871019	783.1081355	567.8564857	569.1256279	663.2079106	922.7044688	755.2564539	787.6423821
872.5349463	962.779627	1080.541926	581.529724	920.2508813	752.7156537	1092.573902	897.7896008	804.7862597
299.7812064	346.1172492	329.9554157	242.6295395	415.39394	257.1793144	411.9869098	328.4539907	142.2744961
332.6296516	396.7043549	386.4988352	230.4481226	376.8162729	317.3170878	316.7265057	469.8719215	345.8266755
1094.903598	865.148823	769.0141939	688.7426599	824.540197	806.7079027	958.0740703	920.4963861	828.3005874
0.001403199	60.2391485	56.94384242	36.35186454	31.10639327	75.21111512	0.001403199	70.8607929	0.001403199
1256.02055	1235.264374	1410.895454	1222.464113	1324.176305	1104.927809	1228.576084	1119.121676	1159.570862
2309.201624	2519.34029	2428.417235	2373.791987	2200.30841	2163.024248	2437.167693	2112.172483	2019.915956
1364.537145	1089.855095	1422.091257	982.9322386	1428.638891	1396.342313	1582.343555	1449.95655	1466.545427
2504.345807	2291.736265	1695.062898	1624.145	1945.497961	2162.695496	2768.995487	2174.847946	2064.200516
33.85520147	35.94008782	64.06766066	27.35351012	0.001403199	30.53756442	0.001403199	30.62493515	0.001403199
811.1063664	916.1874105	719.2716633	923.147994	873.9958874	864.2743206	908.7053401	791.864022	872.9105513
50729.55376	58998.79459	45694.02308	50256.6155	49684.18662	60208.43807	46642.03186	54133.08396	54698.45264
5573.596929	6302.711627	5431.046844	4455.654519	5459.385264	5210.311988	7789.879692	6202.22487	6343.959809
167.864956	608.4729513	370.5788468	2469.959257	2629.251417	3807.473687	433.3124128	665.5342393	631.9806056
205.4727144	0.001403199	340.9205239	1259.1759	1592.150827	2400.651568	257.200157	142.9015961	370.1566347
2092.573281	2040.567593	1387.354006	1399.653652	1489.111718	1686.834547	2118.750423	1890.458878	1726.270341
6372.713863	5663.681216	4160.919046	5163.103824	5980.748701	5899.662738	4871.941911	5125.949717	4951.516471
3375.030562	3697.071836	2473.203671	3972.919114	2984.683767	4866.073981	2697.716324	2920.65344	3314.728211
1669.181537	1758.358758	1187.663308	1184.476272	1172.867969	1330.882108	1931.460033	1785.590697	1618.384652
1205.605629	1292.56329	904.5456579	871.7309238	790.780793	890.890557	1286.817591	1209.869629	1038.597941
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151.7946874	231.8529566	136.0801892	207.0866604	154.3462406	217.1350206	223.7680343	190.1480976	193.196619
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2527.087572	2869.12377	2456.620268	2991.969888	3340.48377	3286.460158	3833.618619	3156.79748	3177.62548
1830.080281	2074.817554	1402.254679	1510.246548	1422.089404	1473.248399	1786.023956	1815.738331	1480.420098
2016.503636	2358.866401	1449.318216	2153.106334	1911.044793	2183.615967	2371.67858	2370.973739	1867.900669
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5618.595432	6659.965671	7553.090365	7437.839102	6188.780833	6452.61179	5655.80476	7320.097217	5960.362418
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2861.441698	2975.22552	2785.443685	2490.664879	2198.037468	2843.796369	2526.106812	3805.721932	2537.451875
1409.372047	999.6668469	1414.182504	1667.321	1393.3427447	1383.60608	1202.892041	2056.206578	1418.567571
793.3544202	788.7747535	551.5283252	682.7727966	687.3704739	802.9502749	898.8262771	914.9945507	632.4174054
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3.69_190.0031m/z	190.0030851	3.6941	pos
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3.69_215.9793m/z	215.9792538	3.6941	pos
3.69_243.1825m/z	243.1825448	3.6941	pos
3.69_243.6843m/z	243.6842565	3.6941	pos
3.69_255.1216n	256.1288272	3.6941	pos
3.69_273.9752m/z	273.9752358	3.6941	pos
3.72_101.0600m/z	101.0600011	3.716333333	pos
3.72_120.0235m/z	120.0235022	3.716333333	pos
3.72_164.0471n	165.0544632	3.716333333	pos
3.72_177.1271m/z	177.1270799	3.716333333	pos
3.72_302.0690m/z	302.0689583	3.716333333	pos
3.72_302.1958m/z	302.1958082	3.716333333	pos
3.72_366.0558n	367.0630521	3.716333333	pos
3.72_399.0003m/z	399.0002623	3.716333333	pos
3.72_474.7403m/z	474.7403459	3.716333333	pos
3.72_475.2417m/z	475.2417215	3.716333333	pos
3.74_113.9605m/z	113.9604774	3.73775	pos
3.74_177.0497m/z	177.049659	3.73775	pos
3.74_241.1042m/z	241.1041596	3.73775	pos
3.74_304.0142n	305.0214319	3.73775	pos
3.74_403.2321m/z	403.232099	3.73775	pos
3.74_465.6448m/z	465.6448288	3.73775	pos
3.74_584.2652m/z	584.2651629	3.73775	pos
3.76_114.0468n	132.0806497	3.759483333	pos
3.76_115.0633m/z	115.0632716	3.759483333	pos
3.76_146.1174m/z	146.1173607	3.759483333	pos
3.76_197.9922m/z	197.9922385	3.759483333	pos
3.76_206.1002m/z	206.1002109	3.759483333	pos
3.76_247.0874n	270.0766209	3.759483333	pos
3.76_294.9928m/z	294.9928419	3.759483333	pos
3.76_296.9897m/z	296.9897282	3.759483333	pos
3.76_373.6018m/z	373.6018401	3.759483333	pos
3.76_374.1033m/z	374.1033066	3.759483333	pos
3.76_416.1155m/z	416.1155481	3.759483333	pos
3.76_474.1721m/z	474.1720965	3.759483333	pos
3.78_122.0317m/z	122.0317448	3.781933333	pos
3.78_157.0757m/z	157.0757416	3.781933333	pos
3.78_194.0784m/z	194.078369	3.781933333	pos
3.78_211.0573m/z	211.0573221	3.781933333	pos
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3.78_242.6653m/z	242.6653435	3.781933333	pos
3.78_326.1318m/z	326.131807	3.781933333	pos
3.78_332.0325m/z	332.0324782	3.781933333	pos
3.78_385.1461m/z	385.1461201	3.781933333	pos
3.80_182.0751m/z	182.0750588	3.80375	pos
3.80_225.0354m/z	225.0353903	3.80375	pos
3.80_229.1043m/z	229.1043055	3.80375	pos
3.80_280.9963m/z	280.9963011	3.80375	pos
3.80_328.0252m/z	328.0252448	3.80375	pos
3.80_347.0612n	348.0684441	3.80375	pos
3.80_361.1024m/z	361.1023623	3.80375	pos
3.80_380.0055m/z	380.0054799	3.80375	pos
3.83_124.0504m/z	124.0504457	3.825583333	pos
3.83_143.0701m/z	143.0701313	3.825583333	pos
3.83_182.0133n	200.0469944	3.825583333	pos
3.83_184.0101n	202.0439436	3.825583333	pos
3.83_201.9641m/z	201.9641206	3.825583333	pos
3.83_222.0981m/z	222.0981382	3.825583333	pos
3.83_243.1199m/z	243.1198665	3.825583333	pos
3.83_243.1825m/z	243.1825089	3.825583333	pos
3.83_243.6842m/z	243.6841597	3.825583333	pos
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3.83_354.1880m/z	354.1880259	3.825583333	pos
3.85_138.0224m/z	138.0223918	3.845583333	pos
3.85_154.0365m/z	154.0364697	3.845583333	pos
3.85_154.0416m/z	154.041564	3.845583333	pos
3.85_157.0420m/z	157.041959	3.845583333	pos
3.85_184.6179m/z	184.6179229	3.845583333	pos
3.85_299.9716m/z	299.9716462	3.845583333	pos
3.85_300.1332n	301.1404322	3.845583333	pos
3.85_311.9977m/z	311.9977144	3.845583333	pos
3.85_321.9534m/z	321.9533827	3.845583333	pos
3.85_340.9980m/z	340.9980428	3.845583333	pos
3.85_379.9852m/z	379.9852029	3.845583333	pos
3.85_465.0324m/z	465.0323954	3.845583333	pos
3.85_467.0291m/z	467.0290791	3.845583333	pos
3.87_133.0283m/z	133.0283034	3.866916667	pos
3.87_219.0601m/z	219.0601096	3.866916667	pos
3.87_220.0943n	243.0835005	3.866916667	pos
3.87_221.6714m/z	221.6713731	3.866916667	pos
3.87_227.0288m/z	227.0287532	3.866916667	pos
3.87_238.1412n	261.1305372	3.866916667	pos
3.87_268.0746m/z	268.074561	3.866916667	pos
3.87_278.0105m/z	278.010538	3.866916667	pos
3.87_316.0787n	339.068104	3.866916667	pos
3.87_334.1754m/z	334.1753871	3.866916667	pos
3.89_138.5544m/z	138.5544392	3.889633333	pos
3.89_146.9611m/z	146.9610742	3.889633333	pos
3.89_155.1056n	156.1129097	3.889633333	pos
3.89_173.1050n	196.0942384	3.889633333	pos
3.89_175.0961m/z	175.096145	3.889633333	pos
3.89_189.0132m/z	189.0131876	3.889633333	pos
3.89_199.0938m/z	199.0937538	3.889633333	pos
3.89_203.9545m/z	203.9544794	3.889633333	pos
3.89_210.9952m/z	210.9951508	3.889633333	pos
3.89_233.0719n	256.0610198	3.889633333	pos
3.89_254.0107m/z	254.0106592	3.889633333	pos
3.89_271.0134m/z	271.0133641	3.889633333	pos
3.89_306.9855m/z	306.9855051	3.889633333	pos
3.89_323.9525m/z	323.9524902	3.889633333	pos
3.89_403.2318m/z	403.2318072	3.889633333	pos
3.89_816.8577m/z	816.8576904	3.889633333	pos
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46.11308539	50.31647542	21.68669023	14.83218647	49.60240723	17.85704768	65.25079553	16.91605663	42.29875116
36.92435981	0.001403199	31.66118503	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	60.45670375
365.3809072	114.0675726	420.6381404	329.1643308	209.7242884	384.7917359	59.24990173	388.1794241	227.6647907
483.6321433	415.3483451	487.100035	620.470641	467.0344712	525.1723419	509.4382726	411.0717311	392.0615389
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809.4102959	927.7866299	714.6169415	1034.265413	812.5162844	872.6443549	963.0335118	933.2762527	753.6266884
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186.7551222	289.7403826	213.1579222	295.1548906	297.8178357	254.6880613	339.2664949	332.2875165	333.1255903
1919.241237	2143.713074	2101.513846	1447.710156	1423.29905	1238.779398	1287.736588	1364.182352	1534.901124
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447.4752318	507.6865032	516.3578419	657.6347862	579.5191807	513.5570481	535.4712042	513.7594836	495.5329858
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489.0685395	388.1003437	339.1959074	336.4417011	320.5183217	333.9282728	412.0844669	289.0203074	331.4642917
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10722.52342	11304.10745	11335.99505	25585.94739	23818.69036	21305.7244	14304.01662	15522.22896	15454.01818
50891.38026	57821.30943	56285.26664	15808.1686	17293.8307	13837.28539	36934.68721	42041.35954	41202.51371
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626.3819077	729.5937026	524.5755716	1262.406137	1217.842999	723.4224579	540.9507153	511.2731857	635.3278134
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5057.023183	5663.985042	5579.204469	5159.783976	4435.960437	4304.911429	3461.053009	4823.051391	4233.940322
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18.70939135	15.16363693	14.34291626	13.07734019	36.06248338	58.79795021	17.08166663	11.69630527	18.34310807
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188.1200852	79.2054675	236.6549348	151.09337	136.446062	152.803377	78.52759576	218.6839447	193.6664917
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1754.445363	1677.644324	1800.653925	2510.822096	2158.16265	1947.62756	1423.519734	1378.494331	1532.119654
4938.346086	4960.460078	5143.247254	504.3732664	499.4748754	373.3513117	2690.943674	2944.51832	2653.437238
593.9682968	225.1904593	792.7388265	294.8364477	276.2900947	695.4350999	103.4863686	454.3396998	591.5047498
1540.633544	855.4754974	1885.661598	1551.297112	2005.575503	1946.319231	779.4403077	1520.752563	1560.063039
1202.830119	263.1455471	1048.661533	0.001403199	0.001403199	70.70286899	0.001403199	610.7969995	582.7778772
2538.94249	2684.555912	2536.197772	1542.972723	1470.655634	1465.529351	2937.654749	4091.637607	4188.375331
25909.95495	27626.89116	30739.49493	30123.03363	28826.46206	27643.14811	30163.20001	33093.01974	31670.69468
3169.533688	2819.880818	3339.339853	3263.342726	3013.539694	3161.479033	3546.948747	4201.445827	3652.793126
3753.736599	2815.736073	2013.331058	2497.827043	484.4946388	1040.778629	1394.20171	1599.384391	1678.705407
2167.31605	2099.5881	2582.407869	2448.81646	2200.502204	2208.358735	2246.487003	2556.786584	2383.66065
1446.435945	1262.405266	1410.481837	2575.394509	1884.385113	1739.089806	1420.672342	2669.063135	2143.729932
81476.66084	87050.03523	92355.53729	7602.450942	8299.993735	7067.953759	75548.93402	88343.42527	81261.51234
541.5651254	814.5055792	584.2925923	96.4346377	205.9788001	295.4381285	188.8063887	238.4968948	315.4586199
1093.768456	168.591741	1523.05433	0.001403199	0.001403199	0.001403199	1014.986045	1889.569928	1238.331684
1521.913577	1744.706287	1981.330644	1965.175653	1968.614103	1690.76398	1805.648632	1935.737485	2002.936719
1533.552301	1493.560818	1516.538702	1136.068924	1143.436766	1111.16304	746.0910537	732.6517743	1139.509077
1951931.291	2088506.236	2151203.767	2293360.31	2458114.895	2260737.632	2467379.618	2334514.016	2417639.383
655112.78	698333.2976	725326.3849	756477.7413	816720.1734	760762.5403	832217.6238	782467.1815	806907.5597
345.4813455	293.2877799	461.7730568	637.0914	609.8381649	690.0784012	180.4234177	752.2368681	593.2905308
648.8772572	680.277814	642.346935	261.6299105	586.5136339	542.4219234	491.0474291	799.2240524	628.7488671
1823.857376	2205.955003	2321.325221	2470.053877	2136.989719	2093.906712	1521.762673	2098.622948	2236.67085
2418.430432	2856.903173	3485.052506	3187.304596	3176.695876	4028.708828	3346.823925	4429.525404	3450.216763
569.0516749	861.7409073	962.3510428	931.8062838	739.5554835	438.3969762	881.7053488	1156.675476	842.3845353
16733.86958	16523.63641	20100.971	22081.96965	21465.31418	19759.98838	21696.24927	25463.82451	23645.28526
5688.985802	6298.778628	6955.751266	7428.594257	5872.469221	7018.731029	5416.009225	7771.87889	6819.031703
587.3665066	617.5486122	678.8803244	630.3663244	831.6881676	559.7853853	810.5697222	728.3111258	619.4623768
68.01840973	319.7360291	551.8047746	0.001403199	44.99685993	19.10166159	915.9892889	695.3606321	163.0209039
460718.5216	504235.3987	525151.2255	559489.1944	592448.758	539972.9707	602869.3953	565886.043	572316.0919
12710.24556	13685.53137	14316.68001	15842.63294	16221.38596	14701.10346	16369.60525	15350.61497	16017.32885
968.8157536	1244.495293	763.1561012	1790.046292	1175.300586	1173.375699	1335.537502	1320.78289	1520.247398
3010.416681	3097.146276	3479.319811	3850.41588	3533.814817	3276.910608	3056.588996	3249.787148	4770.373158
61864.68677	55997.23074	53733.4064	69495.39911	66023.1384	64554.6317	60948.56126	61054.90003	59866.69092
3859.741858	2717.940311	2900.807066	3992.101501	2949.701719	3549.365657	2910.851498	2821.18056	5292.19423
1452.150246	196.9813713	1281.541054	337.7673437	1119.074491	109.9480658	851.3990667	1307.227089	2426.94325
2278.204112	999.6966819	1690.197434	889.2041629	1569.24148	1319.172524	941.9032211	1461.357626	2395.680094
7608.27474	5683.028069	5648.646451	5566.037718	6026.141291	6434.227567	5405.616695	6537.721988	9679.359101
4161.933122	4209.858709	3829.967218	6052.489645	3971.684314	3743.045619	4721.304905	4241.287537	10167.72054
2037.682654	1732.1253	2187.545879	785.8996051	3749.002527	1892.395612	885.3002951	3384.380574	5146.849744
49.50272009	59.68500176	23.51205987	70.66331253	51.42446159	103.2132536	63.97181368	67.23905373	115.8215539
742.315272	729.8300402	775.0566232	967.6995928	869.2513867	922.7504079	736.9496068	1365.538392	1194.839199
5167.596275	5552.896889	5824.036615	6469.152774	5714.909536	5665.350233	3836.704417	5447.475714	5014.163127
0.001403199	50.26831876	101.9588921	161.3635002	27.64221394	79.84042976	105.9238181	72.77478068	74.94661376
6231.72135	6631.343321	6412.210705	2149.928601	2085.554266	1962.66413	6181.941854	7108.248815	6765.370646
44369.18	45913.10297	34538.92856	60658.5547	29107.02301	27939.69021	34426.77403	38040.0912	32799.54785
807.7125578	1031.179587	1128.007814	594.6208547	560.3008889	412.9348157	790.6593921	646.103348	796.4948142
1851.907222	1610.391054	1950.165052	626.0398753	610.2872542	594.5196038	2119.731889	2237.281828	2138.044822
3900.235713	3473.064979	4725.021337	1613.308384	1671.948903	897.340756	2283.093961	2187.454984	2830.309918
1328.705241	534.2394211	1229.247239	362.4759572	643.6152153	615.2628884	1195.420529	1733.351707	2018.34821
41.9205633	16.79506162	13.11258955	31.66146887	27.98428739	15.16660862	15.72793103	29.0961256	12.75322046
1086.690463	1021.403959	1089.341507	1030.852327	1066.555864	1116.24403	1125.194801	1112.907539	1168.214675
262.9161724	273.6496384	213.2261018	240.2327584	137.6772376	217.7117063	182.7126275	305.0122373	170.0497783
7449.771023	7625.417545	7564.390413	1581.707829	1588.235226	1693.888313	4125.527386	4679.551154	3964.185426
333.0301506	284.8029589	297.8053532	280.0994414	335.9369458	260.5546358	293.9173501	308.3559136	350.8918132
1832.175709	1687.700605	1852.660122	2381.864434	2024.85917	1940.122906	1582.832259	1844.984134	1942.001857
3542.043107	3019.142434	2872.752283	3491.443613	3698.078775	3198.186322	2682.44384	2673.650517	2857.186697
208.7567729	259.8005031	144.609563	284.2891594	184.9281335	328.7974676	279.6115248	230.7941519	339.9874182
987.8735534	297.845327	930.3491956	510.9101015	883.7657697	847.976627	734.6708697	788.1652602	847.6485231
1914.410445	1657.960357	2267.16763	4557.302626	4695.441651	4430.537873	5856.912991	6760.679559	6577.026569
6270.899656	6052.323529	6510.220099	8842.424052	8589.484866	8186.931651	7538.964984	8428.175422	8088.378475
543.5386838	530.7312346	661.0624712	716.4354922	727.1796472	796.634084	675.4212671	803.1241073	668.1402221
4067.083634	4187.978695	4291.174332	3201.221122	3653.821661	3136.126549	3368.267862	3414.908691	3396.158384
410.7340783	340.1490316	685.2763781	682.2887695	575.901961	454.1042847	351.3229514	895.6033016	1048.629144
2265.395901	2425.44649	2399.671314	2076.93483	2184.726232	2194.934867	2327.741975	2443.312528	2829.945481
1714.549895	1895.199979	2146.458235	1586.242884	2994.727104	3016.14791	1457.235981	2151.260058	2234.48901
1159.558845	1279.713023	1693.547521	1090.809154	941.5150986	1475.137405	843.7092954	980.887558	577.7146629

3.91_131.9669m/z	131.9669394	3.911966667	pos	23.44114497	11.77755068	19.51814625	59.17414349	28.85278061	16.87025147	48.37230766	49.98479891	41.79585925		
3.91_139.9821m/z	139.9820553	3.911966667	pos	2565.196152	2366.116876	2485.772026	2157.241246	2527.64574	2561.334733	2601.328808	2413.850807	2556.318801		
3.91_144.0370m/z	144.0370141	3.911966667	pos	0.001403199	33.31996032	26.24732129	15.81950792	32.57136002	0.001403199	0.001403199	32.17513037	26.47713441		
3.91_157.0970m/z	157.0970308	3.911966667	pos	107.039124	93.72740139	57.42612117	84.23928984	124.6495159	34.29988608	80.64495727	84.39912033	168.940558		
3.91_159.9619m/z	159.9619076	3.911966667	pos	33.27981724	21.00932062	111.7841227	67.62882585	166.6326576	220.2695924	56.42965503	79.29942799	76.19494989		
3.91_188.0917m/z	188.0916569	3.911966667	pos	6570.626016	6114.902427	6562.644238	6868.281171	6745.511159	6859.934983	6745.555543	6238.678708	6420.497615		
3.91_194.0786m/z	194.0785663	3.911966667	pos	1593.417213	1172.091907	1275.818029	979.3295852	1319.964441	1165.781607	1391.917162	1358.310474	1367.897609		
3.91_195.1377m/z	195.1376918	3.911966667	pos	801.9118193	833.0571864	655.2530825	803.2490501	743.5241765	664.6168063	959.8261648	810.6769908	665.3802928		
3.91_203.1429m/z	203.1428827	3.911966667	pos	1025.140478	856.9113509	980.1512401	844.9905031	829.7404647	708.1682335	901.8244495	823.5608071	696.7134829		
3.91_218.0844m/z	218.084398	3.911966667	pos	194.605395	235.1098305	268.6430631	1623.587283	1524.836993	1442.467706	1532.302693	1748.761638	1794.278491		
3.91_239.0886m/z	239.0886183	3.911966667	pos	3445.133001	3951.391875	3926.144106	2809.094873	2465.278498	2357.633437	3635.774645	3896.217709	3809.719921		
3.91_260.0867m/z	260.0867381	3.911966667	pos	526.0279856	629.2717334	775.836279	407.9164513	473.0358771	320.0612649	410.6331113	649.34693	576.6459844		
3.91_262.0033m/z	262.0032933	3.911966667	pos	2204.63178	2366.356704	2361.72023	9.998986232	43.73305783	93.79344224	1936.730264	2112.922196	1797.519298		
3.91_302.0635n	303.0708221	3.911966667	pos	11119.33245	11216.40132	12036.73506	517.3539695	568.0793817	452.7439439	9545.399072	10491.57116	9745.415813		
3.91_344.9317m/z	344.9316791	3.911966667	pos	2448.966907	2256.460191	2932.074753	252.1041486	274.3045421	206.9074193	1874.002202	1926.835214	2070.008734		
3.91_346.0272n	347.0345264	3.911966667	pos	15347.19049	15564.05891	16650.27661	1590.225546	2018.4613	2176.648014	13781.98976	15221.27848	14655.03177		
3.91_398.0165m/z	398.0164519	3.911966667	pos	11451.14926	11943.77822	13128.44336	311.6765516	404.3428292	266.3784905	9610.687918	10719.5609	9580.682208		
3.93_132.1018m/z	132.1017923	3.9343	pos	2702.358641	2459.739292	2208.765772	1845.724219	2107.720415	2125.244575	2363.59412	2237.641863	2318.070905		
3.93_152.0422m/z	152.0422262	3.9343	pos	210.2779634	205.8293563	229.9127585	40.48888154	23.70491263	34.19425885	93.44756516	154.6476645	136.3486082		
3.93_180.0990m/z	180.0989768	3.9343	pos	315.2605221	318.8186345	328.0644739	169.6086469	175.0078772	275.5255388	306.7355342	334.9226655	280.4481376		
3.93_184.1022m/z	184.1021942	3.9343	pos	255.1334032	139.4994924	198.506546	72.81971048	99.75821589	135.0854219	151.8463718	170.7957009	89.38594462		
3.93_203.1519n	204.159238	3.9343	pos	2904.733159	3242.887581	3520.719312	3180.477723	3032.310243	2899.212373	3099.888548	3368.828906	3236.887775		
3.93_224.0113m/z	224.011323	3.9343	pos	7666.84085	6585.680419	6128.92024	6887.971001	7055.030117	7026.44545	6626.411678	6424.897474	7182.361949		
3.93_255.0585m/z	255.0584825	3.9343	pos	1200.980095	1053.487932	1016.501754	977.7594855	1048.073405	886.6631654	1400.938167	958.0750656	1090.574297		
3.93_284.1297m/z	284.1297318	3.9343	pos	359.3011089	323.3077265	451.1141381	500.4838409	358.8135067	360.5302114	419.3997145	516.1203113	480.5605092		
3.93_290.6768m/z	290.676797	3.9343	pos	2530.260162	2787.181202	3271.627897	2645.830051	2813.916657	2661.258151	2430.516451	2938.809636	2585.895788		
3.93_291.1786m/z	291.1785976	3.9343	pos	830.7934946	1000.308207	980.7707999	682.7531062	989.6200135	957.3378524	809.2603724	876.1740723	826.2499905		
3.93_378.0758m/z	378.075755	3.9343	pos	265.3421564	266.5763635	219.4792985	238.5583437	161.1801652	234.6105526	269.2790533	235.0818798	221.6265115		
3.96_104.0709m/z	104.0708513	3.956866667	pos	281.4375235	219.714673	228.079514	190.2367791	213.7720149	216.1450031	259.9201354	239.9476616	193.4103945		
3.96_114.9716m/z	114.9716343	3.956866667	pos	137.257103	146.1727246	122.475316	142.2051011	162.3580656	123.1284619	176.7602867	184.2248678	158.113606		
3.96_138.9951m/z	138.9951386	3.956866667	pos	1846.793584	1758.576111	1641.968448	1742.405842	1805.028526	1576.801419	1924.671443	1609.597653	2075.412581		
3.96_147.0439m/z	147.043914	3.956866667	pos	849.6880761	832.420045	757.8478961	573.3723536	538.7275437	528.485622	673.2121278	711.2183332	664.8394255		
3.96_178.9904m/z	178.9904479	3.956866667	pos	604.5247995	624.8652451	535.9772486	588.8600701	634.3365931	608.9108366	626.9565188	611.9911531	645.7805924		
3.96_232.0321n	233.039378	3.956866667	pos	3850.544313	3870.675955	3604.686156	7623.251082	7512.926472	8059.613183	4439.105238	4664.478578	4481.445544		
3.96_236.1621n	254.1958862	3.956866667	pos	10946.67587	9837.387108	5597.001194	9283.94229	3843.358859	4914.431687	7777.476858	7427.028806	5919.2606		
3.96_279.6859m/z	279.685892	3.956866667	pos	5396.659001	5754.81355	5931.173637	6372.44439	6120.755067	5681.178957	5045.909695	6376.754507	5433.133276		
3.96_284.0214m/z	284.0213698	3.956866667	pos	916.3733933	1072.869258	1107.044706	1780.831151	1755.545212	2023.420941	1109.037479	1224.610357	1193.642856		
3.96_319.8812m/z	319.8811755	3.956866667	pos	1065.230407	1245.033405	1171.439501	1509.642344	1502.783888	1215.706966	1360.553078	1196.039688	1227.053822		
3.96_324.1914m/z	324.1914254	3.956866667	pos	1036.786324	817.5972314	1098.247649	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199		
3.98_110.0171m/z	110.0171247	3.979183333	pos	9.838068609	71.77139062	14.75575553	11.93980506	5.613023181	6.903460624	69.3451496	7.682695389	5.636044441		
3.98_216.0865m/z	216.0864622	3.979183333	pos	209.6768477	192.5450171	176.7652904	143.2410116	182.1086071	182.39669	163.8508906	217.6160959	156.8906271		
3.98_247.0876n	248.0948474	3.979183333	pos	604.9696494	722.6225831	689.7322674	4728.080733	4450.223434	4341.732053	5174.62229	6152.955025	5422.310431		
3.98_286.9570m/z	286.9569804	3.979183333	pos	1549.85348	1848.658881	1533.985207	393.7305551	260.0744447	357.8049171	1501.36814	1621.890534	1360.532708		
3.98_310.9779m/z	310.9779003	3.979183333	pos	4640.595765	5061.640111	4561.231246	1343.386497	1484.453869	1375.276316	3701.989745	4621.504051	4545.784846		
3.98_332.1813m/z	332.1812922	3.979183333	pos	2284.679221	2545.861347	2383.193635	2688.611116	2524.768718	2302.571828	1780.808575	2260.162392	2103.619454		
3.98_344.2064m/z	344.2063679	3.979183333	pos	5088.774595	5508.135746	5673.090934	10001.61938	10103.11476	10291.99637	6550.263435	7199.640552	6922.485062		
3.98_392.2153n	393.2225766	3.979183333	pos	12731.23671	13397.11359	13771.0568	16696.75065	15919.07761	16238.73941	15771.08088	17596.99715	16357.15603		
3.98_395.2279m/z	395.2279455	3.979183333	pos	111.600871	146.3222624	310.0495054	197.2150156	164.542745	265.0758705	271.1388249	338.9763891	280.6646157		
4.00_116.0529m/z	116.0528702	4.002016667	pos	383.3538212	443.1017403	462.7745101	499.498634	535.4170487	472.232833	485.9696063	540.0988391	440.9203088		
4.00_153.9979m/z	153.9978798	4.002016667	pos	1344.822844	1507.863601	1371.79221	1364.429487	1609.634495	1504.816762	1436.913094	1425.511356	1455.247637		
4.00_169.9654m/z	169.9654041	4.002016667	pos	338.1620173	159.1592136	196.9725733	81.0583797	255.9473606	402.0243741	498.6156524	382.9264565	303.2126968		
4.00_178.9706m/z	178.9705798	4.002016667	pos	1706.416685	1654.131927	1416.62227	1551.352373	1717.937545	1386.693047	1470.208949	1284.933833	1684.159399		
4.00_190.0895m/z	190.0895393	4.002016667	pos	45.69775038	31.40437446	21.63559672	44.0881817	23.36148904	87.48689273	60.17246291	60.31019402	50.22481753		
4.00_197.1170m/z	197.1169913	4.002016667	pos	1016.640235	864.9676175	883.6125795	825.3743226	817.8698873	779.9191551	941.87575	893.2586734	991.9458501		
4.00_204.0606m/z	204.0606328	4.002016667	pos	2048.870398	2272.963425	2130.94449	2941.588362	2661.126032	2694.893334	3080.419282	3116.39693	3078.641221		
4.00_229.0865m/z	229.0864674	4.002016667	pos	247.8691968	205.0334431	308.8692485	142.2473274	259.1805656	289.6314062	289.1407395	450.2851078	575.5235116		
4.00_249.0668n	272.0559786	4.002016667	pos	53808.28079	56500.62414	58739.86823	35814.87	32131.69342	32274.59113	36806.12349	39543.01547	38358.382		
4.00_293.0306n	294.0378698	4.002016667	pos	5638.793259	5713.626183	6135.004082	4288.170767	3555.456724	3552.093826	4396.774947	4263.669283	3960.756377		
4.00_303.9935m/z	303.9934985	4.002016667	pos	1010.519533	972.760767	1045.696834	610.301137	638.8170613	543.716247	701.080404	748.7527999	588.8635994		
4.00_443.1648m/z	443.1648202	4.002016667	pos	1879.616009	1681.169228	2036.807168	2573.013759	2231.808425	1678.921777	1749.760745	2128.370398	1600.422636		
4.00_443.6662m/z	443.6662323	4.002016667	pos	658.0831992	569.5389207	544.6615689	981.6631781	638.7829706	725.7563598	674.0165395	716.0740585	750.8955486		
4.00_762.8681m/z	762.8680558	4.002016667	pos	366.2385714	599.0004691	995.0438739	1138.259291	860.2609528	1137.004538	1171.71588	880.0830012	666.8301573		
4.00_763.3698m/z	763.369837	4.002016667	pos	200.8802519	331.9521026	507.5663131	963.2953514	749.2463192	893.1103596	211.8697456	456.2797612	269.7330194		
4.00_773.8605m/z	773.8604882	4.002016667	pos	398.148406	613.1056845	715.985283	1592.654538	240.1951651	1498.656673	465.5776055	0.001403199	220.071981		
4.02_114.5584m/z	114.5584161	4.024633333	pos	242.8051497	230.0223633	223.2723828	216.7831556	257.8501137	186.7358379	270.9933952	219.9175182	279.4221737		
4.02_116.9720m/z	116.9719961	4.024633333	pos	274.4822431	191.3327346	220.6679859	265.3782201	254.8790308	277.0975895	230.4598901	290.7928901	233.1910787		
4.02_119.5229m/z	119.5229118	4.024633333	pos	114.7784836	186.3652461	185.8064559	315.784286	315.807093	338.4474628	229.3161448	237.2842245	337.8527048		
4.02_175.0340m/z	175.0340097	4.024633333	pos	1491.821504	1588.183811	1545.640872	2653.169165	2524.662058	2254.091301	2113.306392	2161.595558	2131.530982		
4.02_175.0962m/z	175.0962311	4.024633333	pos	127.0664558	147.188863	195.8133422	192.8968537	158.4459943	223.6127259	172.4608714	143.7775989	100.1728208		
4.02_198.1366n	199.1438725	4.024633333	pos	1667.485029	1458.230284	1780.784491	1902.515927	2152.948457	2047.156201	1579.323968	1756.947871	1877.040314		
4.02_202.1127m/z	202.1127394	4.024633333	pos	2023.908682	1736.995101	1282.740972	1712.712687	1809.246892	1592.839979	2119.866839	1361.682387	1890.39344		
4.02_222.0983m/z	222.0982988	4.024633333	pos	1822.097912	1647.581536	1837.070829	1819.570712	1663.197182	1736.314291	1919.314602	1893.020668	2309.549016		
4.02_243.9965m/z	243.9965417	4.024633333	pos	1620.508891	1585.910783	1911.669067	1818.74951	2027.33626	1932.355259	2150.124451	1912.312831	1964.418134		
4.02_312.0509m/z	312.0508973	4.024633333	pos	1416.577112	1339.819946	1479.015302	625.2391335	557.8635616	501.4294596	485.0846542	770.995752	493.4464937		
4.02_316.0827m/z	316.0827191	4.024633333	pos	226.0359687	116.2237243	219.835643	260.7420588	228.3459176	331.9882785	191.2183585	142.7042732	293.2114588		
4.02_354.1894m/z	354.1893838	4.024633333	pos	786.1259216	1060.672608	867.8627194	716.2565322	581.8421135	849.8591278	932.3100815	1138.048683	1216.079991		
4.02_364.0891m/z	364.0890945	4.024633333	pos	161.7310024	117.9803386	106.1475318	297.3100812	144.4120303	216.5485045	190.1987167	66.88873291	215.6378708		
4.02_384.0662m/z	384.0662166	4.024633333	pos	1303.172596	1578.156356	1380.529331	1764.576878	1798.935453	1899.238319	1437.006436	1711.872934	1768.979875		
4.05_165.0544m/z	165.0544316	4.046633333	pos	2141.426163	1745.632381	2087.390007	1389.385729	1561.409274	1584.629422	1797.539474	1802.453051	1670.765888		
4.05_169.9974m/z	169.9974138	4.046633333	pos	1506.790559	1506.986981	1528.343629	1390.58207	1464.689485	1439.026659	1530.71409	1503.85232	1887.148536		
4.05_185.0807m/z	185.0806508	4.046633333	pos	2187.78307	1999.265993	2020.894715	1821.690563	1905.926784	2196.532867	1974.413072	2067.93997	2073.28722		
4.05_201.1095m/z	201.1094637	4.046633333	pos	36141.12463	26402.57586	25080.02964	26169.4299	31335.89465	29516.79467	33551.75447	26394.07374	29381.85726		
4.05_201.1482m/z	201.1481888	4.046633333	pos	556.2258624	425.8476492	456.1983678	503.1096271	474.4482731	473.8924152	469.8049727	625.0166007	552.6845223		
4.05_207.0319n	245.9944322	4.046633333	pos	2437.381493	2580.184636	2366.795456	2706.940644	2606.361864	2517.924269	3053.089199	2689.020352	2921.088816		
4.05_217.9983m/z	217.9982943	4.046633333	pos	554.7029483	542.9191547	455.3530005	509.6195433	496.6988511	486.4778025	547.6853267	574.5359442	664.769227		
4.05_224.0680m/z	224.0679977	4.046633333	pos	1927.208907	2041.480778	1675.057353	1835.560029	1946.245197	2085.538255	2216.752145	1852.072553	2080.677608		
4.05_225.0245m/z	225.0244639	4.046633333	pos	2632.257154	2679.436493	2680.260904	4528.155857	4369.574861	4229.29094	3095.067332	3356.171399	3251.937928		
4.05_262.1105m/z	262.1105357	4.046633333	pos	2295.26878	2572.065032	2552.693398	3555.212041	3123.842862	3074.055279	2174.166006	2598.005552	2549.256797		
4.05_278.0065m/z	278.0065362	4.046633333	pos	77.86075549	66.49402458	104.1712973	175.0302713	167.1673259	153.5829383	37.65288587	71.59289932	115.2135002		
4.05_507.6862m/z	507.6861506	4.046633333	pos	1770.361269	1318.784016	1814.394342	2206.760998	2125.611795	1998.151274	1356.221057	1479.427366	1733.472953		
4.05_508.1876m/z	508.1876406	4.046633333	pos	866.8432002	743.3551476	905.3372318	1124.013686	784.1562379	791.4662041	397.4396213	837.6602592	964.7922443		
4.07_190.0711m/z	190.0711094	4.069116667	pos	133.8755619	130.7103824	81.67404406	84.91277634	134.4120505	109.3254113	200.0753594	120.8489324	222.6307202		
4.07_190.4784m/z	190.4783794	4.069116667	pos	3731.811235	2975.53186	2925.428672	3089.627773	3059.976901	3311.579599	3242.699519	3035.168788	3272.10994		
4.07_191.1066m/z	191.1066149	4.069116667	pos	950.5836457	830.1980666	826.2604405	1022.536561	1098.89894	1185.143878	961.7799147	1004.553239	1068.495752		
4.07_210.0888m/z	210.088825	4.069116667	pos	20.30629591	0.001403199	0.001403199	0.001403199	181.64364	82.86223891	22.40717772	33.0570032	76.44649298		
4.07_213.9826m/z	213.9826231	4.069116667	pos	11948.99142	9642.196098	9623.662595	9272.249792	9196.956473	9333.686156	10327.927	9328.867512	10195.10547		
4.07_215.0889m/z	215.0889203	4.069116667	pos	4134.06641	2998.103064	3475.9266	2942.838491	3321.323283	3698.836306	3433.329231	2816.106488	3548.906902		
4.07_234.1334m/z	234.1333684	4.069116667	pos	1088.822621	1241.102187	1072.091929	1159.160569	1192.891678	1097.967495	910.3565027	1065.159186	1184.536466		
4.07_253.1429m/z	253.1428794	4.069116667	pos	365.3803787	413.6176528	349.9019784	388.78079	283.294852	396.0994023	323.5936924	303.2800127	374.7339653		
4.07_293.6922m/z	293.6922368	4.069116667	pos	530.3392572	768.3197417	900.4943987	693.8467184	563.8608055	738.8292119	726.8198744	711.2864747	881.0055429		
4.07_312.1316n	330.165432	4.069116667	pos	3793.693718	4474.987139	4538.670699	5670.168368	5358.221074	5070.204222	3405.463923	3945.08217	4136.880329		
4.07_318.2020m/z	318.2020081	4.069116667	pos	1974.498646	1724.234197	2098.8519	1019.59411	1024 3.35188	10728.23369	2284.729798	2623.203859	2463.576724		
4.07_379.1365m/z	379.1364947	4.069116667	pos	303.0025905	365.6466456	313.9633141	342.2071362	498.2939412	455.5525477	308.7755868	351.0901816	295.5989138		
4.07_928.4106m/z	928.4106413	4.069116667	pos	358.312763	1242.646937	1118.813258	1439.102976	1135.0889	1788.475865	0.001403199	264.0463867	0.001403199		
4.09_147.1166m/z	147.1165825	4.091916667	pos	432.6552725	387.62339	371.6831204	375.4773811	379.0704259	382.2894889	381.2901665	309.796976	426.1388911		
4.09_159.9643m/z	159.9642862	4.091916667	pos	639.46728	615.5917416	691.8608539	709.5113294	862.9553613	720.5017926	744.6497208	517.2910568	774.935219		
4.09_225.0865m/z	225.0865056	4.091916667	pos	84.80742671	142.3847559	166.4109132	117.228988	88.12768701	131.9675931	58.96881338	82.11239052	175.8707766		

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4.34_190.0565m/z	190.0565376	4.33965	pos	0.001403199	39.56445143	0.785516868	125.1289246	150.5046465	167.6301799	85.31372011	36.28653622	40.04683127
4.34_216.1592m/z	216.1591847	4.33965	pos	402.0784336	459.9144789	388.4572033	276.1120031	216.1414385	272.6687988	330.974053	273.1350031	387.6582034
4.34_225.0080m/z	225.0079639	4.33965	pos	51.61051056	95.27888507	188.3843026	137.0332367	106.0224862	77.27523788	146.3502517	75.99013901	108.5727799
4.34_225.1230m/z	225.1230428	4.33965	pos	1383.006767	1491.044765	1347.986357	844.0397374	812.0101729	890.402272	852.4636684	782.0968709	922.811241
4.34_227.0886m/z	227.0885774	4.33965	pos	712.0225975	795.1535375	785.7594042	635.3224272	578.9812873	758.1205377	504.2725059	566.9749585	657.3900727
4.34_234.9923m/z	234.9923499	4.33965	pos	401.6430767	869.7569558	974.5790343	951.2054399	823.6003893	683.408539	745.6006261	911.1471154	836.7635888
4.34_287.1728n	288.1801084	4.33965	pos	2436.099968	3321.376619	3775.069388	2276.931931	1752.632809	1666.838034	2272.519124	2843.504102	2515.625556
4.34_332.9928m/z	332.9928046	4.33965	pos	2231.557764	2151.850366	2419.228168	2587.356002	2602.587967	2925.155673	2217.227692	2774.568543	2428.708532
4.34_382.1185m/z	382.1184624	4.33965	pos	262.0820895	194.1097399	387.4911986	191.6141395	63.32204314	81.64081945	270.6420298	307.6457329	276.7168332
4.34_392.0713n	393.078543	4.33965	pos	36410.64315	39100.96495	40672.76066	11013.91986	10985.2249	11744.40271	28982.04051	33479.93893	31944.99261
4.34_466.0424m/z	466.0424306	4.33965	pos	773.2473276	2400.9362	2404.52381	596.776884	614.3066627	190.0806666	1718.259178	1761.732552	1720.534887
4.36_140.9510m/z	140.9510333	4.3623	pos	269.0667482	256.4808176	308.6825152	368.3824565	307.6432138	304.900412	271.5261226	289.8865746	268.3301673
4.36_178.9705m/z	178.970512	4.3623	pos	258.4255554	161.8314564	254.9186831	330.5222879	254.5967998	218.160807	301.1982605	194.2647657	222.8132837
4.36_244.1284n	245.1356366	4.3623	pos	125369.3378	121981.2621	83832.59591	111413.3744	62734.04844	57333.16524	101312.9556	88731.92915	70928.89924
4.36_247.0916m/z	247.0916082	4.3623	pos	364.6364246	324.3681342	434.1468865	461.3170168	300.1803525	411.340664	253.1160469	280.9223149	348.5233571
4.36_251.0843m/z	251.0842667	4.3623	pos	163.7082099	969.4102254	899.1694119	1041.433087	987.7134262	350.8263346	702.1839705	817.5018679	675.072244
4.36_268.2114m/z	268.2113814	4.3623	pos	4590.124197	3287.933432	2420.888479	4147.325847	2525.73679	2215.957776	3028.459243	2968.700198	2416.92261
4.36_276.1261m/z	276.1260575	4.3623	pos	7900.683485	8039.468134	9016.946891	12601.25511	11109.9163	11478.50123	7483.184461	8816.859614	9093.024972
4.36_300.1981m/z	300.1981297	4.3623	pos	1793.178585	3389.848123	2918.439144	2855.049928	2766.707942	2309.211497	2617.227864	3064.31907	2372.81767
4.36_300.7003m/z	300.700263	4.3623	pos	193.1897955	424.0523847	402.7434733	366.9052503	211.7302781	319.8109203	265.6065383	201.2785919	436.7287454
4.36_330.1906m/z	330.1906421	4.3623	pos	13562.37462	14502.696	16128.19937	21719.75721	19581.52169	19475.75502	14329.22653	17925.81066	16508.34972
4.36_387.1621m/z	387.1620511	4.3623	pos	3282.529759	3871.822188	4015.275155	3813.096234	3072.212312	3460.511253	2668.74835	3694.420536	3528.027262
4.36_415.0064m/z	415.0064496	4.3623	pos	3776.89213	3451.524515	3872.384729	1828.688949	1328.359857	1780.470767	2194.884045	2173.373096	2554.249686
4.38_160.0221m/z	160.022053	4.384366667	pos	484.7877186	653.9320273	795.1627266	680.80965	738.1093536	600.0391366	926.3804896	1048.66844	892.0179739
4.38_180.5354m/z	180.5353506	4.384366667	pos	9608.618374	10211.28995	10266.04317	7994.800747	7504.312359	8018.022026	10688.98223	10363.7086	10044.60743
4.38_181.5544m/z	181.5544389	4.384366667	pos	1643.754671	1738.880799	1570.846881	1388.866179	1393.858449	1120.192024	1992.338114	2073.957619	1854.81366
4.38_193.5643m/z	193.5642726	4.384366667	pos	572.7294956	358.7863861	319.4845372	383.2037706	299.3953245	192.1966551	358.3139199	454.0228551	500.0976064
4.38_201.0486m/z	201.0486484	4.384366667	pos	7272.545673	7438.061368	7905.672179	5129.484608	4530.892283	5112.494506	6412.104704	6602.163025	6874.00632
4.38_201.5503m/z	201.5503123	4.384366667	pos	561.0341917	322.9093729	580.0102236	398.6282737	426.2928306	383.9832438	644.2089104	585.9548492	412.8951937
4.38_259.1150m/z	259.1149761	4.384366667	pos	3682.992297	3727.654666	2812.555424	4435.439987	1514.905638	1635.859454	2049.138722	2358.886369	2054.999515
4.38_284.5931m/z	284.5930598	4.384366667	pos	1035.806861	1330.718999	1267.970549	770.7523727	426.825424	713.401905	1291.23595	1387.994093	1553.093759
4.38_336.0398m/z	336.03981	4.384366667	pos	7344.898988	7273.363009	6971.097702	5792.305786	4959.95941	5510.80897	7955.428053	9089.976607	7893.172256
4.38_364.0344m/z	364.0344393	4.384366667	pos	13570.69858	14938.42454	13963.82551	10696.47405	9653.143803	10484.60333	15372.42549	15050.21481	15848.48017
4.38_377.0667n	360.0634382	4.384366667	pos	30256.7263	31400.04384	30807.02899	28411.65652	25830.74499	25809.22244	27720.18508	29966.7592	29767.36018
4.38_383.1307m/z	383.1306626	4.384366667	pos	4386.075533	4928.968415	4564.084716	2821.28773	2775.665712	2749.298397	4973.173273	4436.127187	4706.530125
4.38_387.0241m/z	387.0240666	4.384366667	pos	2833.667308	1847.630086	2407.503371	2899.976398	2809.439149	2297.22143	2581.269249	2693.250565	3278.161009
4.38_407.0170n	408.0243044	4.384366667	pos	11193.66843	10574.16859	10966.44267	9746.55356	9624.343002	9252.854857	10949.96826	12805.82763	12275.75378
4.38_437.0120m/z	437.0120071	4.384366667	pos	6061.429779	4357.064176	4732.659996	0.001403199	0.001403199	90.25589207	2744.158221	3440.347903	3410.546837
4.38_663.1612m/z	663.1611539	4.384366667	pos	2038.091452	4941.156087	3895.445302	3762.324177	3224.296737	4079.16309	6180.57847	6711.300812	4243.651511
4.38_738.2196m/z	738.2195809	4.384366667	pos	1883.101002	3184.662378	1995.367798	667.8823917	986.509759	1004.512225	3416.520033	5797.653315	3778.886278
4.38_738.7205m/z	738.7205345	4.384366667	pos	1361.744447	1191.970672	405.2165463	594.4934169	740.7521524	377.2571217	1993.034581	3581.180908	1875.414014
4.38_838.7390m/z	838.7389761	4.384366667	pos	2937.613053	702.5555954	2426.728288	598.0341177	0.001403199	0.001403199	2920.01853	800.335144	3587.316989
4.38_881.2660m/z	881.2659987	4.384366667	pos	8875.226302	12670.69885	11940.87824	4568.290247	3616.147438	5114.25369	12256.11737	23038.36238	15779.45727
4.41_129.0909m/z	129.0909181	4.4062	pos	1597.220618	1532.228491	1358.974353	1723.413597	1291.295535	1368.581321	1580.200222	1468.417353	1403.130497
4.41_139.9820m/z	139.981989	4.4062	pos	433.9858116	291.1191495	316.6249705	478.9923136	396.9428926	389.1138034	268.4254303	296.670461	318.7499844
4.41_172.5491m/z	172.5490577	4.4062	pos	399.4309626	500.3348664	579.6335936	566.1418682	442.882936	404.5389147	458.1355459	526.7406285	614.1300226
4.41_173.0499n	196.0391298	4.4062	pos	3033.616223	2876.008697	3401.442284	1461.737701	1628.802967	1528.207605	2291.32402	2454.148797	2454.486065
4.41_184.0725m/z	184.072535	4.4062	pos	151.4997314	416.8418583	245.7688489	78.18039718	228.2930193	86.66145677	255.3779303	395.259716	224.7933851
4.41_209.1533m/z	209.1533095	4.4062	pos	2104.592252	2100.123729	1578.149425	1581.967648	1385.839261	1095.931425	1605.83408	1493.75336	1409.405844
4.41_239.0886m/z	239.0885838	4.4062	pos	2802.301961	2953.688267	2958.680155	4684.743067	3677.536933	4355.849181	2826.354289	3265.081156	2614.077286
4.41_241.5649m/z	241.5648915	4.4062	pos	1638.098049	1778.26563	1583.720252	477.2555779	656.863992	688.6209081	1325.131127	1578.720467	1466.728778
4.41_242.0665m/z	242.0665368	4.4062	pos	170.6474298	363.3827546	392.1062904	195.4507289	181.0765825	194.1787989	282.4971426	233.4348488	334.4133955
4.41_265.2422m/z	265.2422352	4.4062	pos	132.6512681	603.6197918	959.0069152	643.3891053	459.8115896	106.7028169	327.7551368	490.1482574	514.5664537
4.41_271.1255m/z	271.1255336	4.4062	pos	148.692846	1445.664189	1149.553863	863.4681482	757.1002052	488.4790449	1235.315315	1138.124557	911.9703716
4.41_276.1027m/z	276.1027374	4.4062	pos	293.8562834	668.2007643	583.5106829	289.1400998	345.9498987	228.0942776	704.9483709	572.0081707	675.8331941
4.41_339.0950n	340.1022844	4.4062	pos	9734.078737	10879.1624	11165.45535	7222.315981	7053.809942	7540.457274	10593.00039	12329.35181	10538.84085
4.41_342.2483m/z	342.2483306	4.4062	pos	240.1811066	742.115436	94.07988594	5054.401487	0.001403199	0.001403199	0.001403199	549.0569782	3.080440776
4.41_395.0401m/z	395.0401237	4.4062	pos	430.9376733	2063.374202	2020.339104	835.0755698	1319.143558	464.0079454	2090.68303	2046.681931	1950.266377
4.41_487.1324n	510.1217524	4.4062	pos	31888.26047	32387.21288	35468.97037	16657.75783	14787.1855	14357.20247	28193.23216	29479.82479	30947.64691
4.41_497.0873n	498.0945892	4.4062	pos	13099.74228	17005.22004	17924.06598	5495.049319	5259.475905	4768.459551	11306.49202	13946.60627	14523.59233
4.41_665.2509m/z	665.2509288	4.4062	pos	0.001403199	3437.089754	3148.466194	528.7198589	1365.030284	0.001403199	2454.766616	3414.399131	1562.693599
4.41_796.2126m/z	796.2126486	4.4062	pos	5091.762216	7733.521406	7007.192306	3231.874162	2536.936193	1618.648241	4919.868982	5385.360399	7434.420121
4.41_796.7145m/z	796.7144728	4.4062	pos	1207.022188	934.8669121	1299.789152	0.001403199	0.001403199	0.001403199	0.001403199	896.7208895	0.001403199
4.41_839.2413m/z	839.2412728	4.4062	pos	984.1540187	790.807275	2733.664487	666.9786561	0.001403199	0.001403199	1531.439072	0.001403199	1616.587963
4.43_119.0685m/z	119.068526	4.42815	pos	1757.398631	1959.18796	1857.134393	796.7415953	726.6141766	722.8343363	1139.26442	1477.651569	1465.896492
4.43_158.5224m/z	158.5223738	4.42815	pos	592.3941911	917.4004562	830.6019696	463.5907076	457.8862285	446.2756331	643.2617974	710.8422828	639.0365173
4.43_167.0815m/z	167.0814628	4.42815	pos	169.8686976	290.112702	221.1452326	165.1071411	115.901131	114.3850075	221.1161216	210.6671313	246.0503091
4.43_170.9848m/z	170.9848289	4.42815	pos	179.6434984	163.8893154	102.4614359	70.90057993	65.80788493	100.2174356	86.01518321	110.3140079	126.306808
4.43_177.0497m/z	177.0496904	4.42815	pos	749.7312637	754.2149494	865.5394649	2196.028323	2122.112789	2168.766774	1022.044872	1113.046411	904.0887505
4.43_179.0356m/z	179.0356194	4.42815	pos	79.15170452	68.70604824	101.6029044	95.95537704	66.32118716	47.60011766	178.306144	149.0122468	80.55574602
4.43_224.0291m/z	224.0290608	4.42815	pos	40969.27174	41112.56887	41316.07688	24230.09093	22148.2441	23790.28748	31649.83788	35384.92094	33148.11429
4.43_235.1326m/z	235.1326146	4.42815	pos	1059.91034	941.8327879	778.0907879	1111.048925	813.8645022	1014.185453	544.8760209	719.2223522	582.3329367
4.43_274.0478m/z	274.0478428	4.42815	pos	203.7437564	1862.606019	1365.518162	573.8701997	781.8568082	196.5135002	1020.031032	1317.401074	732.8969494
4.43_277.0758n	316.0374291	4.42815	pos	11460.47422	13579.57786	12943.1096	6371.960032	5345.60028	5461.578489	9787.542991	11402.42123	9320.577232
4.43_278.9906m/z	278.9906472	4.42815	pos	6178.646642	6510.426837	6859.942139	1770.177197	1392.993625	1407.998793	5258.634273	6354.975706	5421.311718
4.43_301.9717m/z	301.9716594	4.42815	pos	372.1833715	888.7409322	769.3135672	471.8432747	604.2860475	354.540227	507.9925008	738.3338287	658.7893307
4.43_311.1210m/z	311.1210246	4.42815	pos	2108.93343	2374.718564	3076.630151	3548.43961	3574.991405	3581.052691	2306.798415	2676.294353	2626.196353
4.43_314.1270n	353.0838658	4.42815	pos	6250.953894	7382.670927	7673.53379	3567.005423	3130.323993	2968.798002	6239.144033	6902.296413	7065.967771
4.43_316.0142m/z	316.0142338	4.42815	pos	619.111815	669.9130821	582.9565715	516.318492	376.4015753	492.6468805	339.9949569	740.6508892	419.1081738
4.43_326.2201n	327.2273737	4.42815	pos	2203.904911	3931.300245	3771.388112	2001.052004	1696.164566	1717.453163	2100.158141	2502.181065	2574.491903
4.43_344.1134m/z	344.1133782	4.42815	pos	204.7640572	405.5290082	647.9515507	817.9705697	868.101352	598.1636589	770.4634345	845.1271404	648.9273587
4.43_360.0035m/z	360.0034736	4.42815	pos	3633.315044	3391.032508	3198.846887	2738.320532	2418.359685	2406.451804	3427.424784	3173.474841	2851.596309
4.43_402.0798n	425.0688685	4.42815	pos	21867.36183	24212.71351	22015.1308	7539.913889	5848.301052	5887.777826	13754.37614	16110.36593	14856.26989
4.43_403.2323m/z	403.2322857	4.42815	pos	3145.50074	3588.332681	3547.433964	2669.333823	2763.417574	2552.011761	3786.728455	2799.972617	2810.743884
4.43_412.0350n	413.0422351	4.42815	pos	4563.438838	7243.169651	6809.20215	1890.906512	1351.422488	1239.414725	3253.024155	4500.50864	4278.398568
4.43_414.2696m/z	414.2695652	4.42815	pos	575.0100273	663.8201219	222.9567	627.032427	641.6659958	606.5533187	516.1661497	785.1879636	656.6492027
4.43_427.1570m/z	427.1569924	4.42815	pos	3515.598101	4507.279802	3700.613522	9341.14945	6990.504009	7451.511093	4315.913553	5103.536216	4651.9762
4.43_433.2652m/z	433.2651998	4.42815	pos	639.7021898	2364.83175	2402.100182	2354.357076	2372.665739	1759.81247	1847.296585	2284.24901	2462.352396
4.45_132.1018m/z	132.1017915	4.451133333	pos	1353.26905	1174.777375	1110.707181	1065.990785	946.0482913	911.7393628	1079.288914	1195.024186	1171.533839
4.45_180.0444m/z	180.0443502	4.451133333	pos	475.917616	239.0645767	192.9330058	304.2839209	435.7013835	409.6068133	217.3266751	203.2138601	335.4737196
4.45_226.1178n	227.1250669	4.451133333	pos	13508.68402	14001.58701	15005.38489	10790.48585	9264.940245	9659.721876	11509.47979	13495.88438	13034.93745
4.45_229.1543m/z	229.1543131	4.451133333	pos	132.1033997	240.3180285	225.7322546	162.8225343	136.6569465	155.5601395	134.4896397	93.66540909	108.3458412
4.45_236.1496m/z	236.1496479	4.451133333	pos	987.1139106	1080.998979	890.7789805	944.3893625	953.7017035	984.9204907	922.3214762	983.6999812	950.8180788
4.45_268.1419n	269.1491976	4.451133333	pos	2083.800625	2804.962195	2350.70952	2166.041979	1908.996117	1877.546382	2732.736728	3343.395412	2859.855684
4.45_283.1516m/z	283.1516257	4.451133333	pos	1185.174134	914.6879959	860.014367	806.3019018	666.3265696	898.3332903	769.2757735	862.8199649	886.8428905
4.45_293.1358m/z	293.1357614	4.451133333	pos	511.8727867	370.8796331	453.315588	516.7747008	354.1799798	481.007105	276.66287	425.1019566	379.6075147
4.45_314.1709m/z	314.1708882	4.451133333	pos	836.695478	1008.89669	1197.157195	1057.981487	1019.50275	897.8113689	836.8747958	1024.592895	878.8273154
4.45_428.2098m/z	428.2097712	4.451133333	pos	2374.536713	1724.014626	1901.97437	1834.547562	1572.13649	1776.64384	1671.112351	2057.610026	1902.178136
4.47_117.0547m/z	117.0546674	4.473983333	pos	199.2190219	175.2568841	135.9660769	184.323128	203.378093	217.4302677	189.250635	189.5375303	214.9958586
4.47_161.5572m/z	161.5572034	4.473983333	pos	24.62376044	25.09715615	0.001403199	55.33138019	63.37676476	74.52347152	43.08121972	36.56035137	26.35468083
4.47_164.9203m/z	164.9202655	4.473983333	pos	559.0583962	569.3958162	487.7833467	681.2008575	712.6297651	695.6878239	641.3539774	585.4094929	613.6690581
4.47_169.5433m/z	169.543344	4.473983333	pos	203.7560305	182.7077655	155.0801274	537.7537698	461.8968898	500.6087865	169.9547231	260.9111713	254.3684919
4.47_201.0731m/z	201.0730977	4.473983333	pos	1145.139697	917.4045914	908.6899456	1007.64539	960.8981938	1036.52896	1327.410241	1080.728374	1063.946169
4.47_202.9509m/z	202.9509184	4.473983333	pos	6817.880319	6866.993871	6485.780463	6932.098244	7993.476487	6717.748276	8115.651929	6555.412939	7153.983708
4.47_249.1032n	272.0923655	4.473983333	pos	12079.47643	11705.62633	12039.93467	25623.72676	22742.53789	22340.7845	25845.09059	27691.06173	26729.00626
4.47_287.1679m/z	287.167862	4.473983333	pos	541.8530243	680.6018759	580.8854593	385.624015	308.1790429	221.6012867	560.6494652	569.97497	470.0539233
4.50_104.0305m/z	104.0305332	4.496783333	pos	536.3170312	516.0465142	461.9288305	682.9508024	661.9081453	555.4924604	632.442694	509.3956383	572.4867261

4.50_115.0633m/z	115.0633001	4.496783333	pos							15.55636994	51.80630964	54.96108504	65.38095417	37.06460431	34.90217549	45.04372893	38.18138535	32.24374286
4.50_125.9862m/z	125.9862164	4.496783333	pos							1983.342664	1855.263834	1870.286891	2127.376263	2432.720399	2071.719571	2366.192112	1921.090326	2014.137532
4.50_192.6052m/z	192.6051923	4.496783333	pos							506.7063027	550.7861396	437.3955013	280.1173544	281.0858249	340.353996	501.4171983	570.3602692	537.916297
4.50_197.9924m/z	197.9924403	4.496783333	pos							825.8703983	739.6683014	693.1921744	676.9713024	734.4687369	732.634441	792.4200247	711.7261123	706.5323754
4.50_201.1362n	224.1253262	4.496783333	pos							9458.59815	8113.908144	8070.65431	8237.186417	7879.529046	8551.498754	8491.070668	7480.046444	7930.649778
4.50_205.0445m/z	205.0444694	4.496783333	pos							254.3001746	368.5123754	316.2161648	323.2013206	363.9352751	355.6299024	368.8727778	326.7056662	251.6019347
4.50_208.0392m/z	208.0392332	4.496783333	pos							1091.457317	997.7859511	846.3820003	853.7076295	856.5171153	902.2576855	1232.863162	866.6292723	904.0047889
4.50_224.0114m/z	224.0113905	4.496783333	pos							1515.156137	1550.549934	1394.788459	1189.780661	1219.053795	1307.309213	1898.144106	1449.43102	1388.1512
4.50_227.1500m/z	227.1499914	4.496783333	pos							431.588426	223.2789095	137.9144661	174.6223328	294.6571553	272.6235233	250.8422531	99.1482439	286.387923
4.50_259.9763m/z	259.9763165	4.496783333	pos							57.74429974	90.45791687	153.9161542	0.001403199	0.001403199	0.001403199	65.82508982	103.7864038	94.23708233
4.50_283.1746m/z	283.1746486	4.496783333	pos							1018.741603	919.3784232	819.9241785	735.5773577	730.0843133	736.5434576	1128.574116	914.5786922	822.517134
4.50_318.2271m/z	318.2270946	4.496783333	pos							1015.374529	1228.70247	1194.144591	1078.0789	1117.876362	667.6452391	1075.268783	1098.175859	1013.093665
4.50_339.2518n	362.2408688	4.496783333	pos							158.6688025	3866.225359	637.1738709	468.1565259	673.7546062	184.3417298	790.0668881	580.0336609	454.0726583
4.50_349.1388m/z	349.1388257	4.496783333	pos							1985.549949	1746.55674	1527.484194	2666.045037	1846.972151	2155.122423	1793.191429	1886.883409	2147.518232
4.52_110.0171m/z	110.0171162	4.51925	pos							28.57121329	0.001403199	30.47616148	19.5744143	0.001403199	0.001403199	37.39576741	0.001403199	20.73475993
4.52_147.1166m/z	147.1166003	4.51925	pos							1207.209328	1121.82738	1109.048667	1174.712027	1126.21195	1039.335734	1211.518155	1045.202449	994.0760675
4.52_178.9904m/z	178.9903866	4.51925	pos							884.3228193	942.3322602	831.2397946	843.9950925	863.1854683	884.9565875	1041.705638	820.6783829	863.3754978
4.52_185.5295m/z	185.5294667	4.51925	pos							157.7789701	307.9437961	189.4852517	232.4437038	184.5869512	195.7839334	239.6975507	231.6164754	272.8084175
4.52_263.0202m/z	263.0201888	4.51925	pos							406.2817745	285.3323913	345.1014109	1176.154314	978.5360356	1126.216889	363.0027951	339.7628433	285.2547848
4.52_310.0119n	333.0011304	4.51925	pos							8316.69861	8512.093512	9188.734673	5286.178108	5119.871248	5034.142499	14841.72948	16160.95953	16056.89378
4.54_136.0214m/z	136.021425	4.542216667	pos							508.6837267	419.5413692	452.3124375	428.284912	436.1806884	456.8354491	580.8152408	412.4138541	416.6545108
4.54_159.9644m/z	159.9643653	4.542216667	pos							48.759342	114.760358	79.19316457	77.44327836	206.0389924	141.3685823	190.772401	79.95718688	112.2341704
4.54_170.5566m/z	170.5566285	4.542216667	pos							81.28350476	21.28350294	48.34928791	321.1084001	151.247423	170.726943	43.87438259	34.31888819	41.40374478
4.54_171.0624m/z	171.0623516	4.542216667	pos							458.1336201	476.1200056	447.2882767	594.6388735	542.4871549	444.2199618	625.7270276	438.4357025	484.1700705
4.54_189.0657m/z	189.065675	4.542216667	pos							964.3525323	846.6851646	662.1255885	494.6549505	432.3491591	388.9565339	700.0823808	466.7362524	432.9928029
4.54_190.0393m/z	190.0393072	4.542216667	pos							49.02282682	0.001403199	366.8384277	15.53846211	0.001403199	0.001403199	0.001403199	0.001403199	41.59468157
4.54_192.1361n	215.1251761	4.542216667	pos							16123.61046	11897.66216	11964.87482	12507.43742	16605.67854	16216.92122	15743.21683	11949.78432	14117.75119
4.54_238.2010m/z	238.2009509	4.542216667	pos							301.5911068	260.5023283	214.1208767	326.2836123	331.4843809	315.2100226	463.6195903	264.8430155	295.4843063
4.54_241.1044m/z	241.1043903	4.542216667	pos							2516.791864	2584.623764	3009.204133	2893.29568	2613.531719	2707.816744	2248.122615	2440.539191	2273.856414
4.54_265.6443m/z	265.6442739	4.542216667	pos							123.0032153	236.2372716	110.6739045	170.8603708	140.269083	191.7110337	203.9219622	250.7170982	210.0818406
4.54_266.1726n	289.1617666	4.542216667	pos							79581.43527	96916.38625	53902.60458	116771.0517	1881.070915	17169.67139	32914.85221	56099.32936	27412.39008
4.54_273.0611n	274.0683278	4.542216667	pos							1580.467894	2590.210541	2740.395836	1781.663865	1646.212564	1587.667852	1888.486242	1754.631481	1762.632537
4.54_286.0555n	287.0628056	4.542216667	pos							7243.338402	1044.378461	29379.51347	1498.986533	1189.121894	1256.560525	1534.949197	1279.29759	3529.594075
4.54_296.1369n	279.133576	4.542216667	pos							5516.231637	5848.544601	6456.859924	3945.976031	3941.143184	3578.105494	3042.322308	3455.717247	2897.457654
4.54_338.0446m/z	338.0445825	4.542216667	pos							659.3774123	0.001403199	2368.054958	162.4050387	115.2674749	130.8524492	87.99741281	102.7207304	240.6083063
4.54_340.2092n	363.1982849	4.542216667	pos							1227.608455	2143.644636	830.4032067	11786.60391	58.35692645	203.0533632	293.1565001	2294.520787	86.99107695
4.54_414.2461n	437.2352612	4.542216667	pos							10363.21714	8839.980466	10593.21747	9132.700147	9145.28709	8462.990849	9311.968521	9141.842812	8515.645222
4.57_113.0347m/z	113.0346941	4.565116667	pos							554.6195657	537.5045743	519.6548465	637.3093284	666.4987772	490.4073872	723.5574908	510.9103962	544.7179852
4.57_165.0544m/z	165.0544495	4.565116667	pos							1142.802422	1075.52256	1229.566374	1521.97	1583.549064	1223.100914	1303.35713	1175.126272	1405.683739
4.57_213.9826m/z	213.9826018	4.565116667	pos							2233.546756	2361.815285	2162.981048	2335.044308	2703.519908	2130.82853	2743.034274	2121.443944	2255.94349
4.57_227.0288m/z	227.0287596	4.565116667	pos							2991.375584	3228.053307	3483.16966	3297.101825	2960.736947	3062.177443	2952.587169	2698.647099	2589.5599
4.57_243.9415m/z	243.9414601	4.565116667	pos							1794.86859	1715.67002	1750.246754	2145.032572	1933.467203	1981.991749	2840.801074	1710.223565	2008.146364
4.57_282.1317m/z	282.1316722	4.565116667	pos							477.49478	345.6510912	417.2067078	555.0513245	509.4803994	455.2738178	648.7321304	481.0461884	492.3733634
4.57_307.0783m/z	307.078322	4.565116667	pos							527.919041	579.6509027	611.7044159	243.0519062	277.9439953	255.3401066	628.0453479	587.9705776	598.5486202
4.57_440.2402m/z	440.2401903	4.565116667	pos							349.8663356	461.1699315	530.85838	511.0893566	513.83777212	574.498938	451.4986505	540.2773666	611.6986886
4.59_154.0416m/z	154.0415887	4.58805	pos							306.7259551	296.2227447	406.9707525	407.4701634	467.2855454	391.5762128	415.1413678	317.8362527	419.3959547
4.59_155.0700m/z	155.0700294	4.58805	pos							469.4422599	447.4100871	453.4353588	593.2783571	445.7736153	407.5705298	625.6682294	437.179373	441.1218046
4.59_169.0494m/z	169.0493562	4.58805	pos							230.020605	323.4503237	349.5628741	217.5053965	326.1578103	231.1069013	310.9697403	260.2027338	247.4067997
4.59_176.9717m/z	176.9717463	4.58805	pos							2758.747074	2811.848143	2722.246282	3044.006895	3562.009273	2864.278718	3276.514015	2690.44535	2849.872092
4.59_186.1205m/z	186.1204788	4.58805	pos							99.86533851	123.6590575	160.0513518	124.7068642	153.5624805	160.9771784	49.93193057	126.8093901	128.7814658
4.59_202.1072m/z	202.1072252	4.58805	pos							1634.635993	1691.137664	1615.696621	1499.747435	1467.499085	1314.790426	1616.986148	1303.173002	1411.094892
4.59_224.1571m/z	224.1571074	4.58805	pos							98.21996743	102.3146738	64.22314732	76.86843384	56.49081182	0.001403199	86.55892773	115.9767426	29.31941344
4.59_234.0080m/z	234.0080487	4.58805	pos							980.003315	1149.166112	1093.950751	1273.635969	1279.097471	1258.713357	1259.132383	1273.819565	1281.587489
4.59_236.0051m/z	236.0050882	4.58805	pos							565.1525542	761.3550081	709.515677	756.7647358	802.7285992	753.1404972	810.3421497	725.9435897	756.2247246
4.59_240.1802m/z	240.1802239	4.58805	pos							707.2651468	756.9233995	613.469977	667.7653833	680.941977	524.2811706	865.8132839	628.0448179	636.0719474
4.59_248.0948m/z	248.0948092	4.58805	pos							483.8765287	477.1384361	461.8317163	596.3703133	482.1238285	528.359838	570.7227175	642.8641122	519.5657559
4.59_259.1149m/z	259.1148505	4.58805	pos							1332.053855	1482.886698	1022.889754	1941.004275	1579.029705	928.2559938	1485.459248	1051.136944	1135.886124
4.59_268.2115m/z	268.2114913	4.58805	pos							1972.671076	1868.494796	1694.791141	2015.174414	1978.180842	1439.492955	2499.619348	1654.879914	1561.4114
4.59_359.0612n	360.0684822	4.58805	pos							25286.61481	28994.04814	29144.37269	32781.00982	32907.60548	30599.26316	26466.3684	29030.49007	28391.24195
4.59_363.0034m/z	363.0033914	4.58805	pos							0.001403199	690.1870368	716.4497716	283.0525727	670.6220335	139.2105323	280.3511708	419.1544354	269.0741207
4.59_385.1465m/z	385.1464693	4.58805	pos							4626.919622	4466.153852	4789.748157	3235.237201	3387.64065	2831.431684	5005.995143	4643.493324	4261.986257
4.61_163.1172m/z	163.1171881	4.610866667	pos							429.8520609	173.8740768	280.0727203	94.37256322	35.77800353	20.4417775	244.4452556	14.47824287	158.3595556
4.61_166.0836m/z	166.0835994	4.610866667	pos							468.8248167	438.0314886	390.5529088	420.7165938	555.1527152	476.6258929	468.3982259	384.5526799	375.7252664
4.61_182.0753m/z	182.0752518	4.610866667	pos							10.23665898	44.37849784	0.001403199	74.49969066	0.001403199	62.3388825	19.6536523	22.07476616	100.2296875
4.61_208.1080n	226.1434933	4.610866667	pos							5548.374777	5901.021446	6034.547587	4641.522816	5314.666667	4062.576478	4727.348034	4717.438573	4948.527881
4.61_218.1024m/z	218.1024146	4.610866667	pos							938.3871319	814.1260865	673.8920349	657.0415091	753.6860022	822.9433969	596.5054295	565.4261461	545.115725
4.61_220.0821m/z	220.0821381	4.610866667	pos							190.0776485	267.9632878	363.3688612	255.1998707	265.8985899	182.2204585	220.586468	229.6392429	204.5557852
4.61_355.1131m/z	355.1130701	4.610866667	pos							642.5443478	873.1541536	921.7300506	1126.433778	1529.46561	777.9356635	580.0183338	873.0444952	794.6682738
4.63_155.0700m/z	155.0700338	4.63335	pos							766.7486247	698.3564203	664.7014972	877.522015	975.2163868	740.8047409	716.0689441	680.110603	723.2340387
4.63_178.0373n	196.073292	4.63335	pos							97.53794387	101.502529	125.1692226	165.0472707	217.7972973	194.8489981	165.7049078	85.8357954	213.8468917
4.63_178.5430m/z	178.5430246	4.63335	pos							226.7835809	285.6989353	359.4839207	523.9111595	555.1929847	497.3049454	266.22743	325.0522137	348.0219962
4.63_178.9903m/z	178.9902559	4.63335	pos							725.8717847	608.9526385	584.7279263	562.0004131	880.2132692	544.1146309	643.8731283	533.4122581	529.6792511
4.63_199.1327m/z	199.1326835	4.63335	pos							2394.890547	2352.800412	2457.27541	2212.026145	2110.5192	2237.565391	2612.826987	2119.052078	2208.40212
4.63_202.1435m/z	202.1434916	4.63335	pos							1076.505836	1039.254801	1015.46917	1112.236132	1297.89569	1017.504627	999.7190122	1002.551687	989.7862647
4.63_231.1468n	232.15407	4.63335	pos							2920.300183	2645.637497	2609.063853	2575.387965	3141.647119	2490.350437	3223.669897	1989.804726	2683.861605
4.63_319.8812m/z	319.8812196	4.63335	pos							879.8056897	780.3819229	828.7411771	908.3483162	1354.673543	1037.690579	929.78474	845.6557731	1001.881319
4.63_449.1624m/z	449.1623759	4.63335	pos							1594.519588	2560.405308	2239.595407	1835.449526	1842.855078	1696.154318	1816.347041	1442.710617	2030.776482
4.63_451.1563m/z	451.1562714	4.63335	pos							729.9283241	740.0508948	750.4269743	1357.786923	1301.306975	1404.916563	861.3173834	911.1949934	802.6639616
4.66_198.1098m/z	198.1097681	4.656183333	pos							3007.811277	1868.385231	1697.949914	3086.302137	3492.716672	2671.185518	2713.828684	1995.238174	2429.536524
4.66_206.0667m/z	206.0666988	4.656183333	pos							956.393866	1045.505151	1180.386043	1009.255125	1072.197502	907.3225142	1180.624643	1033.956488	999.881134
4.66_315.1912m/z	315.1911961	4.656183333	pos							219.1812932	198.347997	101.6450015	484.2332194	459.7999581	517.0188754	257.030972	188.7148104	174.2098004
4.66_491.8053m/z	491.805258	4.656183333	pos							1233.575573	1566.043591	1403.65419	1378.010077	2292.024886	2224.152254	2055.035701	1682.065224	1741.385125
4.66_492.3069m/z	492.3068593	4.656183333	pos							647.1537306	643.3296373	733.8211206	734.6034138	974.4583638	709.388552	828.3357037	954.8355224	135.30382
4.66_957.0335m/z	957.0335451	4.656183333	pos							671.1540032	1504.486395	1241.0163	2303.430827	1980.46496	1793.451036	534.5383964	829.7339935	858.6088431
4.68_131.9741m/z	131.9741414	4.678916667	pos							662.8199583	747.8887253	762.848128	765.2012697	715.8369904	718.0704241	977.7558061	737.6083374	802.5049897
4.68_157.0758m/z	157.0757704	4.678916667	pos							829.1394603	626.2145212	583.6796931	413.2384084	345.2849201	396.9725638	752.8784658	474.0332543	470.1269512
4.68_169.0912m/z	169.0912401	4.678916667	pos							179.7977713	232.1852385	213.0212698	186.0132537	195.353365	122.1443655	163.0537684	241.1231289	226.0495569
4.68_175.0806m/z	175.0806133	4.678916667	pos							59.09473536	0.001403199	47.46726826	46.10168897	62.80284666	41.3249921	0.001403199	0.001403199	0.001403199
4.68_185.0808m/z	185.0807758	4.678916667	pos							3088.8107	3242.757974	3494.031673	3033.53202	3078.991225	2768.420462	3526.542051	2947.123751	2984.730142
4.68_216.9225m/z	216.9224631	4.678916667	pos							1132.899596	1303.696389	1322.694396	1151.210105	1566.706284	1313.151525	1468.417593	1362.927117	1394.453303
4.68_229.1432m/z	229.1432209	4.678916667	pos							1581.62806	1497.771287	1600.810624	1783.030149	1632.018604	1594.919156	1613.732013	1525.456611	1597.242549
4.68_267.1016m/z	267.1016058	4.678916667	pos							1023.862931	670.9030425	746.138899	859.0717362	1285.713626	978.9566233	817.5901166	704.9720251	726.0738169
4.68_350.0608n	351.0680894	4.678916667	pos							6508.382575	7455.977766	7971.452414	3799.334796	3620.542561	3861.835225	7865.615449	8033.61347	7802.29721
4.68_638.0244m/z	638.0243854	4.678916667	pos							7265.631409	12809.28128	9645.147099	12333.70944	11758.68271	8753.342085	7583.271698	9644.795555	10761.44958
4.68_638.3585m/z	638.3584857	4.678916667	pos							6439.794343	10641.74169	8729.241294	10658.57482	10007.24274	9630.218243	5930.476439	8061.485272	9280.770493
4.68_638.6928m/z	638.692815	4.678916667	pos							4281.301218	5135.904997	3861.805417	6514.858061	5465.324849	4514.773425	3276.63191	3847.076088	4330.423909
4.68_956.5323m/z	956.5322786	4.678916667	pos							1662.430768	2190.540938	1516.721512	2843.169062	1483.4724	2096.287105	1644.100111	1808.567284	1581.100361
4.70_147.0631m/z	147.0630657	4.701116667	pos							20.58547087	124.9613628	86.56422811	7.924744955	0.001403199	0.001403199	0.001403199	0.001403199	4.910721781
4.70_183.1377m/z	183.1377132	4.701116667	pos							1405.023029	1268.661712	1118.35763	1289.332796	1262.268041	1004.50438	1397.412539	1156.159189	1181.059141
4.70_232.0917m/z	232.0916953	4.701116667	pos							15879.12177	14469.09903	13728.01733	15683.21844	15427.17641	15693.48209	16654.66157	14576.48275	14777.75104
4.70_238.0446m/z	238.0445966	4.701116667	pos							252.6986693	704.3088161	800.0154802	86.78360012	140.107078	218.2270187	714.0117334	923.0304681	880.0354924
4.70_291.1184m/z	291.118382	4.701116667	pos							1304.069578	1339.797296	1179.285483	1760.730874	1746.35573	1567.063105	1132.396662	1383.114236	1311.952669
4.70_300.0786m/z	300.0785619	4.701116667	pos							1464.271971	1374.555108	867.9908977	1426.178386	1435.971706	1554.222662	1528.846989	1406.465244	1409.123183
4.70_310.1987n	333.19787	4.701116667	pos							14930.13153	36625.51884	13212.54656	12163.61159	224.3119396	1330.264159	5370.554587	21552.47881	2381.946613
4.70_590.3400m/z	590.3400019	4.701116667	pos							280.2153666	381.1772299	429.4596391	461.0860226	192.9179181	402.8930536	237.9284442	262.2232218	206.3309037
4.72_180.0215m/z	180.0215377	4.723666667	pos							225.2753946	222.5879467	238.7831696	201.0322926	147.5477914	186.4165736	285.8299065	212.3747813	251.5753642
4.72_182.0751m/z	182.0751166	4.723666667	pos							25.80531031	20.00772799	66.1210352	22.02793741	46.52131438	0.001403199	0.001403199	45.14678574	23.97491703

4.72_217.0445m/z	217.0445455	4.723666667	pos																
4.72_249.1475m/z	249.1475267	4.723666667	pos																
4.72_265.0159m/z	265.0159479	4.723666667	pos																
4.72_322.1681m/z	322.1680631	4.723666667	pos																
4.72_520.3321m/z	520.3320678	4.723666667	pos																
4.75_127.9667m/z	127.9667118	4.7456	pos																
4.75_141.5540m/z	141.5540239	4.7456	pos																
4.75_149.5402m/z	149.5402383	4.7456	pos																
4.75_162.5690m/z	162.5689819	4.7456	pos																
4.75_164.5700m/z	164.5700432	4.7456	pos																
4.75_170.0535m/z	170.0534785	4.7456	pos																
4.75_186.1204m/z	186.1204195	4.7456	pos																
4.75_211.0935m/z	211.0935079	4.7456	pos																
4.75_224.0115m/z	224.0114608	4.7456	pos																
4.75_234.0080m/z	234.0079927	4.7456	pos																
4.75_236.0051m/z	236.0050691	4.7456	pos																
4.75_236.1620n	259.1513149	4.7456	pos																
4.75_259.1117n	298.0733218	4.7456	pos																
4.75_264.0946n	247.0913203	4.7456	pos																
4.75_285.0052m/z	285.0052081	4.7456	pos																
4.75_346.1600n	369.1514398	4.7456	pos																
4.75_352.2088m/z	352.208797	4.7456	pos																
4.75_403.2323m/z	403.232252	4.7456	pos																
4.75_445.1195m/z	445.1194643	4.7456	pos																
4.75_448.2044n	449.2117084	4.7456	pos																
4.75_458.1587m/z	458.1586794	4.7456	pos																
4.75_473.2258n	474.2330388	4.7456	pos																
4.75_525.2874m/z	525.2873764	4.7456	pos																
4.77_104.0708m/z	104.0708422	4.768333333	pos																
4.77_172.5796m/z	172.5795727	4.768333333	pos																
4.77_174.1487m/z	174.1486837	4.768333333	pos																
4.77_193.1433m/z	193.1432774	4.768333333	pos																
4.77_195.5824m/z	195.5823938	4.768333333	pos																
4.77_207.0868n	208.094072	4.768333333	pos																
4.77_215.1250m/z	215.1250371	4.768333333	pos																
4.77_221.1156m/z	221.1155862	4.768333333	pos																
4.77_244.0521m/z	244.0520752	4.768333333	pos																
4.77_265.0946n	266.1018839	4.768333333	pos																
4.77_475.3249m/z	475.3248699	4.768333333	pos																
4.79_104.0305m/z	104.0305237	4.7912	pos																
4.79_217.6235m/z	217.6234981	4.7912	pos																
4.79_233.0758m/z	233.0758473	4.7912	pos																
4.79_241.1043m/z	241.1043179	4.7912	pos																
4.79_274.0118m/z	274.0118025	4.7912	pos																
4.79_289.2273n	312.2165443	4.7912	pos																
4.79_292.1575m/z	292.1574853	4.7912	pos																
4.79_296.1381n	297.1454141	4.7912	pos																
4.79_328.1189m/z	328.1188767	4.7912	pos																
4.79_337.1815m/z	337.1815313	4.7912	pos																
4.79_344.2063m/z	344.2063138	4.7912	pos																
4.79_351.0949n	374.084135	4.7912	pos																
4.79_382.1234n	383.1306816	4.7912	pos																
4.79_558.2670n	559.2742644	4.7912	pos																
4.81_143.9589m/z	143.9588588	4.814066667	pos																
4.81_172.9562m/z	172.9562316	4.814066667	pos																
4.81_176.9717m/z	176.9717065	4.814066667	pos																
4.81_181.0859m/z	181.0859093	4.814066667	pos																
4.81_184.1048m/z	184.1047796	4.814066667	pos																
4.81_193.0063m/z	193.0062767	4.814066667	pos																
4.81_244.1308n	267.1202255	4.814066667	pos																
4.81_255.1200m/z	255.1199536	4.814066667	pos																
4.81_283.1516m/z	283.1515809	4.814066667	pos																
4.81_302.1421m/z	302.1420519	4.814066667	pos																
4.81_334.1615m/z	334.1615142	4.814066667	pos																
4.81_354.2250n	377.2141924	4.814066667	pos																
4.84_117.0573m/z	117.0573454	4.836966667	pos																
4.84_155.0699m/z	155.0699215	4.836966667	pos																
4.84_177.0788n	216.0415736	4.836966667	pos																
4.84_222.0865n	223.0937528	4.836966667	pos																
4.84_237.0731m/z	237.073092	4.836966667	pos																
4.84_246.1338m/z	246.1337835	4.836966667	pos																
4.84_730.2435m/z	730.2435316	4.836966667	pos																
4.86_164.0471n	165.0544764	4.8596	pos																
4.86_200.0870n	218.120736	4.8596	pos																
4.86_201.1000n	184.0966878	4.8596	pos																
4.86_225.1482m/z	225.1482471	4.8596	pos																
4.86_230.5779m/z	230.5779279	4.8596	pos																
4.86_239.1253m/z	239.1253262	4.8596	pos																
4.86_239.5642m/z	239.5641542	4.8596	pos																
4.86_261.1307m/z	261.1307293	4.8596	pos																
4.86_286.1341m/z	286.1341062	4.8596	pos																
4.86_362.1572n	363.1646003	4.8596	pos																
4.86_394.1703m/z	394.1702989	4.8596	pos																
4.86_406.1648m/z	406.1648225	4.8596	pos																
4.86_473.2441n	456.240791	4.8596	pos																
4.86_684.1786n	707.1678528	4.8596	pos																
4.88_140.0629m/z	140.0628609	4.882333333	pos																
4.88_202.9508m/z	202.9508001	4.882333333	pos																
4.88_207.0439m/z	207.0439222	4.882333333	pos																
4.88_218.0528n	219.0601162	4.882333333	pos																
4.88_226.1046m/z	226.104642	4.882333333	pos																
4.88_230.0785m/z	230.0784505	4.882333333	pos																
4.88_270.0420m/z	270.0420124	4.882333333	pos																
4.88_300.1179m/z	300.1178771	4.882333333	pos																
4.88_308.1182m/z	308.1182286	4.882333333	pos																
4.88_408.0376m/z	408.037569	4.882333333	pos																
4.88_475.2600n	458.2566798	4.882333333	pos																
4.90_113.0346m/z	113.03462	4.904516667	pos																
4.90_172.0968m/z	172.0967934	4.904516667	pos																
4.90_176.5510m/z	176.5510379	4.904516667	pos																
4.90_203.1427m/z	203.1426988	4.904516667	pos																
4.90_243.9412m/z	243.9412458	4.904516667	pos																
4.90_256.1419n	257.1491616	4.904516667	pos																
4.90_295.1513m/z	295.1513437	4.904516667	pos																
4.90_301.1617m/z	301.1617006	4.904516667	pos																
4.93_122.0318m/z	122.031763	4.927016667	pos																
4.93_169.9973m/z	169.9973486	4.927016667	pos																

285.5612818	1130.424242	1109.805145	677.0536334	994.0628297	913.616991	827.2726558	835.2321213	837.4811636											
397.6061021	378.4381715	468.6418959	415.9524675	255.1851897	390.7793056	481.5853983	363.6845318	372.9136449											
0.001403199	0.001403199	0.001403199	163.2389668	151.868673	112.6480017	0.001403199	54.53774847	0.001403199											
2313.152034	2579.477128	2340.605209	3073.869264	3045.247675	2975.02603	1574.778334	1642.739574	1749.712105											
1191.41163	966.902982	1029.719355	999.0944037	741.7111489	547.4079871	649.7484734	765.2769523	780.7189662											
258.6570428	239.7760017	277.1695784	286.7661211	202.4753724	247.2808765	348.0867452	254.2580905	326.5606901											
138.2728362	159.9057445	160.1493356	141.7885956	154.7119639	114.4273551	153.9149803	154.6773824	167.8231059											
1079.417413	1097.229364	1159.174329	936.4960363	901.8059728	916.3259527	926.7191805	1156.058314	1007.311642											
105.0717834	104.324053	96.39409066	102.1901351	94.68056692	101.1695102	87.21487984	130.6330681	123.9773062											
83.17532407	14.57222381	57.45257884	42.37931159	101.2563038	54.93346868	32.17717254	49.61771584	59.94554916											
795.7738635	855.1282837	964.4974266	849.2627239	724.6134805	718.9382459	690.6921342	701.0136325	809.7019974											
1118.882453	1169.49984	1196.177174	1132.191597	759.3779209	788.9218337	1021.232146	1162.31113	941.4964663											
2779.536617	3036.757604	3451.177814	2004.78633	2020.00673	1745.09527	2207.926344	2005.797903	1986.238645											
2261.926235	2134.374777	2583.267031	1887.684234	1524.919531	1728.397134	2459.848873	1823.175298	1902.362678											
3067.120621	3036.156889	3339.660755	3469.917268	3947.829799	3462.846757	3977.357654	3892.544998	3625.80838											
2525.338471	2477.273898	2511.924933	2548.4026	3081.208635	2593.935177	2855.089114	2776.138858	2878.838311											
42668.03344	40758.18821	29539.07822	36611.21195	21832.12473	19093.22481	34066.14207	27635.96382	22637.45185											
10389.69187	12280.46795	13417.20796	9270.080092	8798.404835	8640.817859	10309.06307	12029.39419	10898.93858											
29261.90121	30643.4861	30351.48655	25550.31082	24536.40548	22973.47378	25115.49771	29188.03137	25785.03797											
1233.453431	1542.663325	1670.637765	1951.077503	1814.902237	1883.673953	1434.556922	1960.064031	1827.439933											
5833.250434	5903.426506	5759.701387	6704.841919	2775.991516	3085.25047	4631.467513	5217.372547	4413.804246											
433.474899	1524.342402	1519.461267	954.0302308	1110.956696	1328.898087	935.5502674	1367.8938	1188.236949											
2490.507239	2467.047457	2451.610692	2252.515992	1664.180468	2012.379701	3393.182788	2417.485224	2317.332795											
1834.776599	306.3921227	254.2014775	0.001403199	133.0873474	401.3063377	414.5612177	311.5566164	234.5482793											
9004.756503	9538.62746	10084.45695	6352.288702	5193.419543	5776.418118	5580.474915	7934.01388	5817.817198											
1345.281544	1391.859956	1707.411806	1164.014094	808.6710151	848.7347225	762.6909221	1431.016401	1007.140988											
10388.10936	12725.40033	13892.66561	7649.229736	8068.837126	7658.474187	10658.44855	11747.74948	10929.06427											
249.3810199	2045.252312	2939.739846	210.7860706	736.3989559	809.0032635	1582.121373	1635.288406	1639.481326											
2572.100911	2215.356575	2180.179168	1754.246307	1653.959768	1525.659613	2123.178681	1812.670696	1837.887101											
91.57701426	130.1243922	157.249069	977.9856675	1185.090366	1197.597802	159.956341	179.9240009	177.8939928											
350.0283072	331.6426691	458.186616	279.226422	172.8830072	248.1559373	393.8584245	299.3397822	250.146601											
66.87552771	49.60199675	20.9662405	52.20469492	113.5480886	141.2178248	91.28042345	16.84406185	108.6845823											
156.8204945	307.4232015	222.541541	1957.217077	1998.473307	1941.242676	222.3740235	243.7968435	202.4617736											
2396.69796	2350.244678	2796.205033	2182.663951	1987.90618	2203.930164	2461.088113	2279.272908	2452.730107											
2810.243808	1610.607083	1759.805112	1742.877874	3277.532945	3564.603389	2730.732221	1989.849145	2623.10679											
568.9518846	480.066532	800.0788608	570.1510153	437.3453012	539.3205797	636.4504659	456.9187659	452.4865261											
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8849.378747	9583.312569	10723.95512	6676.204816	6282.561578	6204.551668	8543.790471	9648.145328	9113.197018											
121.8852626	2664.772596	466.7313844	181.7656577	201.8693225	531.1159441	290.4022788	291.7664528	312.1472044											
326.5933451	386.6253242	404.871878	385.8417401	314.0445176	391.7659396	413.4250769	449.8910286	419.4845603											
319.1735429	418.8007428	416.8277462	826.429686	639.6376683	717.9528661	313.4161024	359.0322237	348.7590802											
176.3120298	66.50693587	148.2456734	138.6536031	116.5174578	105.7588787	91.59240061	118.5317814	121.3079766											
2332.742596	2648.978498	2936.689075	3406.233082	2871.92762	2779.982648	2233.184316	2607.797784	2376.841236											
1617.292981	1136.109146	1652.164871	639.5016661	426.4771837	485.071532	715.7068692	570.8631439	513.3870638											
5521.338214	6511.639394	6893.31808	10670.31201	10631.31201	10118.07382	4653.113298	6010.871161	5790.074786											
3045.920742	3404.47675	3612.893859	5683.799209	5276.74651	5380.407352	2905.11786	3457.585417	3435.613444											
3911.183946	4659.768702	4910.43582	2810.039498	2286.770688	2586.519914	2973.278453	3141.525465	2915.731196											
425.0387881	543.4128377	745.2277247	806.8930485	607.6961002	726.2715648	622.5377826	778.2312393	760.0168191											
248.6289828	452.0349132	698.8259296	213.8518299	187.0497594	317.796606	270.4954267	230.2775755	209.4276094											
11680.88947	12205.44952	12477.09583	19093.68543	17777.90253	17887.18534	10373.92753	11783.00236	10583.74178											
94993.75412	98567.04553	103592.3591	162198.4374	146888.4924	144362.7379	76505.51087	89007.79955	82228.33357											
112621.1581	117535.7863	122028.8122	103121.0446	96442.59513	95737.61346	107461.1464	116361.6935	113145.1196											
10398.84149	9627.22041	11726.87717	15636.50699	12590.16342	13598.14921	10168.50824	10767.58554	10068.62414											
18.20650222	13.85759594	45.19449646	42.74174544	28.60692078	12.55794475	51.30723027	0.001403199	46.23875292											
1285.193549	1232.371001	1570.243379	1137.854337	1192.574026	1129.173421	1215.965393	1088.081646	1469.026332											
1151.931348	1132.53426	1523.523983	1087.227702	1053.5938216	1174.392494	1249.632265	1125.238622	1124.159024											
1229.237623	1375.547761	1603.880664	1122.621394	956.017811	1085.704172	1242.34119	1369.39875	1327.929834											
109.2215648	81.72370365	99.30050188	150.4690075	103.3699648	122.8833663	46.40203481	113.7758627	122.0439269											
266.8686313	189.8368797	213.318749	183.5841974	148.911348	193.8275881	259.9330276	146.6096381	237.5970118											
26887.13662	28793.21279	30409.38201	37609.43213	34633.65699	35889.97899	26027.36674	27474.06601	27737.83698											
1053.933915	1453.08294	1660.200431	1330.074763	1193.687403	1295.486426	1229.509491	1341.644797	1196.085702											
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8659.627096	9503.449212	9204.76912	13138.24451	11305.94394	11683.96908	8377.589021	9384.946374	8987.242065											
852.7683688	871.7841498	1026.384328	418.9799323	441.380807	530.6050166	514.7618634	767.4629755	607.665747											
1585.969499	4928.710939	1374.413278	26007.77668	0.001403199	6.778705819	151.3835284	3852.874021	0.001403199											
623.6167273	472.1977254	415.9362837	218.4335789	199.8929099	200.3184242	333.4655268	280.3391852	306.4943946											
558.2837385	539.4924975	567.5773093	564.5753939	509.821013	476.4817097	571.7493278	554.364636	693.0559192											
712.5137512	779.9191677	691.7170965	834.7356879	837.5380939	813.5903553	633.8791946	606.190166	477.9287299											
16348.52339	17506.68612	17913.30401	18420.74743	16360.44067	17097.82169	13432.1588	14401.65602	14319.22479											
1352.61365	1308.504839	1444.618937	2115.387109	2045.211396	1968.239291	1331.083172	1432.411463	1374.215312											
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26527.62766	152.459552	0.001403199	40.7707036	386.3621729	0.001403199	0.001403199	0.001403199	0.001403199											
1463.439472	1759.647782	1985.380335	1438.213364	1349.983321	1408.534281	1729.921898	1501.226553	1723.734003											
3697.359657	3784.484052	3828.796058	6031.871542	5739.720543	5461.150724	3255.370839	3565.42129	3669.83106											
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878.7958423	903.7038128	947.346854	760.5075089	830.2530212	866.8717011	870.5960163	778.9652217	800.1833193											
1007.328879	911.675246	1012.487131	1133.070356	1128.147911	1087.635273	1285.190055	1212.626907	1172.542946											
2303.693134	1884.994032	2496.86929	2546.853065	1808.432759	2080.796526	1650.557405	1668.612925	1865.179838											
441.078194	468.7419776	450.5404384	455.1946337	449.0045846	429.7850292	546.0195763	604.2534586	481.9504878											
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472616.5232	995.478489	604.3330083	631.7057786	1094.783736	1578.126426	1855.861217	1134.205911	1480.686243											
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267.158644	2458.37218	3365.920342	2509.828402	2668.771485	2693.188169	2684.389468	2490.270296	3178.205181											
286.8870925	393.4077545	320.207401	315.3195333	225.8436469	264.0935427	174.5056595	217.5150709	215.5910291											
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180.0053067	486.4332968	244.0522113	311.5414827	361.6874395	316.3672088	390.504041	502.0291252	518.1471317											
934.8764171	990.6829698	1111.985231	528.2071098	508.0365343	503.8420482	854.7889106	609.3668249	887.9452592											
5212.516168	5494.022597	5392.566956	5350.179387	4811.390458	5070.436391	3849.852994	4981.360162	3692.682486											
682.094884	774.9646759	644.5051136	383.5165916	407.3852815	410.0543656	865.2963912	803.3254186	632.841205											
298.6216929	394.8124295	325.1639514	456.6051547	414.6069586	452.0463874	355.9941236	389.2263451	316.2634728											
434.0409831	370.1316394	385.8427605	0.001403199	0.001403199	0.001403199	744.1492433	796.3471133	860.846462											
6237.554121	6992.596238	6057.346482	5223.553096	5144.029809	5213.131564	6337.208843	6727.066791	6512.572977											
881.924854	937.8903138	1022.504111	967.6950146	901.2569331	840.1057428	944.2920807	920.0213013	1090.646945											
3231.940437	3411.063081	3728.702034	3776.439963	3765.3645	3926.056625	3173.575868	3170.101223	3190.858818											
91.20867305	100.7694308	162.8542342	226.6594702	242.2380786	259.1212728	113.9066686	138.1757755	125.1515778											
1344.831732	1059.603436	1391.734921	1207.796268	1191.562065	1072.222001	1236.532339	1004.104997	1256.679288											
2190.5212	1926.983474	1763.63587	1749.347389	1991.642599	2023.115187	2168.004361	1827.626312	2484.298766											
54282.09833	53349.02881	57403.26932	89330.12754	77658.60187	79628.82135	53320.87276	55598.91867	53979.11357											
3708.348498	3986.018031	5027.026742	3280.684184	3315.226581	3008.840633	2651.43613	2916.28724	3152.194243											
2684.587975	3736.411937	2408.122898	2065.573614	124.8511696	293.5472232	1748.565025	2271.905282	1568.687364											
209.1174463	221.7900896	211.7176165	20.55130149	16.44484779	0.001403199	16.34856096	40.17245245	32.58065088											
1223.59645	1106.476558	1022.936977	1050.882051	1196.215773	1156.703304	1149.129778	1193.154426	1194.640903											

4.93_203.0652m/z	203.0652149	4.927016667	pos							202.5603901	340.1404341	187.3261883	242.4037999	546.0636425	351.8347297	393.9983973	705.2323373	730.4621526	
4.93_330.2269m/z	330.2269345	4.927016667	pos							21784.05211	23524.75346	23710.87838	27955.89593	25130.8221	25584.25882	20714.50113	22929.14693	22394.54608	
4.93_339.1773m/z	339.177306	4.927016667	pos							1637.738049	1456.792392	1773.574652	1281.518607	1246.381485	1258.530212	842.6790256	1078.233569	1276.148814	
4.93_445.1194m/z	445.1193815	4.927016667	pos							2932.913609	318.2927219	90.01560982	262.6779103	351.6308075	181.9459192	257.8612791	314.8907078	83.15355988	
4.93_500.1650n	501.1722373	4.927016667	pos							95870.35239	103198.9524	103457.3062	185.823009	350.4587309	245.7980001	56779.10701	62938.77253	60506.68806	
4.95_130.0862m/z	130.0861807	4.948983333	pos							782.8749061	799.3072183	761.3605283	755.2135473	642.5407588	662.1537565	749.5564702	755.6290757	725.2245589	
4.95_133.0646m/z	133.0646475	4.948983333	pos							1284.447816	1184.455978	1145.01439	765.9829127	796.9496898	808.4174687	1008.62014	1035.244676	1023.801559	
4.95_163.0386m/z	163.038642	4.948983333	pos							846.1292336	712.3280994	773.9401583	666.2090884	768.742396	733.1690368	867.23359	637.0342582	624.265318	
4.95_273.1934n	274.2007983	4.948983333	pos							6123.199878	6918.015425	6197.257286	5851.349709	6266.43842	6138.371212	4904.216001	5526.264757	5723.643529	
4.95_297.1936n	280.190294	4.948983333	pos							115540.1747	127602.4043	125469.0092	84695.67468	70006.32807	71621.49326	91504.34632	105963.7862	101852.8484	
4.95_317.1566m/z	317.156579	4.948983333	pos							2923.68742	4728.858661	3452.363949	8037.805934	320.6530662	816.8203689	1431.036829	2395.950178	1520.142838	
4.95_403.2319m/z	403.2319154	4.948983333	pos							5271.342182	4923.90621	4702.855351	5262.400592	4649.434949	4763.346676	5137.089987	4786.517181	5085.114896	
4.97_146.5699m/z	146.5699484	4.970833333	pos							1028.957442	825.1342163	1170.786224	981.9871148	822.6430816	922.3670832	1095.665678	765.2148278	1085.659031	
4.97_154.5562m/z	154.556165	4.970833333	pos							2230.976056	2086.338323	2190.761139	2245.054216	2065.415947	2107.153537	2355.839085	2338.12943	2372.968109	
4.97_209.1534m/z	209.1534381	4.970833333	pos							1363.521175	1349.740421	1147.163846	860.4836284	859.4428008	772.8697342	1228.38847	1156.978243	1029.662764	
4.97_253.6520m/z	253.6520437	4.970833333	pos							153.9631765	182.6261193	266.1412782	338.8606712	218.1512887	162.8123874	0.001403199	120.7495632	55.44507493	
4.97_265.1039m/z	265.1038913	4.970833333	pos							7531.158869	9113.71819	7844.571197	10443.36801	11342.6968	11671.71205	7912.195537	9242.788977	8737.644051	
4.97_474.2327m/z	474.2327028	4.970833333	pos							5919.534109	7137.042991	6187.561391	4400.999562	4485.458269	4840.668469	5282.156256	6962.857577	5863.042969	
4.99_104.0305m/z	104.030498	4.991816667	pos							193.6709775	178.5130489	197.2878248	184.4070637	192.6210186	189.4948257	170.2261751	162.1287615	195.2975481	
4.99_111.5409m/z	111.5408619	4.991816667	pos							116.786336	53.31647063	107.213208	113.1706715	113.085422	97.37106724	87.2330061	103.9052008	92.96745738	
4.99_153.1271m/z	153.1270843	4.991816667	pos							1020.264284	1026.726402	919.6841653	772.4677404	986.1985547	848.2428299	964.4306689	1048.69613	1023.848709	
4.99_171.1257n	194.1149353	4.991816667	pos							1559657.121	1486043.115	1473320.427	1462577.319	1528661.118	1479348.181	1701154.984	1492645.093	1591399.992	
4.99_172.1268m/z	172.1267786	4.991816667	pos							39.07597762	113.994554	175.0142177	361.2114684	336.9162098	258.9216807	208.6307906	257.5509086	195.2652785	
4.99_212.1254m/z	212.1253876	4.991816667	pos							151000.7228	144661.2473	141706.8052	143699.5164	152278.1872	149484.9031	168691.6243	149939.3169	160308.6222	
4.99_230.0528n	231.0600625	4.991816667	pos							2607.978811	2432.342082	2964.926658	3948.451207	3550.28617	4023.145767	2931.065342	3075.861979	3301.280001	
4.99_239.0885m/z	239.0885473	4.991816667	pos							5586.128801	5210.821942	5833.020982	6611.631997	6282.976168	6449.442867	5253.507342	5942.102742	5404.832422	
4.99_359.0968m/z	359.096779	4.991816667	pos							2771.625537	3194.642431	3607.556135	481.6465332	494.1942523	486.6060538	2167.964764	2397.584032	2517.217312	
4.99_385.1463m/z	385.1462911	4.991816667	pos							47344.82844	49084.17551	54958.43694	53731.47321	49920.69676	51090.11477	43859.74227	49438.12471	47653.27217	
4.99_521.1129n	522.1202075	4.991816667	pos							8011.174984	8555.135703	9086.650987	0.001403199	0.001403199	0.001403199	508.0470796	253.6594925	0.001403199	
5.01_123.1168m/z	123.1168147	5.013433333	pos							1615.114952	1630.553836	1694.422197	1541.905721	1478.059807	1515.836216	1477.833094	1606.098656	1565.879512	
5.01_268.2014m/z	268.2014237	5.013433333	pos							884.7899208	852.1213156	943.1166879	298.4120103	460.2663197	326.5320977	467.0222165	743.5434761	646.2290336	
5.01_289.1019m/z	289.1018929	5.013433333	pos							493.4526147	538.6055601	555.3257071	855.4492024	557.4433932	734.4401022	502.3146097	494.0911625	569.834476	
5.01_324.2143n	347.2035753	5.013433333	pos							9772.288326	23391.72514	12508.24517	73698.72171	19.8803397	924.3131115	4091.176226	13756.8957	1749.415534	
5.01_362.1903m/z	362.1902766	5.013433333	pos							380.3722767	228.9495941	1099.078723	411.29982	1207.202207	402.5271667	0.001403199	259.0529969	129.2683101	
5.01_413.6519m/z	413.6518517	5.013433333	pos							883.2608636	1087.921115	1089.404905	1019.88759	1395.601448	1122.736064	1180.251953	853.7009946	1236.004046	
5.04_194.1079m/z	194.1078657	5.035783333	pos							2264.296494	1719.191074	1846.922179	1242.194999	609.900357	1117.893082	1315.58909	447.2131002	787.7807599	
5.04_263.1188n	264.1260912	5.035783333	pos							6047.172838	5838.938303	6793.33228	7947.032121	7084.351722	7483.741714	6789.394786	7395.474689	7692.245078	
5.04_279.1103n	280.1176248	5.035783333	pos							1673.966734	2048.607808	1892.022539	3113.991025	3041.119656	3286.704153	2352.512819	2375.160255	2576.17411	
5.04_354.2270m/z	354.2269606	5.035783333	pos							1494.83354	1795.843298	1938.495434	4451.881616	3104.261826	3173.633159	1860.477865	2220.627213	2282.858621	
5.06_124.0534m/z	124.0534232	5.058233333	pos							0.001403199	0.001403199	0.001403199	6499.723393	6276.79007	6186.338401	0.001403199	0.001403199	0.001403199	
5.06_124.5551m/z	124.5550846	5.058233333	pos							0.001403199	0.001403199	0.001403199	858.5668555	888.4785466	770.2246491	0.001403199	0.001403199	0.001403199	
5.06_141.9585m/z	141.95846	5.058233333	pos							1212.031428	1212.512373	1188.356815	1173.196397	1290.678963	1217.926808	1328.880914	1254.203253	1298.181123	
5.06_144.5665m/z	144.566522	5.058233333	pos							313.9917589	749.6153714	304.8612789	3286.40199	3482.036226	3187.136245	470.4345854	666.7308306	481.5090926	
5.06_174.1122m/z	174.1121796	5.058233333	pos							1406.942688	1480.787242	1405.042744	1575.569456	1598.82392	1637.463173	1109.696818	1280.952821	1116.998444	
5.06_229.0655n	247.0993254	5.058233333	pos							71.57554761	197.3555463	79.97382897	59044.72206	53044.23561	53684.695	71.18290388	126.6804877	68.64655133	
5.06_231.0625n	249.0963676	5.058233333	pos							0.582677945	0.001403199	0.001403199	18419.41256	16190.8668	16290.22826	0.001403199	0.001403199	0.001403199	
5.06_237.1690m/z	237.1689916	5.058233333	pos							659.4617797	1359.785136	504.478391	640.7509554	920.7615069	418.2259023	898.7594702	878.7515411	522.3636842	
5.06_246.1333m/z	246.1332907	5.058233333	pos							301.6763086	439.2335219	308.5138797	268.5283178	187.4839535	157.1376026	312.0917062	359.0561928	154.1576411	
5.06_257.1453n	280.1346209	5.058233333	pos							1642.490344	1547.52494	1828.02849	1866.514376	1523.312536	1708.730696	1747.640204	1516.693125	1635.246143	
5.06_261.1480m/z	261.1479813	5.058233333	pos							668.2310525	560.9710569	775.7781617	1081.555437	777.3080596	843.9681753	588.229184	730.2252016	604.3048742	
5.06_278.1054m/z	278.1053977	5.058233333	pos							2301.056341	2698.722085	2522.225589	4305.266038	3772.814305	3656.270427	2195.670104	2354.118906	2472.272052	
5.06_372.1446m/z	372.1446204	5.058233333	pos							301.2821862	300.4331098	187.2469499	716.9984293	795.8959048	736.7128907	324.0902625	141.4569863	161.1010196	
5.08_186.1206m/z	186.1206098	5.081	pos							154.9838395	231.6260083	114.7599125	152.9595195	71.15910726	55.23593293	130.8350403	160.1115669	164.4218281	
5.08_213.1119m/z	213.1118503	5.081	pos							536.2559991	556.7493095	475.1250682	567.3699239	614.1114041	527.3764624	447.6182453	498.3669103	499.7750865	
5.08_224.0113m/z	224.0112999	5.081	pos							913.4754361	933.9736416	850.061986	805.9410148	1035.598655	835.3937153	894.0936464	788.0162201	912.2032471	
5.08_302.1958m/z	302.1958429	5.081	pos							5173.242054	4913.506512	5754.732654	9413.587971	9828.293467	9091.521584	5189.707954	5588.984622	5462.849631	
5.08_327.2042n	328.2114345	5.081	pos							30176.84464	31052.57188	33925.54514	45075.41746	40880.16126	40884.91666	32296.2922	35526.00754	35295.66217	
5.08_446.1895n	469.1794363	5.081	pos							6768.305163	7272.793654	7270.940197	14538.07605	15400.16178	15478.83477	8505.422219	8940.450031	8369.300031	
5.10_215.0887m/z	215.0887421	5.103066667	pos							636.9527326	603.3600563	617.1591517	600.7858866	625.7114859	609.2698085	757.4931327	623.2500842	630.2764661	
5.10_247.1074m/z	247.1073666	5.103066667	pos							1912.953814	2167.286671	1841.064079	2061.898383	2326.850706	2297.140927	2507.389703	2205.375084	1969.529293	
5.10_259.1516n	259.1516151	5.103066667	pos							720.6364956	569.9182924	829.5603783	1106.636554	1165.718107	507.4704556	636.5755905	591.4626217	529.8993036	
5.10_384.1777n	407.1671009	5.103066667	pos							8015.034154	7818.93837	9721.36622	5789.316272	5056.413442	5598.453681	9654.871379	7607.969979	8452.894259	
5.13_110.0171m/z	110.0171099	5.125733333	pos							5.969386199	0.001403199	10.99928071	0.001403199	0.001403199	0.001403199	7.480563227	5.57447588	7.364093504	
5.13_119.0492m/z	119.0491843	5.125733333	pos							85.63771344	165.4063953	94.86010303	89.70564873	219.0857651	153.1795828	183.1107706	222.7533031	138.7034362	
5.13_165.0545m/z	165.054481	5.125733333	pos							305.1467766	310.444315	199.423744	272.0976707	218.9687862	205.1550503	298.1336118	290.47501	211.9488972	
5.13_171.0344m/z	171.0343755	5.125733333	pos							369.4451004	358.6900625	309.0703332	343.3167784	373.1733287	352.4162595	375.765037	298.9493461	280.63111	
5.13_250.0447m/z	250.0447233	5.125733333	pos							2555.139705	2735.885548	2539.960583	4864.575603	4965.637772	4559.86199	5527.869617	4621.915742	4416.385634	
5.13_257.1374m/z	257.1373799	5.125733333	pos							638.1595364	753.8169365	777.4660408	856.3379588	854.1783273	889.7476809	683.734483	812.6644518	624.0827741	
5.13_261.1306m/z	261.1305682	5.125733333	pos							848.2859459	913.7788508	843.6948292	365.0313776	825.2042872	663.4734728	916.2777689	704.5740207	839.9471471	
5.13_270.1576n	271.1648524	5.125733333	pos							3807.202349	4160.41195	4133.187886	7305.436286	7094.861233	7133.843344	4624.533759	3634.48888	3665.077742	
5.13_288.1082n	289.1155209	5.125733333	pos							14667.73366	14823.57914	14684.14532	10482.16501	9997.600986	10442.21734	19028.35757	15193.73436	14841.19982	
5.13_342.1342m/z	342.1342026	5.125733333	pos							343.0939812	282.6548551	408.6150576	602.2252375	407.1320986	353.024723	421.1213682	492.6985076	525.472692	
5.13_358.1236n	359.1308872	5.125733333	pos							16306.23653	18945.58169	16622.16571	23980.1024	22161.65275	23298.66638	20155.56818	15879.36615	15655.30032	
5.13_362.1991m/z	362.1991197	5.125733333	pos							4612.251521	3634.605561	4991.010801	4600.891285	3692.929758	4295.017635	3026.492043	2716.180388	3290.626721	
5.13_472.1915n	473.1989184	5.125733333	pos							22571.49201	23971.8147	24623.13593	28412.6361	27188.19165	29687.26776	27283.54608	26718.54852	25158.82812	
5.15_113.0346m/z	113.0346394	5.148116667	pos							639.8533871	670.1414182	612.2375295	607.5099367	632.3168285	570.3383905	658.0258172	591.0730743	673.5652058	
5.15_137.1323n	137.1323016	5.148116667	pos							364.8898607	342.5734536	328.9283506	276.3126204	281.8118358	280.6455754	402.3548726	324.5579834	321.1015757	
5.15_163.0388n	163.0388449	5.148116667	pos							1074.961971	897.8351891	810.8437502	768.8412311	846.0115013	816.4300286	852.0128251	877.6370163	782.9424563	
5.15_170.1254m/z	170.1254361	5.148116667	pos							78.35877754	54.60294718	41.62425299	86.11524266	73.75433895	43.87609294	19.20975543	83.3753109	57.86308389	
5.15_185.0807m/z	185.0806754	5.148116667	pos							2794.94824	2685.259945	2679.322095	2335.503424	2546.092138	2403.885725	2998.37258	2509.854102	2760.059381	
5.15_201.1362n	202.1434493	5.148116667	pos							3887.176752	3914.76503	3701.213692	3543.212932	3499.12203	3440.049812	4274.789647	3407.995617	3797.220733	
5.15_244.1308n	267.1200822	5.148116667	pos							18032.77463	17974.40868	17999.92145	27289.17556	25938.52506	25244.30039	18357.76595	20416.4634	19917.39132	
5.15_253.6521m/z	253.652099	5.148116667	pos							164.9718305	151.7664871	176.8667828	208.3230392	186.7566408	168.7206661	110.8317696	95.4562227	67.51040874	
5.15_258.1577n	281.1468437	5.148116667	pos							11903.32842	10592.57638	10931.87675	18330.94232	17127.4369	17055.20163	10855.55579	11647.31796	11842.4731	
5.15_260.9801m/z	260.9800749	5.148116667	pos							3734.420779	3310.523901	3671.580399	0.001403199	35.48414739	15.18492293	2843.558891	2948.908101	2775.98479	
5.15_283.1527m/z	283.1527018	5.148116667	pos							590.0692516	728.8658528	661.8421279	627.2862966	524.2687038	609.4885901	548.5373651	673.5385251	630.0604384	
5.15_313.1619m/z	313.1619469	5.148116667	pos							1493.248503	1465.029022	1571.14097	1370.146039	1382.111998	1284.214269	1127.220124	1406.074455	1315.339039	
5.15_347.1696m/z	347.1696453	5.148116667	pos							1276.970383	1801.622174	1485.505506	634.6772318	694.5026547	696.8421696	1612.960737	1028.755098	1616.347685	
5.17_128.9710m/z	128.97098	5.1709	pos							192.5666794	157.9451291	160.5570577	146.6220563	215.001161	160.55914	193.4473532	179.5381605	163.1283157	
5.17_136.0836m/z	136.0836116	5.1709	pos							101.8749555	23.99847043	50.83819744	48.28392651	70.28891177	45.69021413	35.3295419	68.30725813	81.70405639	
5.17_184.0029m/z	184.0029315	5.1709	pos							524.5819177	479.4025044	488.2393942	541.1142987	614.8640011	560.7887334	664.3710912	554.5135078	564.8700366	
5.17_201.0731m/z	201.0731245	5.1709	pos							627.1056654	547.4684993	506.9388886	538.4428939	514.4355801	503.2346477	557.5400225	577.6762314	532.250923	
5.17_202.1025n	220.1363712	5.1709	pos							27738.99431	27902.48902	28825.34686	42777.34627	41399.83423	39481.51156	23346.28762	26417.70527	29152.09477	
5.17_262.1470m/z	262.1470048	5.1709	pos							305.9128831	291.6912764	409.3924665	389.4776108	383.7796717	425.146466	147.6497385	417.8152662	352.465338	
5.17_295.1514m/z	295.1513541	5.1709	pos							9962.101924	10610.15446	10828.49143	9828.600669	8539.394434	8334.865341	8022.713654	7912.115749	8292.953806	
5.17_317.1335m/z	317.1334592	5.1709	pos							675.7400164	580.4585711	600.5518717	521.3708528	500.3619525	500.530759	404.0286532	376.2519154	531.1162254	
5.17_442.2132n	443.2204549	5.1709	pos							147680.8879	147344.4216	154759.2792	93221.44367	84172.08725	81548.88382	124655.3819	138712.4024	133414.4893	
5.17_486.1731n	509.162478	5.1709	pos							79061.59339	76960.63417	79574.64664	78927.30294	75240.35773	72538.34498	66829.70466	74754.31372	73218.46466	
5.19_125.9862m/z	125.9861763	5.193566667	pos							738.7008504	695.976968	673.8152119	680.4646953	711.0997185	702.6471295	989.9588045	696.4706738	718.2220551	
5.19_131.0612m/z	131.0611575	5.193566667	pos							576.9532287	591.8286174	534.336159	8017.074512	7847.044239	7933.296471	610.9500949	477.6908998	512.1427273	
5.19_230.0728m/z	230.0727822	5.193566667	pos							33.45018047	1.43659463	0.064852129	20513.27033	20769.33522	18948.48226	0.027408677	0.001403199	0.001403199	
5.19_243.9774m/z	243.977412	5.193566667	pos							6115.4144	5372.138051	5404.69705	5499.220316	5639.014567	5585.302198	6702.051014	5352.499664	5647.485542	
5.19_334.2044m/z	334.2043949	5.193566667	pos							1841.230208	1956.762658	2248.647838	2241.212728	2303.16186	2199.272145	1497.359503	1396.141791	1592.444227	
5.22_131.5628m/z	131.5627928	5.21595	pos							0.001403199	0.001403199	0.001403199	0.001403199	1087.923317	1072.256386	1185.427051	0.001403199	0.001403199	
5.22_151.5743m/z	151.5743447	5.21595	pos							0.001403199	0.001403199	0.001403199	1806.386311	1897.97631	1897.989298	0.001403199	0.001403199	0.001403199	
5.22_152.0759m/z	152.0758945	5.21595	pos							14.98265637	0.001403199	22.76183386	183.9859961	201.9822889	249.5445677	2.409905811	14.30096145	0.001403199	
5.22_202.9509m/z	202.9508665	5.21595	pos							1646.52343	1588.957676	1532.534997	1572.047337	1615.883299	1554.123963	2065.775642	1472.863251	1703.486847	

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5.50_372.2376m/z	372.2375645	5.49815	pos
5.50_385.1464m/z	385.1463907	5.49815	pos
5.52_231.5667m/z	231.5666629	5.5209	pos
5.52_296.2429m/z	296.2428777	5.5209	pos
5.52_362.0972n	363.1044319	5.5209	pos
5.52_438.0690m/z	438.069048	5.5209	pos
5.52_453.0738m/z	453.0737513	5.5209	pos
5.54_152.1149m/z	152.1148881	5.543066667	pos
5.54_180.0443m/z	180.0443388	5.543066667	pos
5.54_242.0575m/z	242.0575154	5.543066667	pos
5.54_395.0416m/z	395.0416411	5.543066667	pos
5.54_443.0453m/z	443.0452941	5.543066667	pos
5.54_445.0420m/z	445.0419668	5.543066667	pos
5.56_120.0237m/z	120.0237444	5.56405	pos
5.56_142.0699m/z	142.069912	5.56405	pos
5.56_224.9327m/z	224.9327196	5.56405	pos
5.56_304.1575m/z	304.1574608	5.56405	pos
5.56_387.1623m/z	387.1622708	5.56405	pos
5.56_525.2691m/z	525.2690975	5.56405	pos
5.58_123.1168m/z	123.1168183	5.581883333	pos
5.58_130.0862m/z	130.0861639	5.581883333	pos
5.58_180.1591m/z	180.1591495	5.581883333	pos
5.58_190.1203n	173.117055	5.581883333	pos
5.58_268.1284n	269.1356463	5.581883333	pos
5.58_645.2013m/z	645.2013464	5.581883333	pos
5.58_654.2203n	637.2169691	5.581883333	pos
5.59_107.9670m/z	107.9670163	5.590966667	pos
5.59_276.1626m/z	276.1625622	5.590966667	pos
5.59_277.1345n	278.1417527	5.590966667	pos
5.59_310.6108m/z	310.6108353	5.590966667	pos
5.59_335.1460m/z	335.1459608	5.590966667	pos
5.61_208.6268m/z	208.6267529	5.613933333	pos
5.61_244.1307n	267.1199571	5.613933333	pos
5.61_253.1504m/z	253.1503524	5.613933333	pos
5.61_253.6520m/z	253.651988	5.613933333	pos
5.61_282.1580n	283.1653037	5.613933333	pos
5.61_289.1018m/z	289.10183	5.613933333	pos
5.63_141.9585m/z	141.9584995	5.633433333	pos
5.63_178.9904m/z	178.9903805	5.633433333	pos
5.63_185.1414n	208.1305489	5.633433333	pos
5.63_197.9922m/z	197.9922329	5.633433333	pos
5.63_239.0886m/z	239.0885904	5.633433333	pos
5.63_243.9413m/z	243.9413433	5.633433333	pos
5.63_302.2321m/z	302.2320551	5.633433333	pos
5.63_364.1962m/z	364.1962454	5.633433333	pos
5.66_104.0305m/z	104.0305204	5.656316667	pos
5.66_182.1417n	205.130911	5.656316667	pos
5.66_185.0808m/z	185.0807745	5.656316667	pos
5.66_243.9774m/z	243.9774195	5.656316667	pos
5.66_369.2244m/z	369.2244236	5.656316667	pos
5.66_431.1884m/z	431.1884038	5.656316667	pos
5.66_467.1880m/z	467.1879704	5.656316667	pos
5.68_155.0700m/z	155.0700134	5.675716667	pos
5.68_173.0852m/z	173.0851535	5.675716667	pos
5.68_221.1160m/z	221.1160244	5.675716667	pos
5.68_313.1752m/z	313.1751661	5.675716667	pos
5.68_347.2303n	330.2270226	5.675716667	pos
5.68_400.2688m/z	400.2688237	5.675716667	pos
5.68_459.1806m/z	459.1806475	5.675716667	pos
5.70_113.1074m/z	113.1074463	5.69755	pos
5.70_215.0887m/z	215.0886842	5.69755	pos
5.70_270.1697m/z	270.1697331	5.69755	pos
5.70_287.2205n	310.2095911	5.69755	pos
5.70_297.1670m/z	297.1669636	5.69755	pos
5.70_385.1464m/z	385.1463537	5.69755	pos
5.70_387.1622m/z	387.162238	5.69755	pos
5.72_104.0708m/z	104.0708486	5.720466667	pos
5.72_243.1570m/z	243.1569952	5.720466667	pos
5.72_270.1576n	293.1466986	5.720466667	pos
5.72_311.1729n	294.1696462	5.720466667	pos
5.72_470.1577m/z	470.1577073	5.720466667	pos
5.72_562.2380n	585.2274476	5.720466667	pos
5.72_635.2011m/z	635.2010768	5.720466667	pos
5.74_130.0862m/z	130.0861907	5.743266667	pos
5.74_199.0937m/z	199.0937339	5.743266667	pos
5.74_233.1049n	234.1121847	5.743266667	pos
5.74_366.2043m/z	366.204307	5.743266667	pos
5.74_542.2721n	565.2613138	5.743266667	pos
5.77_228.1187n	246.1519679	5.7661	pos
5.78_121.0284m/z	121.0284176	5.778566667	pos
5.78_131.5522m/z	131.5522441	5.778566667	pos
5.78_180.0443m/z	180.0442775	5.778566667	pos
5.78_184.0028m/z	184.0028152	5.778566667	pos
5.78_216.9226m/z	216.9225564	5.778566667	pos
5.78_256.5935m/z	256.5934728	5.778566667	pos
5.78_403.2323m/z	403.2323317	5.778566667	pos
5.79_129.1273m/z	129.1273036	5.790983333	pos
5.79_224.0114m/z	224.0114136	5.790983333	pos
5.79_224.9325m/z	224.9324801	5.790983333	pos
5.79_287.1752m/z	287.1752037	5.790983333	pos
5.80_206.1516n	229.1407528	5.799666667	pos
5.80_455.2242m/z	455.2242073	5.799666667	pos
5.82_161.5611m/z	161.5611411	5.821	pos
5.82_181.5727m/z	181.5727341	5.821	pos
5.82_207.1588m/z	207.1588201	5.821	pos
5.82_251.1849m/z	251.1848961	5.821	pos
5.82_296.0577m/z	296.0577304	5.821	pos
5.84_176.9716m/z	176.9715737	5.843716667	pos
5.84_257.6012m/z	257.6012043	5.843716667	pos
5.84_258.1030m/z	258.1030087	5.843716667	pos
5.84_313.1754m/z	313.1754292	5.843716667	pos
5.84_478.1787n	479.1859284	5.843716667	pos
5.84_488.1334m/z	488.1333529	5.843716667	pos
5.84_511.1227m/z	511.1226694	5.843716667	pos
5.87_125.9862m/z	125.9861933	5.8665	pos
5.87_163.0388m/z	163.038754	5.8665	pos
5.87_302.2226m/z	302.2225838	5.8665	pos

3050.745323	3653.396057	4284.317871	2805.849486	2674.237121	2699.583332	2185.912356	2462.32871	2586.213213	
12720.17295	15099.06174	14690.50188	11636.8063	11625.60891	11470.68764	13572.18294	13725.84165	13132.48131	
382.6406293	366.1973421	342.5623588	146.24757	106.4952587	143.1463539	391.2158912	342.655947	412.6073037	
728.6275258	928.9572114	793.679251	689.272454	706.8978035	536.6685416	963.3858433	802.6885837	645.469061	
186177.5005	199226.6128	211328.5934	64743.18168	61204.36697	64988.21662	180881.4995	164969.2664	171665.4912	
829.0837971	973.8797456	851.1310899	128.2917718	129.753861	0.001403199	632.9469665	653.2048244	765.1806062	
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156.9369324	185.1955806	165.8355931	145.5453779	151.4356552	162.2770852	166.5730458	174.217514	204.8002466	
970.7590966	905.9957545	956.5777986	668.3614044	727.9772584	712.3444777	1086.973976	887.3081966	787.8144842	
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1994.013279	1979.165246	1819.487143	626.6105983	552.3228591	641.2095928	1882.648359	1788.755591	1762.424166	
491.6930516	579.4684579	475.2674296	125.5090367	180.9296638	202.1978683	570.2788	451.1612644	276.8811494	
343.0042369	359.7641626	313.9494958	285.8122223	303.6618253	308.8264339	284.4884401	363.47948	395.3788654	
133.552966	112.2925101	161.8373841	112.8397249	139.667009	157.3246558	197.7498131	152.5457821	170.1018433	
1559.756969	1238.933598	1459.31171	1138.675129	1196.066593	1199.789707	1737.460354	1584.856502	1256.764857	
2317.379064	2443.503127	2407.141588	2452.971583	2294.87308	2450.942778	2908.751696	2862.203591	2815.471973	
2478.159161	3153.484074	1984.986054	2695.881062	2965.574046	2756.75214	2621.006999	2350.324171	2162.928891	
2873.308408	2254.448984	1612.652245	2896.014494	3005.298234	2860.812091	2074.498758	2160.872255	2019.25271	
448.8460548	406.7634942	363.4311189	291.0550494	403.9316689	257.4738806	403.5251526	364.020267	369.607018	
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1948.361644	1876.687376	1758.069693	1625.324573	1790.579144	1654.065707	2277.822505	2100.710016	2026.396165	
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939.865417	1281.433716	1688.37389	2141.066779	2242.802546	1965.486824	1204.635383	1613.224405	1175.191185	
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7312.703504	7411.883809	8308.488796	13937.15499	13643.56982	15627.70586	8005.608023	9071.247099	9306.665686	
4853.449772	5089.878826	5635.046205	7513.322601	7175.683045	8645.151405	6778.345771	6751.219987	8037.507227	
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20.61897117	21.88082105	50.9956708	55.52714758	33.33205561	58.27848355	0.001403199	23.07266903	38.20131181	
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748.5065708	790.1279492	662.1953557	1561.826854	1474.243803	1901.739272	599.1057597	557.4215252	764.6808254	
190.9634014	230.8250414	79.12642274	312.7742153	323.2410135	482.6843409	137.665239	156.6726856	155.0749287	
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320.7803484	318.0671691	215.4493287	351.8785217	437.4733769	423.4666646	420.8447424	274.9743455	343.5791326	
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1175.836552	1100.454373	893.6570939	922.5279071	1359.390486	1092.260835	1369.829908	997.4305219	993.5950637	
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681.304794	1017.219212	662.2302162	558.8377655	589.2469674	645.1535415	490.602444	455.0664207	715.3005365	
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717.7274834	686.3095983	494.2988286	644.3231635	782.0917029	726.233903	916.9811636	603.2889435	640.1431156	
573.7166518	543.3440547	418.3333867	393.1773437	544.60089	505.1251645	560.5936907	377.1763392	644.0705591	
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71806.3491	72135.08808	73307.83386	99776.93675	113028.3639	100804.3766	69418.12665	64359.33977	67124.79621	
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239.2550514	208.9105784	175.4357356	312.830712	308.9679564	305.1552361	334.3909013	249.9620237	283.6164205	
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373.7629232	460.5151947	334.8510189	256.5860674	320.4347578	229.5965491	355.4781362	227.9232332	297.0985384	
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9258.990631	9182.957265	9060.520298	8949.675639	8889.923356	7888.172476	6478.860947	5405.143703	5559.773639	
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16555.88922	16518.12964	15669.69362	37469.41039	34853.65839	32568.47753	21186.16403	16142.48768	16084.19407	
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1099.427293	1308.338054	1257.936488	2583.425802	2243.03592	2404.94781	1996.03929	1441.94388	1192.15814	
17829.29188	16575.11597	17607.00083	21240.56427	21683.24041	19897.47185	17546.81688	15564.0201	15755.57906	
4833.051634	4304.826757	4667.103907	5255.737323	5577.277488	4505.261534	4034.362681	4314.962269	3488.775091	
868.3567144	660.8296938	635.7700592	776.3739786	780.1416326	558.8900589	795.1777514	628.3585606	641.0396904	
2015.29891	1597.418366	1783.691824	1794.812032	1690.965632	1410.367988	1979.251152	1530.528693	1536.657172	
5954.003888	5928.251383	6117.883865	4837.266693	4613.098426	4287.181688	10596.62054	8112.020476	8706.103851	
766.896735	497.2914912	970.1994228	602.4111425	497.7299642	438.3978364	686.776944	562.5284231	681.387962	
119828.0602	124405.555	121633.2233	153214.2841	150708.0343	144043.2726	134769.6159	113383.827	115998.7562	
2232.047504	1899.470589	2103.038655	4563.15466	3696.926083	3723.174222	2214.051595	2152.708909	2132.029251	
308.1192397	297.1964379	284.4317239	280.5278038	275.7933372	275.9252958	334.7736307	377.2546075	377.9171243	
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432.5506475	503.3178914	384.0045135	451.4933623	304.0140805	422.787017	646.6290655	444.7236073	366.9676599	
3628.425403	2370.592462	2972.874603	4305.181852	3788.608	3407.539148	3395.658287	3235.445038	3180.524424	
899.1384986	674.2150054	645.3290672	762.5059125	855.2745951	755.0688412	895.6582992	656.634002	770.9897604	
1212.831463	817.3049938	1151.65808	1078.045562	1178.2351183	1045.643954	1026.854252	1092.777095	1061.539861	
1222.014398	986.109242	1268.833703	1304.437276	1346.741481	1239.080935	1246.346459	1217.603226	1329.771006	
620.2843443	513.2754639	585.9956114	235.847589	330.6953257	381.8064977	473.3967307	579.7302094	485.9333494	
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21.57170917	29.52989559	52.84890062	16.70940003	40.88966771	12.49095684	17.78296306	16.63209629	0.001403199	
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856.2438755	981.7552344	717.6941214	351.3522381	820.4497926	956.1027492	699.4331818	647.1274481	874.7093062	
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3865.204938	3973.823598	5049.041962	2889.751032	3056.816834	3174.38512	1811.411808	2397.988086	2779.315725	
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5.87_363.1783m/z	363.1782586	5.8665	pos
5.89_136.0214m/z	136.0213669	5.888383333	pos
5.89_297.1669m/z	297.1669108	5.888383333	pos
5.89_411.1621m/z	411.1620595	5.888383333	pos
5.91_185.0808m/z	185.0807611	5.9112	pos
5.91_201.0731m/z	201.0730887	5.9112	pos
5.91_210.0888m/z	210.0887921	5.9112	pos
5.91_223.1495m/z	223.1495293	5.9112	pos
5.91_236.1044m/z	236.1044062	5.9112	pos
5.91_246.1519m/z	246.1519195	5.9112	pos
5.91_267.1200m/z	267.1199541	5.9112	pos
5.91_369.2246m/z	369.2246068	5.9112	pos
5.93_277.1789m/z	277.1788808	5.933983333	pos
5.93_303.1432m/z	303.1432315	5.933983333	pos
5.93_330.2270m/z	330.2270264	5.933983333	pos
5.93_491.1415m/z	491.1415006	5.933983333	pos
5.93_542.2722n	565.2610652	5.933983333	pos
5.93_587.2430m/z	587.2429968	5.933983333	pos
5.96_202.1153m/z	202.115251	5.956833333	pos
5.98_113.0347m/z	113.0346789	5.97975	pos
5.98_144.0654m/z	144.0653743	5.97975	pos
5.98_180.0442m/z	180.0442006	5.97975	pos
6.00_104.0306m/z	104.0305577	5.995733333	pos
6.00_155.0701m/z	155.0700946	5.995733333	pos
6.00_170.9775m/z	170.9774527	5.995733333	pos
6.00_197.1171m/z	197.1170656	5.995733333	pos
6.00_217.9982m/z	217.9982259	5.995733333	pos
6.00_243.9774m/z	243.9774274	5.995733333	pos
6.00_425.2138m/z	425.213835	5.995733333	pos
6.00_562.2384n	563.2456333	5.995733333	pos
6.01_216.9226m/z	216.9225523	6.01315	pos
6.01_549.2664m/z	549.266386	6.01315	pos
6.02_111.5369m/z	111.536854	6.02225	pos
6.02_273.1802m/z	273.1801836	6.02225	pos
6.02_424.1995m/z	424.1994712	6.02225	pos
6.03_110.1047m/z	110.1046616	6.03205	pos
6.03_181.1584m/z	181.1583905	6.03205	pos
6.03_208.0391m/z	208.0391202	6.03205	pos
6.03_237.1483m/z	237.1482934	6.03205	pos
6.03_455.1882m/z	455.188185	6.03205	pos
6.03_531.2038m/z	531.2037877	6.03205	pos
6.04_210.0890m/z	210.0890265	6.041083333	pos
6.04_216.9224m/z	216.9223915	6.041083333	pos
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6.05_164.9203m/z	164.9203292	6.0535	pos
6.05_193.9989m/z	193.9988668	6.0535	pos
6.05_297.1670m/z	297.1669796	6.0535	pos
6.05_410.1549n	411.1621758	6.0535	pos
6.05_412.1706n	413.1778587	6.0535	pos
6.07_186.1487m/z	186.1486546	6.071983333	pos
6.07_239.1485m/z	239.1485067	6.071983333	pos
6.07_319.8811m/z	319.8811059	6.071983333	pos
6.07_360.2640m/z	360.264033	6.071983333	pos
6.07_402.2846m/z	402.2846044	6.071983333	pos
6.07_406.2068m/z	406.2067507	6.071983333	pos
6.08_141.9586m/z	141.9585626	6.084383333	pos
6.08_176.0828m/z	176.0827643	6.084383333	pos
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6.09_111.5368m/z	111.5368443	6.093533333	pos
6.09_130.0862m/z	130.0862277	6.093533333	pos
6.09_331.2088m/z	331.208809	6.093533333	pos
6.09_408.2223m/z	408.2223341	6.093533333	pos
6.10_125.9862m/z	125.9862396	6.104466667	pos
6.10_190.0033m/z	190.0032811	6.104466667	pos
6.11_244.1541m/z	244.154096	6.113683333	pos
6.11_270.1519m/z	270.1519249	6.113683333	pos
6.11_464.1912m/z	464.1911934	6.113683333	pos
6.13_104.0305m/z	104.03054	6.128133333	pos
6.13_227.1638m/z	227.1638381	6.128133333	pos
6.13_403.2323m/z	403.2323401	6.128133333	pos
6.14_184.0029m/z	184.0028573	6.140733333	pos
6.14_217.9982m/z	217.9982134	6.140733333	pos
6.14_294.9388m/z	294.9388093	6.140733333	pos
6.15_123.1169m/z	123.1168624	6.149866667	pos
6.15_163.9881m/z	163.9881191	6.149866667	pos
6.15_189.0656m/z	189.0656442	6.149866667	pos
6.15_216.9225m/z	216.9224649	6.149866667	pos
6.15_420.1027n	421.1099874	6.149866667	pos
6.16_113.0347m/z	113.0347284	6.162416667	pos
6.16_362.0973n	363.1045517	6.162416667	pos
6.17_319.8809m/z	319.8809393	6.17335	pos
6.17_529.2614m/z	529.261375	6.17335	pos
6.18_144.0654m/z	144.0653727	6.182466667	pos
6.18_203.1429m/z	203.1428956	6.182466667	pos
6.18_296.1730n	297.1802871	6.182466667	pos
6.20_125.9862m/z	125.9861913	6.1979	pos
6.21_123.1168m/z	123.1168393	6.20705	pos
6.21_131.9742m/z	131.9741648	6.20705	pos
6.21_140.9511m/z	140.951077	6.20705	pos
6.21_176.9717m/z	176.9717437	6.20705	pos
6.21_190.0034m/z	190.0033754	6.20705	pos
6.21_281.2261m/z	281.2260949	6.20705	pos
6.21_286.2373m/z	286.2372663	6.20705	pos
6.22_209.1535m/z	209.1534578	6.216316667	pos
6.22_269.1743m/z	269.1743265	6.216316667	pos
6.22_310.1524n	311.1597027	6.216316667	pos
6.23_204.0865m/z	204.086461	6.22895	pos
6.23_210.0889m/z	210.0888966	6.22895	pos
6.23_217.9982m/z	217.9981694	6.22895	pos
6.23_578.2026m/z	578.2026209	6.22895	pos
6.24_509.2851m/z	509.2850968	6.23805	pos
6.24_585.1807m/z	585.1807201	6.23805	pos
6.24_621.2306m/z	621.2305519	6.23805	pos
6.24_653.3995m/z	653.3995421	6.23805	pos
6.25_107.9670m/z	107.9669941	6.2535	pos

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548.4759497	500.6927552	476.8031269	456.1585018	508.4327337	492.5814536	634.2145451	440.7206681	558.1937631	
7591.700126	7665.22462	8096.192931	7118.089166	6646.099519	6438.962751	4160.606068	4557.196683	4522.41152	
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2595.149305	1974.484003	2163.183102	2321.123406	2274.89769	2448.225122	2283.77757	2441.713296	2543.021079	
56.03070338	81.83710571	71.61406281	96.11271485	66.9824463	189.0047581	153.1234557	107.2257332	121.9496229	
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5825.74376	6870.543527	6449.070662	9430.847903	9153.692705	9649.697263	5191.603034	5619.059887	5886.176307	
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6953.424109	6921.56714	7129.799063	11108.8559	11414.96362	11586.76796	10603.97819	12111.84512	10072.50153	
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6.26_176.9717m/z	176.9717042	6.262533333	pos
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6.31_164.9203m/z	164.9202782	6.308766667	pos
6.31_266.5876m/z	266.5875978	6.308766667	pos
6.31_488.1332m/z	488.1332136	6.308766667	pos
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6.32_107.9670m/z	107.9669981	6.323133333	pos
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6.36_289.0946n	290.1018693	6.355166667	pos
6.36_403.2320m/z	403.2320417	6.355166667	pos
6.37_178.9905m/z	178.9904509	6.366016667	pos
6.37_413.1778m/z	413.17782	6.366016667	pos
6.38_113.1074m/z	113.1074404	6.3814	pos
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6.38_136.0215m/z	136.0214623	6.3814	pos
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6.39_184.0029m/z	184.0028646	6.392283333	pos
6.39_292.1573m/z	292.1572504	6.392283333	pos
6.39_297.1672m/z	297.1672327	6.392283333	pos
6.39_415.1830m/z	415.1830052	6.392283333	pos
6.41_133.0647m/z	133.0647374	6.406516667	pos
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6.41_164.9203m/z	164.9202545	6.406516667	pos
6.41_176.9716m/z	176.9716151	6.406516667	pos
6.42_305.1293n	328.1184313	6.422383333	pos
6.42_358.2480m/z	358.248024	6.422383333	pos
6.44_102.0133m/z	102.0132639	6.43815	pos
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6.45_199.1570n	222.1461543	6.45055	pos
6.45_403.2320m/z	403.2320108	6.45055	pos
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6.48_113.0346m/z	113.0345731	6.476883333	pos
6.48_114.1278m/z	114.1277957	6.476883333	pos
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6.48_193.0062m/z	193.0062091	6.476883333	pos
6.49_161.1363m/z	161.1363337	6.485983333	pos
6.49_197.1170m/z	197.1170319	6.485983333	pos
6.49_208.0391m/z	208.0390998	6.485983333	pos
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6.50_190.0032m/z	190.003157	6.4952	pos
6.50_210.0889m/z	210.0888787	6.4952	pos
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6.51_634.3779m/z	634.3779015	6.509583333	pos
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6.52_167.1429m/z	167.142899	6.523916667	pos
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6.52_261.1305m/z	261.1305245	6.523916667	pos
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6.53_125.9862m/z	125.9861919	6.533083333	pos
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6.53_213.1484m/z	213.1484138	6.533083333	pos
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6.55_123.1168m/z	123.116798	6.5509	pos
6.55_201.0730m/z	201.0730334	6.5509	pos
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6.57_307.2010m/z	307.2010368	6.568316667	pos
6.58_104.0708m/z	104.0708346	6.584266667	pos
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6.58_184.0029m/z	184.0028699	6.584266667	pos
6.58_270.1697m/z	270.1696673	6.584266667	pos
6.58_292.1936m/z	292.1936409	6.584266667	pos
6.58_470.2147n	493.2037481	6.584266667	pos
6.60_140.9510m/z	140.9510122	6.599816667	pos
6.60_187.9875m/z	187.987537	6.599816667	pos
6.60_326.1956m/z	326.1956246	6.599816667	pos
6.61_104.0305m/z	104.0304841	6.613233333	pos
6.63_170.9774m/z	170.9774295	6.627483333	pos
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6.64_136.0214m/z	136.0214432	6.638433333	pos
6.64_210.0888m/z	210.0888461	6.638433333	pos
6.64_217.9982m/z	217.9981814	6.638433333	pos
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6.65_119.0492m/z	119.0491665	6.647516667	pos
6.65_297.1675m/z	297.1675146	6.647516667	pos
6.65_627.3610n	650.3499018	6.647516667	pos
6.66_511.2509m/z	511.2509318	6.657916667	pos
6.67_117.0573m/z	117.0573177	6.670416667	pos
6.67_216.9225m/z	216.922463	6.670416667	pos
6.67_403.2321m/z	403.2320897	6.670416667	pos
6.68_104.0305m/z	104.0305216	6.679616667	pos
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6.68_215.0888m/z	215.0887751	6.679616667	pos
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6.69_190.0033m/z	190.003286	6.690566667	pos

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340.8005273	424.0703183	384.3908403	333.5136556	436.0393377	528.9562469	260.3882823	418.4932176	234.5128119
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111.0868581	53.83272043	62.54437311	87.91710799	42.80151816	65.73052027	72.93630451	83.8657744	88.66760495
1940.852101	1652.29396	1317.090675	1470.89526	1882.24097	1536.901238	2052.647612	1934.636548	1819.613361
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8692.566217	10304.12758	9806.028447	13764.12599	13659.86101	13349.27097	8938.491832	10478.60808	8856.288927
496.4538956	524.0118722	432.7377213	569.2953286	580.6304451	695.8398786	690.6835254	552.5162388	702.810431
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97997.00527	98000.21584	81779.52615	128104.605	120074.5388	127128.2009	99297.64318	99931.29327	88721.18964
1396.919469	1236.491012	1060.365563	1597.505246	1433.055167	1654.184875	1038.084219	1250.642517	813.6037546
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86875.64223	85886.0248	76892.65882	75911.26089	81977.79074	79767.81682	97870.94453	87935.70946	86843.04962
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767.3867627	1097.104325	786.807012	755.506383	923.1944498	1069.186787	1215.651798	818.2476541	709.975804
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262.0804245	207.5242348	213.7152906	1149.926282	1376.943966	1632.97551	0.001403199	0.001403199	0.001403199
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6.71_177.1020m/z	177.10202	6.709016667	pos
6.71_243.9414m/z	243.9413663	6.709016667	pos
6.71_504.2796m/z	504.2796022	6.709016667	pos
6.72_113.0346m/z	113.0346344	6.7199	pos
6.72_136.0213m/z	136.0213202	6.7199	pos
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6.72_264.0596m/z	264.0596153	6.7199	pos
6.73_104.0709m/z	104.0708528	6.729133333	pos
6.73_193.0062m/z	193.0062363	6.729133333	pos
6.74_294.9385m/z	294.9384689	6.738266667	pos
6.75_102.0133m/z	102.0133032	6.748833333	pos
6.75_184.0028m/z	184.0027832	6.748833333	pos
6.76_140.9510m/z	140.951024	6.761383333	pos
6.76_190.0032m/z	190.0032487	6.761383333	pos
6.76_202.5089m/z	202.5089337	6.761383333	pos
6.76_202.9508m/z	202.9508245	6.761383333	pos
6.76_247.0914m/z	247.0913565	6.761383333	pos
6.76_403.2320m/z	403.2320454	6.761383333	pos
6.78_115.5572m/z	115.5572004	6.771913333	pos
6.78_393.1664m/z	393.1663688	6.771913333	pos
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6.78_401.1528m/z	401.1527987	6.771913333	pos
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6.78_791.3419m/z	791.3419481	6.771913333	pos
6.79_164.9202m/z	164.9202247	6.7933	pos
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6.79_279.8885m/z	279.8885265	6.7933	pos
6.81_154.9849m/z	154.9848699	6.810883333	pos
6.81_257.6546m/z	257.6545849	6.810883333	pos
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6.84_216.9224m/z	216.9223829	6.8409	pos
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6.86_104.0305m/z	104.0305168	6.8599	pos
6.86_245.2351n	246.2424148	6.8599	pos
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6.90_567.1524m/z	567.152449	6.8951	pos
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6.91_171.0623m/z	171.0623024	6.909216667	pos
6.91_221.0700m/z	221.0699799	6.909216667	pos
6.91_242.5836m/z	242.5836106	6.909216667	pos
6.91_408.1882n	409.1955003	6.909216667	pos
6.91_432.2717m/z	432.271726	6.909216667	pos
6.91_458.1357m/z	458.1356667	6.909216667	pos
6.92_164.9202m/z	164.9202045	6.919716667	pos
6.93_404.2012m/z	404.2012148	6.928783333	pos
6.93_788.5408m/z	788.5408049	6.928783333	pos
6.94_209.1533m/z	209.1533358	6.9443	pos
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6.97_319.8809m/z	319.8808862	6.974116667	pos
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7.03_227.1637m/z	227.1637069	7.025516667	pos
7.04_140.9510m/z	140.9510298	7.03765	pos
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7.04_176.9717m/z	176.9716566	7.03765	pos
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7.04_197.1534m/z	197.1534028	7.03765	pos
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7.07_403.2321m/z	403.2320982	7.069916667	pos
7.07_411.1619m/z	411.1618921	7.069916667	pos
7.08_269.1742m/z	269.1742107	7.078966667	pos
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7.09_164.9203m/z	164.920281	7.089616667	pos
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7.10_184.0027m/z	184.0027471	7.1021	pos
7.10_442.2329m/z	442.2328971	7.1021	pos
7.11_197.1170m/z	197.1169868	7.108583333	pos
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7.12_210.0889m/z	210.0888976	7.117716667	pos
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7.13_140.9511m/z	140.9510739	7.131	pos
7.13_322.1885n	323.1957517	7.131	pos
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7.14_393.1407m/z	393.1406801	7.13965	pos
7.16_132.5366m/z	132.5365643	7.16055	pos
676.3354913	588.3927673	516.9923236	557.2375689	574.3794555	604.4134601	631.2594306	664.63572	677.523863
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2337.851191	2971.331981	2538.790953	2707.65444	2719.513702	3360.894819	203.3392674	180.0549184	353.5559824
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5937.34988	5175.553943	4471.737396	4324.182343	4479.426303	4741.742644	5273.632868	5096.263795	4575.240993
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813.4030339	834.16872	747.0024834	778.7245099	1033.762147	738.7803627	922.8018565	838.8722114	1030.010362
1282.182792	1175.082129	901.1378469	1183.711076	1339.835275	1072.516396	1406.956497	1127.304452	1663.830916
812.3886652	888.1141643	793.9521333	750.9966667	905.7725733	775.13631	827.9793593	725.6421413	906.5510265
1073.480342	1396.859402	981.3513785	1013.066595	1097.831307	1076.120818	1527.281533	1087.954412	1291.684023
280.142726	251.3059539	252.1525567	353.9559928	394.3420835	320.1739296	267.1377004	232.776807	330.3189119
12987.31531	11247.68353	13950.97985	13301.68707	12629.46766	11401.18002	14381.89217	12052.95401	13408.57438
46.03135927	12.75476085	32.29770658	45.56552977	19.02326262	50.16411892	74.41398317	36.69139242	17.37836999
1648.382697	1887.158992	2052.550737	447.812459	440.0292083	473.0902074	1077.766423	744.4978638	1348.394692
581.6114487	878.1803468	903.6635678	46.16662003	226.1859638	121.7544987	348.4835157	206.8284492	412.1710883
1738.823288	1506.098833	1492.896125	88.05222572	150.0669994	254.0960956	730.9408413	789.7605245	809.0486963
165939.6625	158812.7458	177971.367	45665.24544	53074.6955	40838.63275	90522.96697	96299.08822	118205.6852
16714.47083	15462.64086	17504.63511	4502.357007	4275.940627	3469.607294	8525.126562	9101.393851	11845.30102
2275.018067	1981.660551	1951.172842	1757.666174	1899.478779	1761.278562	2487.245117	2006.61895	2330.117665
917.7273048	733.9665094	604.4426938	373.709058	398.7964803	384.5752092	593.6602321	474.5734537	520.7451263
1151.618258	928.8348205	786.8680558	605.980325	806.9202606	682.2750421	1119.715888	770.6649629	1141.816181
49.60214776	16.76761194	27.35691463	0.001403199	9.141096707	0.001403199	0.001403199	0.001403199	0.001403199
524.3568627	477.1588408	669.0471513	763.7189565	728.1922674	865.8895828	431.3906782	430.2517156	574.1671363
7342.342921	6860.159795	6299.684017	12429.9651	13656.36246	11302.64271	5002.876681	5252.00476	6228.459828
34.31897318	37.64402682	49.75029923	106.1336987	125.0694695	99.02692974	78.04241579	65.59271526	76.34993964
3109.492318	2745.052266	2238.523005	2998.427482	4234.499109	2910.366323	3951.948515	2719.256286	4224.374853
46861.71541	46595.35658	49150.4792	63146.1193	66555.76381	56157.62677	54452.31293	56198.67753	60986.8219
257.2120017	330.0279834	229.5146353	397.4054895	435.7607208	403.1274464	327.417888	268.6577995	309.5478259
68329.56814	53333.96373	58849.01064	49993.6499	71892.60314	80039.19078	69625.40052	36336.11568	65557.30685
708.2562369	856.4072634	531.9636565	1178.213854	960.1933936	867.9076031	1055.619214	871.0080853	884.0230417
1271.697713	1486.071498	1315.809142	2970.475098	3049.251351	2495.451028	1384.429124	1287.828479	1361.737354
54161.13609	52885.92851	52431.84215	59884.69964	58269.98907	53005.87526	47915.6634	48003.21653	52594.82931
550.8765691	450.314566	353.7458293	524.0702041	527.5391397	403.3259213	325.9840389	334.3891714	429.8089141
1377.162293	1000.399545	1203.010657	1583.75116	1318.273628	1301.511895	1365.185643	1324.906998	1196.088305
17105.7489	15847.32119	14813.66106	15698.42671	16634.08382	15052.74674	17618.72447	15581.55887	16505.36143
892.9398389	1128.086405	1078.47964	1625.142362	1561.045284	1553.507638	627.2609446	928.0404092	933.6804422
544.1439816	140.428951	2605.935745	0.001403199	91.17982249	0.001403199	0.001403199	131.6380133	154.7278556
2336.792518	143.197225	10525.58341	686.6734512	479.0462897	312.3961952	489.0966166	418.5284845	1172.328389
547.8451845	487.8176701	387.4682854	469.6043678	344.1326294	382.6990085	287.6849282	479.3925285	510.781904
488.5582112	501.8248786	337.6736374	563.7842597	411.5683738	411.1703999	393.964998	300.3677486	384.9863069
466.2567381	19.65115924	2180.17163	44.90895278	49.10955817	65.90710423	118.9044307	71.25114112	307.3967346
220.5847851	0.001403199	828.7716104	25.42238025	0.001403199	53.76340214	0.001403199	27.94374232	94.79580508
330315.9522	81510.85662	1084688.019	99018.08312	84611.80756	86888.74182	96072.22415	93547.13386	205110.5273
715.0168672	0.001403199	5973.767327	110.525635	0.001403199	75.68753527	0.001403199	51.93425941	562.2798529
1391.905945	0.001403199	4930.033331	244.9522151	268.453017	61.30146597	261.4184245	226.7217392	476.6867556
1083.000624	1095.378628	665.3442411	1361.192359	1213.225762	965.0368224	965.4022167	1147.560549	898.3733
533.6743347	580.7005052	992.3258292	539.5762609	530.603859	345.9953344	435.1905425	573.7521356	591.1043398
3899.051278	3067.067817	2215.579933	1873.29901	972.6753284	814.6821085	2365.109072	2276.59425	2489.096527
10151.51057	9723.237816	8067.688444	8457.174408	8660.548623	7863.334838	9780.654525	8587.289975	9072.573408
6974.009043	6703.471484	5755.723821	2640.696472	1915.531843	2371.897024	3322.947804	4447.588256	5397.128676
812.0475115	696.838313	667.716439	543.2274	564.7657406	501.2459459	629.0502256	604.4698895	636.3500099
29194.96903	29683.53163	31078.46884	53277.22438	49807.98595	48103.09638	28763.619	31739.7852	35192.52833
474.6885989	723.4953888	954.1320576	1088.713926	1258.101368	1272.771524	276.9626282	853.1629717	1087.495731
5175.749444	5034.738487	4814.688233	4674.304838	5883.018153	5141.464659	6075.413065	5088.265969	5242.330963
23.88844491	35.06983276	24.08850589	29.22996937	5.984059629	0.001403199	30.65981702	0.001403199	21.78201878
784.8155506	711.0636247	830.0494471	608.5034241	661.5953338	757.1763274	714.2251718	690.7569178	750.7988496
401.7095193	401.8611252	423.2883659	743.2025528	660.4118419	541.6820068	374.560824	325.8612232	414.0842571
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672.6110649	569.3354986	635.950109	622.5698981	776.5058383	735.0050085	829.9324115	635.2322275	623.2583253
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1812.332634	1966.190931	1969.950734	1942.270913	2021.390169	1819.760422	2385.599866	1877.914661	1876.121533
520.4658764	572.0751023	471.9731029	460.3844037	576.3315115	499.2568087	674.1114368	629.1253831	532.4143272
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1545.652013	1261.130295	1220.912875	1156.156005	1151.672696	1072.194202	1298.038746	1224.8203	1348.626822
4601.985471	3921.300691	3827.554062	3559.216913	3721.352348	3372.984572	4346.101274	3547.858418	3699.66494
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87.73439105	118.8629954	121.5784125	175.4140376	176.6975291	126.083578	177.217585	212.3634097	228.8535269
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3147.746382	3621.566253	3809.98071	2466.809415	2572.957664	2157.276138	3895.516847	3450.378848	3105.373465
1521.437666	2066.724754	1704.169607	1655.797275	1983.970719	1708.143684	2318.893181	2093.624988	1845.327708
474.3710288	626.9390345	483.822319	501.7602279	580.2176143	461.8328746	655.7002424	549.9828343	462.7993216
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217.1887153	184.3515918	255.619259	187.3080695	428.9665252	350.0207519	448.4832959	308.9742239	280.937413
2532.884782	3354.06546	3189.036541	3313.375595	4084.69973	3444.195743	5144.399646	3994.430145	4104.383527
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253.2076437	332.0439097	417.4950253	417.6304088	455.6301845	304.4865679	543.0012439	399.3986879	379.5379951
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179.1105068	46.92051842	60.4920394	90.61901522	67.25198904	122.6579956	107.2495717	103.3920782	105.4392012
1854.553487	2094.755987	2082.542566	3218.289019	3153.499662	3403.810408	2636.909966	2886.238199	2832.856497
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7.16_154.1356n	177.1271197	7.16055	pos
7.16_217.9981m/z	217.9981212	7.16055	pos
7.16_243.1831n	226.1797987	7.16055	pos
7.16_453.1725m/z	453.1724551	7.16055	pos
7.18_114.0734m/z	114.0733795	7.182883333	pos
7.18_256.1493n	274.1830726	7.182883333	pos
7.18_360.2643m/z	360.2643475	7.182883333	pos
7.22_113.0346m/z	113.0346213	7.221	pos
7.22_269.1743m/z	269.1743384	7.221	pos
7.23_215.1639m/z	215.1639212	7.230183333	pos
7.25_243.9773m/z	243.9773421	7.246116667	pos
7.26_164.9203m/z	164.9203316	7.25695	pos
7.26_280.6033m/z	280.6032543	7.25695	pos
7.26_480.2797m/z	480.2796769	7.25695	pos
7.27_190.0032m/z	190.0031909	7.274466667	pos
7.27_197.1170m/z	197.1169808	7.274466667	pos
7.27_216.9223m/z	216.9222636	7.274466667	pos
7.27_255.2315m/z	255.2314561	7.274466667	pos
7.27_302.1957m/z	302.1956815	7.274466667	pos
7.29_217.9790m/z	217.9790286	7.294266667	pos
7.29_334.6501m/z	334.6501017	7.294266667	pos
7.29_403.2320m/z	403.231996	7.285366667	pos
7.29_483.0324m/z	483.0324441	7.294266667	pos
7.29_540.9910m/z	540.991007	7.294266667	pos
7.29_577.0413m/z	577.0413476	7.294266667	pos
7.31_104.0305m/z	104.0304891	7.305883333	pos
7.31_125.9861m/z	125.9860903	7.305883333	pos
7.31_203.1429m/z	203.1428538	7.305883333	pos
7.31_210.0888m/z	210.0888149	7.305883333	pos
7.31_261.1306m/z	261.1305703	7.305883333	pos
7.31_342.2093m/z	342.2092736	7.305883333	pos
7.32_140.9510m/z	140.9509923	7.31785	pos
7.32_256.1493n	274.183043	7.31785	pos
7.33_235.1194m/z	235.1194474	7.332033333	pos
7.33_363.1772m/z	363.1771835	7.332033333	pos
7.34_366.2245m/z	366.2245421	7.3446	pos
7.35_161.0708m/z	161.0707816	7.353716667	pos
7.35_319.8809m/z	319.880857	7.353716667	pos
7.37_181.1584m/z	181.1583944	7.366316667	pos
7.37_197.1170m/z	197.1169744	7.366316667	pos
7.37_280.1494n	298.1830906	7.366316667	pos
7.37_614.3653n	597.362032	7.366316667	pos
7.38_125.9862m/z	125.9861663	7.382233333	pos
7.38_164.9203m/z	164.9203244	7.382233333	pos
7.39_215.0886m/z	215.0886101	7.39475	pos
7.39_216.9224m/z	216.9223803	7.39475	pos
7.39_403.2320m/z	403.2320493	7.39475	pos
7.40_209.1533m/z	209.1533213	7.403833333	pos
7.40_261.1303m/z	261.1302894	7.403833333	pos
7.41_197.1533n	197.1533456	7.414583333	pos
7.43_190.1203n	213.1093678	7.432366667	pos
7.43_203.1429m/z	203.1428644	7.432366667	pos
7.45_312.6417m/z	312.6416689	7.448183333	pos
7.45_332.6533m/z	332.6532881	7.448183333	pos
7.45_341.6396m/z	341.6396336	7.448183333	pos
7.45_362.6548m/z	362.6547918	7.448183333	pos
7.45_629.2896m/z	629.289571	7.448183333	pos
7.48_156.9850m/z	156.9850315	7.480483333	pos
7.49_164.9201m/z	164.9201131	7.4907	pos
7.49_169.9972m/z	169.9971783	7.4907	pos
7.49_193.0062m/z	193.0062106	7.4907	pos
7.49_215.1639m/z	215.1638783	7.4907	pos
7.49_217.9792m/z	217.9792039	7.4907	pos
7.49_272.5407m/z	272.5406702	7.4907	pos
7.50_366.2245m/z	366.2244904	7.4998	pos
7.50_368.1440n	391.133203	7.4998	pos
7.50_444.1157m/z	444.1156874	7.4998	pos
7.51_462.1959m/z	462.195922	7.50885	pos
7.52_131.9741m/z	131.9741041	7.5231	pos
7.52_190.0031m/z	190.0031445	7.5231	pos
7.54_158.0179m/z	158.0179167	7.535616667	pos
7.54_213.1845m/z	213.1845448	7.535616667	pos
7.55_444.2353n	445.2423504	7.553266667	pos
7.55_534.2797n	535.2870169	7.553266667	pos
7.58_294.9386m/z	294.9385729	7.5833	pos
7.58_651.3700m/z	651.3700199	7.5833	pos
7.59_651.8644m/z	651.8644321	7.592316667	pos
7.61_133.0647m/z	133.0647418	7.606533333	pos
7.61_216.9223m/z	216.9223315	7.606533333	pos
7.62_164.9202m/z	164.9202219	7.617316667	pos
7.64_270.1463n	293.1354611	7.637083333	pos
7.65_125.9861m/z	125.9861464	7.652983333	pos
7.65_447.2921m/z	447.2921424	7.652983333	pos
7.67_261.1304m/z	261.1304471	7.668366667	pos
7.67_437.8743m/z	437.8742844	7.668366667	pos
7.68_208.0390m/z	208.0390499	7.678416667	pos
7.68_221.1535m/z	221.1534953	7.678416667	pos
7.68_243.9773m/z	243.9773386	7.678416667	pos
7.68_247.1662m/z	247.1662202	7.678416667	pos
7.69_190.0033m/z	190.0032908	7.690416667	pos
7.69_210.0890m/z	210.0889521	7.690416667	pos
7.69_403.2320m/z	403.2320375	7.690416667	pos
7.70_155.1428m/z	155.1427744	7.699383333	pos
7.70_217.9790m/z	217.9790051	7.699383333	pos
7.70_319.8810m/z	319.8810355	7.699383333	pos
7.71_125.9862m/z	125.9861582	7.709666667	pos
7.71_170.9774m/z	170.9774138	7.709666667	pos
7.71_215.9833m/z	215.9832854	7.709666667	pos
7.71_243.9413m/z	243.9413225	7.709666667	pos
7.72_158.0178m/z	158.0178191	7.718733333	pos
7.73_651.3698m/z	651.369769	7.726266667	pos
7.75_128.9710m/z	128.9709669	7.748416667	pos
7.75_651.8645m/z	651.86449	7.748416667	pos
7.76_170.9774m/z	170.977429	7.759183333	pos
7.76_221.1533m/z	221.15333	7.759183333	pos
7.76_269.1741m/z	269.1741363	7.759183333	pos
7.77_156.1202m/z	156.1202126	7.768133333	pos

1151.896325	1429.396925	1454.606192	1513.262395	1520.721637	1546.855269	1668.29849	1493.984448	1557.335367
939.5659513	958.4583388	904.6857209	891.4736023	1235.132051	1190.446325	1443.81115	960.2752228	1275.799994
31922.37654	31093.2005	27392.24307	30443.23058	26246.5665	26609.18781	27783.58743	26961.37746	30644.21184
23842.74753	24619.16769	24504.18527	24758.42064	21979.84647	21745.04086	18642.83623	21751.67892	22128.0272
2165.493376	2073.704882	1942.455678	1894.544502	2114.161035	2110.803953	2497.466268	2062.11985	2190.433793
73299.52654	74071.61002	78984.76174	105269.6939	97042.83339	96987.06087	51749.76763	56279.88397	62403.19666
7604.847516	7275.54333	7817.800574	10097.85648	9007.074521	9099.992198	5795.502166	6675.930164	7089.11574
599.4561517	444.5168184	425.6640543	415.8520158	443.1469245	557.0498321	479.5677204	441.5636499	544.8785532
916.8449289	1075.422961	1029.701366	1197.971685	923.6354905	1059.750515	1113.258849	872.082513	1014.184172
1196.22653	1065.136861	1084.274243	1140.528363	994.9929465	1012.748212	1169.908784	976.4683881	1000.866413
6559.167539	5690.902224	5015.052104	5970.257256	5145.951156	6084.477289	5416.294893	5471.913284	6297.813517
901.8728477	735.0343107	682.5495377	985.9328198	822.2437661	803.2253748	707.8138598	840.7562295	861.7873476
365.4531625	315.1312791	438.4201421	492.1998531	313.7395305	322.5576522	274.3954059	546.4940042	679.5653863
6795.736428	8695.381889	8110.31498	8871.508852	7450.961653	8100.300483	9324.38086	10818.39242	11282.70404
1553.931941	1356.794176	1159.454272	1594.132673	1094.470587	1312.175077	1137.750215	1371.605956	1409.929848
931.2068302	668.4712549	699.2149162	727.8223525	542.835721	516.4257652	607.5761216	584.2369541	600.3987407
2049.137701	2311.690199	1651.911254	2202.854484	1905.207589	1469.433032	2184.592646	1906.505503	2176.352058
1959.173104	2181.165676	1760.406388	3118.821147	2717.29974	2804.697513	2083.842848	2214.151917	2235.040218
198.7879404	360.0666452	321.7564003	541.5762203	522.050114	434.0393271	329.0279952	385.3942627	243.8620262
699.1261691	652.0140026	599.6654531	810.9284773	799.5154649	837.955928	1074.02441	879.9240606	799.6355764
564.7837846	1421.651964	973.7421128	65.22758689	98.78586301	49.44630977	500.9817864	936.8265989	653.7293205
7214.67812	7061.278332	6732.014764	7491.897519	5468.054832	5853.37004	5885.376298	5979.373006	5837.624304
68688.59475	79945.31871	72774.62592	63838.82754	64130.04128	64084.39268	51177.58168	66153.75119	61541.17193
1987.137117	2273.249713	1842.571518	1604.720662	1431.329724	1335.028991	1307.99945	1780.97686	1420.67104
2718.815714	3928.310493	3368.107937	2422.27239	2483.702596	2280.639882	2004.412975	3062.490083	2196.170622
226.1219934	289.5423705	183.4650235	220.8033461	202.1024658	270.2233135	280.8323774	227.6657775	270.7553843
888.5316881	1172.503951	631.5760686	977.8144122	856.7746695	1024.635118	1088.132376	975.6514463	1094.468919
515.1831743	710.61085	533.1004729	625.5377185	538.095919	578.5179553	668.1319715	635.1649409	677.5104597
2078.325556	2161.104331	1948.696329	2296.148153	1981.851028	2056.032093	2151.367233	1973.298603	2223.113472
1491.033503	1632.14199	1178.688037	1547.795084	1219.319196	1315.844086	1621.630783	1485.965684	1360.62657
1623.330492	2025.14214	1705.53991	2608.836359	2535.613112	2712.023561	1799.149442	2006.227832	2015.861954
528.5223188	671.3882321	501.6597094	648.5300346	657.4646079	794.4268981	856.5666855	749.1980247	749.2837917
41443.86021	53804.41924	47169.66296	68180.40394	71325.14888	67570.30181	39997.38581	48894.86357	46792.89972
35.62391175	30.14484648	37.95584221	139.4092274	146.4730664	253.6958865	186.7447053	114.2327299	165.5360026
2755.776539	2585.860418	2838.332055	4886.724351	5195.117789	5136.14504	2079.8002	2492.08503	2093.728205
1367.722679	1286.967812	1345.804546	1679.779808	1690.031423	1969.469548	2112.26176	1638.659843	1869.494987
212.3111964	189.4738257	116.86584	122.022206	127.7996157	111.0219378	188.1395396	188.5047297	129.6053576
1986.160307	1748.258936	1576.664858	1804.609299	2825.159582	2622.796222	2309.76168	2373.734324	2163.533906
463.870031	441.9990874	462.9329508	645.8224171	473.7839061	861.3059719	536.9640627	549.6656269	445.0310178
441.8426714	407.2081982	297.0892454	257.4020782	473.8466014	444.7981434	406.0409955	418.5322709	289.5157917
8782.555431	8681.721722	8611.342945	13866.24016	13613.72137	15616.03532	6832.363343	8642.067645	7872.109508
7583.141146	8076.406989	8174.639471	6799.273879	8646.333027	9466.756145	7430.865626	9414.175066	7152.650804
670.3196477	644.6373723	511.2602138	499.7384981	838.3523958	814.8402113	692.219327	699.2610845	524.0918838
678.6071686	631.1355701	402.9862212	418.0699718	690.464974	671.4848891	466.5354618	710.8636834	477.9051378
731.0726705	601.2930366	569.9851141	585.4934351	857.0999757	824.1305973	721.6107594	917.7451	596.2723398
4578.910728	3849.915859	3641.133869	3826.953247	5950.432054	5045.862131	4747.697442	4781.210386	4281.887378
6919.470715	6381.643035	4743.067472	5108.414447	6980.403106	5876.811486	5357.183448	5833.828251	5156.328983
1196.78508	981.9687705	837.0302831	693.4224289	929.0992805	855.9457486	686.2922143	899.195253	668.5394621
1140.879503	1081.952459	802.8535763	748.098355	1269.723425	1053.423725	822.8965412	1026.925751	881.2914481
861.5391652	756.7904392	729.7419965	484.9725914	861.8389742	794.71566	794.591381	625.6822471	492.2678865
74679.42397	64991.79343	71229.64306	69972.39799	76929.67357	70984.89424	73299.29151	73378.15728	70958.2834
770.1782772	689.0646261	705.5168019	666.843289	838.0250971	625.7596413	811.4020103	696.486179	677.5583197
236.8520099	190.8073377	370.9286925	0.001403199	0.001403199	33.24564131	98.29165517	116.4059229	127.3876957
1069.604234	863.2584878	1174.287147	65.67089804	47.67130692	0.001403199	202.6607462	407.4151802	359.5023688
656.3527875	643.4750492	630.9039449	0.001403199	46.52875189	0.001403199	363.6186947	271.2005862	308.265367
426.8195666	438.3590853	596.6708818	43.52612004	0.001403199	0.001403199	148.7900553	338.923784	185.2609206
31177.57112	30283.41335	37238.85997	5723.839072	5593.232919	4917.978538	13552.8219	15011.5076	14674.95775
11.65044544	18.90701349	19.08556937	31.67047346	33.67868189	33.34272381	12.77393903	53.64027286	42.49239678
836.9122776	797.3381411	712.2986676	883.1837938	633.1997126	620.2463805	677.0331468	859.687994	907.5120706
1233.697518	1247.327211	1206.068347	1225.428504	921.3756353	861.0155803	974.1723927	1202.888153	1312.288799
690.8919526	470.6987168	555.2654946	601.0867074	770.7731232	273.5544788	536.0096945	561.7563188	594.3921274
854.2585024	708.5116737	711.8503203	727.6854563	608.1307176	501.530291	613.3886135	621.9570364	645.5325958
1160.258559	750.8515699	790.3829077	860.4308317	745.9451332	608.8220058	884.546094	733.7512512	778.8207542
461.7915248	564.2993006	417.9563534	343.5782436	434.8604977	407.969292	518.6579821	503.757219	472.2224953
2322.223524	1917.337854	1722.345999	1920.344665	1391.244287	821.1031623	1704.081894	1699.143438	1690.170203
20822.21494	19634.43462	20334.29776	21626.00961	19075.29444	18498.61085	16893.66465	19230.48959	18522.28742
3075.554634	2396.733356	2929.519266	2765.820773	2485.835616	2424.761852	2406.69921	2949.209496	2870.75197
2155.924825	1688.542271	1733.310778	2987.81487	1948.465566	1830.004595	1546.312658	1899.952228	2055.829172
252.0648432	206.8696629	209.2586085	218.1129222	170.2555316	209.0713278	231.4694357	185.6018146	251.9340063
1000.418823	853.9718908	856.5552482	763.9581711	686.2818448	743.2601064	909.0485102	618.9750426	868.8265325
1557.008018	1287.061356	1344.562453	1415.82334	1072.98527	1114.787346	1243.443578	1217.110157	1408.890489
1133.392954	930.5971743	950.4420087	859.6615604	964.913876	1021.349305	1073.840158	870.3979977	888.8402245
5686.940358	5614.141668	5417.593538	7787.088691	5890.836848	6771.023777	7030.833446	7181.868597	8623.974054
55136.76768	53486.737	50793.2679	67454.27009	69142.89797	66608.81553	45510.3406	46203.39053	46534.9349
1333.197295	1236.044629	1339.651061	1300.963786	1312.25834	1715.946496	1286.296925	1288.160255	1096.380493
1054.006135	1109.480537	1312.575154	2170.721786	1689.1988	1610.933199	1239.232721	1442.302913	1532.825561
864.0347173	842.0167838	661.0815978	685.888657	571.1331949	1144.690088	578.5980761	820.9854801	584.1912329
621.5529404	497.0607193	408.2792775	357.9573727	549.6727172	476.260556	571.0857623	501.99799	546.5950801
4429.729605	4052.363515	3897.742711	3712.233481	4873.200658	4668.799997	5147.901541	4042.657135	4310.548091
1492.738327	1306.777528	1227.598834	1319.002749	1924.721625	1347.974019	1934.168405	1468.413489	1492.01546
14393.59265	14457.76169	17144.44435	10723.70372	9361.596569	9443.078016	12774.7134	14391.32468	14781.64188
688.1649431	675.5390967	629.8984228	885.4814982	883.1374722	549.480149	585.4774262	693.7995574	729.3992612
1114.607147	763.6242918	22816.66878	551.7614252	777.7235019	382.9456481	593.4628017	543.2264675	501.8061174
857.4363366	752.9100099	696.0511121	1131.739962	964.2854818	692.3350863	672.7169875	686.8301858	756.9180406
902.6782564	665.3506585	603.7517948	814.1034405	789.090477	671.1695272	561.4404288	797.5442781	881.7062172
12463.28814	10996.1507	11000.25708	10406.4392	11049.88896	9454.383521	11382.67131	10256.48269	10070.21467
830.6236553	807.0783162	732.8113984	932.8294114	853.5092688	598.8030289	632.6648111	841.6724563	984.482235
24872.54888	23380.88569	22529.90707	22587.20124	24916.4583	22733.63625	25772.54533	23043.70047	23159.85535
3678.298856	3502.145471	3393.349921	4089.702191	3720.816851	3369.793161	3523.612749	3521.07849	3654.707776
765.7860573	702.5345908	674.6186802	887.9186459	725.9986157	758.3011395	527.285209	583.8000719	822.8657904
876.9296953	801.6184311	730.5987482	999.4898806	798.8380802	667.1947428	817.3894665	787.2327573	1054.116958
13910.29154	14995.41485	13811.17382	13534.36507	13879.46701	13822.25056	15020.27167	13983.19673	13721.01123
633.9308089	688.8730134	695.7327075	667.1451869	589.3321183	605.096867	517.7881434	616.5490062	579.7248488
944.3931867	922.5503804	787.2476645	1033.857999	836.7164853	751.0638056	906.7752268	846.6845301	1100.799166
2249.666984	2179.114465	2092.622077	2575.154755	1821.004918	2266.233826	1866.419454	2209.493191	1907.598034
830.144628	798.1814079	901.1693288	972.5821503	692.6743859	790.6867015	693.5188881	766.1397095	697.8116944
415.8056087	364.7082842	287.8144148	401.3455717	323.0471788	350.8518656	314.4726651	451.837061	197.1911942
2739.074771	2320.135177	2430.694593	2522.74964	2600.825791	2445.533796	2890.927473	2336.732987	2347.594663
6203.92931	5933.76637	5683.97573	7111.336726	6542.292907	5679.964675	6434.001972	5907.257651	6277.610786
513.7833924	463.5089181	444.3157765	473.8054941	368.5804857	483.9596187	518.0752783	453.858222	492.9768161
1641.138672	2541.363903	1796.689151	3297.328099	2545.351093	2627.640287	2319.702607	3452.68226	2891.108635
264.6944085	295.9479377	269.2297062	292.9832366	293.882334	330.1740617	297.482715	330.0962009	285.6411642
902.5541764	1139.152236	1312.624871	1209.479722	1401.026112	1102.397025	1309.368802	1387.678439	932.4994267
435.0269623	589.1096791	519.8422512	405.5475349	586.233368	505.5077386	634.9091772	576.3205994	494.893669
1099.811527	1342.501598	1233.347469	1190.397242	1206.24168	1169.495893	1150.368037	1179.134928	971.970772
651.0270916	718.3852283	861.7606742	687.0035405	716.66568	755.4698952	618.5507458	759.6735742	697.1559101
214.8276379	257.1705794	258.2701694	218.7957199	254.0885908	254.2950132	238.5131282	188.7274033	207.0478129

7.77_239.1486m/z	239.1486043	7.768133333	pos	1017.08577	1170.396373	1068.056022	852.5001194	1004.563471	980.3206064	1051.420947	1042.133993	929.9581966
7.77_488.2380n	511.2272959	7.768133333	pos	30503.3807	32093.12568	28495.03968	36205.50666	43172.39925	40323.74447	32809.82532	35826.14997	33337.61732
7.77_579.2144m/z	579.2144484	7.768133333	pos	1136.955742	2300.661779	806.1715677	2099.755002	3154.036461	2942.489439	2254.25057	2135.474399	2322.171467
7.77_605.2357m/z	605.2357012	7.768133333	pos	3035.951567	4031.940362	2990.20625	4420.962231	5255.464121	5137.723502	3692.90491	4441.491622	3820.858078
7.78_319.8810m/z	319.8809587	7.780633333	pos	2500.06156	2856.66258	1933.020876	2027.23675	3122.843349	2616.452128	3326.594433	2697.109637	3117.662987
7.79_193.0062m/z	193.0061915	7.791366667	pos	445.7009459	551.6463497	361.8516044	453.5074475	580.4109695	488.0496609	739.0294744	547.5168114	701.0069327
7.79_197.1534m/z	197.1534249	7.791366667	pos	2140.251767	2406.491874	2129.609549	1801.721627	2098.757073	1885.776568	2371.87038	1870.061367	1918.48514
7.79_215.1792m/z	215.1792487	7.791366667	pos	209.1383469	159.1338129	113.5759888	136.3433871	212.7149082	155.8338812	162.2714337	130.1682305	135.0525701
7.79_354.2610m/z	354.2610309	7.791366667	pos	353.5134243	567.6663522	340.888508	363.9818369	567.7790002	516.6825416	524.1685473	417.1670969	611.3619614
7.80_140.9510m/z	140.9510449	7.80375	pos	3527.715673	3102.13409	3069.24896	3145.68041	3218.415396	3066.317392	3498.108209	3160.791187	3198.117892
7.80_169.9973m/z	169.9973213	7.80375	pos	1735.555535	1898.479942	1255.933647	1510.517364	2324.258809	1893.205032	2747.756355	2006.206642	2701.104443
7.80_213.1846m/z	213.1845884	7.80375	pos	1343.159091	1233.978774	1078.847437	1024.204146	1439.87859	1234.314714	1718.829589	1274.764928	1129.923857
7.82_156.1202m/z	156.1201895	7.817466667	pos	444.5817086	367.6685378	330.2005488	339.7949612	364.6344535	362.7385199	419.4717218	310.1903362	370.4244591
7.83_131.9741m/z	131.9741132	7.828216667	pos	228.6707661	162.636092	177.971417	204.9279982	217.358845	154.9348993	241.9801788	180.8556139	238.7410441
7.84_164.9203m/z	164.9202512	7.837283333	pos	1460.401522	1394.773053	1173.800276	1621.93585	1869.480606	1550.44259	2039.097789	1475.225958	1793.939581
7.86_178.9904m/z	178.9904031	7.863116667	pos	1385.14561	1068.629037	1278.802943	1206.808877	849.385924	1091.594029	1229.072231	869.0332947	875.2715312
7.86_216.9224m/z	216.9224378	7.863116667	pos	5328.327873	4759.838947	5053.765433	5025.810559	5291.378292	5209.920064	6049.469828	4404.448853	5218.982169
7.89_258.1651n	276.1988491	7.893783333	pos	35690.66594	38282.0893	50778.669	52626.16703	48366.32965	49339.53074	29904.11897	31009.18058	35068.26505
7.89_261.1306m/z	261.1306303	7.893783333	pos	1066.493524	1093.103197	1121.649635	1046.589025	1034.437697	1098.902494	1219.742744	899.9383316	948.5222004
7.89_319.8809m/z	319.880926	7.893783333	pos	1455.23972	897.6286286	1386.575588	1169.514061	1437.993221	1337.25711	1789.663816	1214.399169	1389.49776
7.91_197.1534m/z	197.153435	7.906183333	pos	1585.024079	993.5446048	1113.397231	1348.728977	1116.319376	1015.881553	1513.760598	1270.338302	1157.575797
7.91_273.6217m/z	273.62168	7.906183333	pos	307.155512	338.4337336	443.9195728	446.8310773	404.7814353	484.4424436	432.5054026	424.5902325	389.3917391
7.91_431.2422m/z	431.2421713	7.906183333	pos	5674.913011	5883.010173	6075.306623	8216.107911	7789.156048	7538.941246	6402.219722	7177.220359	6191.271231
7.92_164.9203m/z	164.9202766	7.915266667	pos	1114.806244	887.2743833	1130.147532	1147.788417	1241.825508	1184.914273	1532.536816	1156.696668	1161.60413
7.92_215.9833m/z	215.9833348	7.915266667	pos	816.6560009	748.8362423	829.8850436	699.8542915	900.9233459	865.2576258	1015.378281	967.4832916	728.2415991
7.92_605.2358m/z	605.2358096	7.915266667	pos	3046.94322	2943.606665	3227.271706	5092.278471	4145.091239	3979.50412	2704.221498	3075.360142	3058.463859
7.93_203.1428m/z	203.1427906	7.927683333	pos	2844.285426	2170.130248	2245.852127	2369.023481	2111.48117	2140.191987	2642.467427	2081.528673	2045.700654
7.93_340.2478m/z	340.2477786	7.927683333	pos	632.8778335	510.4441852	627.3854296	951.8225288	1018.17816	994.8482115	625.6634183	583.5824379	649.0307963
7.93_579.2145m/z	579.2144904	7.927683333	pos	3782.208288	3567.800783	4876.566649	6417.441775	4982.393442	5152.868165	4108.354019	4519.394941	4080.207238
7.96_210.0889m/z	210.0888635	7.9616	pos	1074.874442	802.881722	643.6569443	918.2692662	690.7061969	714.2409564	1076.614636	898.9604519	845.08405
7.96_651.3700m/z	651.3699964	7.9616	pos	2494.380009	3760.467382	3123.437201	4353.244266	3517.975215	2979.19984	2678.448813	3704.311126	2514.603202
7.97_102.5327m/z	102.5327248	7.9736	pos	1388.26689	1296.549797	1420.925017	1403.095302	1481.879805	1514.506013	1620.743686	1384.799833	1511.875762
7.97_271.2414m/z	271.2413981	7.9736	pos	1820.886387	836.0289389	685.6752064	399.1743309	329.9520485	237.3568586	778.872004	530.6630296	369.9959877
7.97_651.8640m/z	651.8639935	7.9736	pos	912.6044059	880.3549852	1250.147424	1669.095494	1333.935198	1807.551353	1850.488246	971.7113869	1333.550893
7.99_261.1305m/z	261.1305345	7.987716667	pos	1596.346481	853.4288115	773.0234206	789.6055838	969.4045447	923.4960582	976.125055	976.6131783	1103.384366
8.00_158.0178m/z	158.017822	7.996616667	pos	476.9832902	532.9760904	454.0675763	345.6180988	452.4329759	455.0257001	503.8860754	457.9373023	460.042174
8.01_199.1691m/z	199.1691108	8.00565	pos	8801.173613	7319.138003	7286.888607	7182.86948	7276.569387	7153.325226	8301.990204	7543.576668	7526.610184
8.01_217.9981m/z	217.9981352	8.00565	pos	898.682156	914.4195439	746.093689	572.6226911	783.3561463	758.1701841	807.613374	827.8499832	755.6826038
8.02_113.0346m/z	113.0345888	8.019366667	pos	514.3602958	597.0807636	511.1416706	437.7758395	435.3602215	531.6919694	534.9749198	532.2316464	604.7048312
8.02_171.0624m/z	171.0624265	8.019366667	pos	533.9540114	570.1046461	516.6724443	458.5561714	597.3210856	513.8056105	565.5317537	458.3228588	583.8408444
8.02_190.0033m/z	190.0032532	8.019366667	pos	983.153659	1083.087687	845.7550215	629.2205524	1081.21091	752.7964141	1007.05091	887.9316505	1115.054446
8.02_193.9988m/z	193.998833	8.019366667	pos	362.2795813	225.6216217	210.1626194	228.8795547	237.3687062	247.6829699	339.298517	277.7911386	294.4852758
8.03_161.0707m/z	161.0707287	8.03173333	pos	284.4103036	300.5987029	308.3034609	214.1458417	236.164443	123.3888446	236.1466967	206.513885	247.1358341
8.03_221.1535m/z	221.1534537	8.03173333	pos	654.7190295	654.1671592	535.421342	609.5865986	630.8795987	512.8198847	504.0276915	513.8611878	647.4134889
8.04_164.9202m/z	164.9202193	8.0438	pos	610.5536449	572.2821533	768.1181611	620.6374444	888.4897272	666.8183824	650.440215	668.1539858	801.1328914
8.04_215.9833m/z	215.9833187	8.0438	pos	1374.69076	1708.057342	1796.040722	1346.741123	1637.686025	1376.003597	1605.619243	1557.679329	1725.709005
8.06_210.0889m/z	210.0888596	8.059583333	pos	385.266139	559.3026752	811.9293199	573.6952322	786.8179279	598.158536	692.931565	618.1938928	757.2055729
8.06_282.1652n	300.1987128	8.059583333	pos	36859.56653	47593.66007	52989.70621	72120.86443	64028.43638	63321.936	34893.36187	36713.98363	41965.15453
8.07_100.0113m/z	100.011332	8.074933333	pos	63.72600774	74.06675571	45.46900694	47.81288487	55.70704821	76.05564001	96.00351774	97.63831126	91.85193857
8.07_264.6446m/z	264.6445781	8.074933333	pos	446.208206	679.5862908	500.5459769	26.22023584	51.8432	28.33475515	250.2384531	291.6444456	271.4854759
8.07_403.2320m/z	403.2320087	8.074933333	pos	9548.141796	9813.45132	9515.941393	8096.603405	9795.564749	8739.274737	9635.538619	9072.13155	9762.307067
8.07_542.2427m/z	542.2427426	8.074933333	pos	5894.305646	7748.540964	8883.49459	628.5403887	439.9170751	518.0176083	3661.583832	3750.631961	4333.797904
8.07_544.2529m/z	544.2529374	8.074933333	pos	445.9880645	686.0945289	665.7855231	0.001403199	0.001403199	0.001403199	0.001403199	223.0870934	95.6351427
8.07_545.2512m/z	545.2512211	8.074933333	pos	9909.269826	13792.02067	15062.96032	1143.197076	1237.971359	1413.400364	6728.275685	6711.288576	7476.036704
8.09_166.0839m/z	166.0839465	8.094616667	pos	103.4052366	228.1690592	120.0462143	163.5966768	196.7963573	173.8931303	176.0844386	163.4535986	149.7537521
8.09_174.1123m/z	174.1122886	8.085633333	pos	164.745914	107.1180969	145.6267072	108.3081814	156.2369723	121.3336455	161.9521599	143.2564815	148.8710229
8.10_104.0709m/z	104.0708706	8.104816667	pos	303.9880051	261.6670425	229.8111073	290.1267452	297.4456158	284.3057743	347.7927227	324.8346993	297.8123728
8.10_213.1458m/z	213.1457777	8.104816667	pos	736.976213	672.6270747	416.5670921	685.9770232	826.8421251	589.8588143	696.5891323	639.2387905	698.9231739
8.10_216.9224m/z	216.9223941	8.104816667	pos	6120.833026	5678.322011	5255.957537	6540.303899	7390.693184	7250.314757	7976.826239	6459.231934	6273.435605
8.12_156.9850m/z	156.9850341	8.117233333	pos	66.34461147	44.87521587	60.25940507	47.74442334	122.5289933	111.2976515	94.32090199	123.7699313	114.5608251
8.12_319.8809m/z	319.8808905	8.117233333	pos	2551.238523	2769.618953	3239.695791	3272.139396	4014.16719	3327.985208	3336.70465	3304.019936	4227.263894
8.13_170.9774m/z	170.9774373	8.13135	pos	1064.727038	1326.497331	1251.448153	1253.34355	1539.165403	1060.227139	1557.733432	1357.385047	1363.864738
8.13_357.2240m/z	357.2239589	8.13135	pos	1188.178921	1349.160026	1502.460809	1770.954967	1282.25017	1311.486511	1277.854731	1587.794585	1116.776551
8.14_169.9972m/z	169.9972087	8.140333333	pos	1971.037569	1845.432401	1552.164787	2253.633781	2439.296856	2276.062181	2382.032414	2085.786046	2196.41069
8.15_209.1533m/z	209.1533365	8.152766667	pos	2610.813101	2167.417469	2001.12027	2106.409009	2304.202767	1645.393528	2880.827108	2172.097072	1906.32738
8.16_197.1533m/z	197.1533404	8.163466667	pos	1128.956453	1108.538874	1035.387649	1046.895827	973.048118	743.8794374	1568.441537	1093.658309	1020.201221
8.17_130.5215m/z	130.5215001	8.173716667	pos	821.8640548	867.6848864	659.0164195	789.721146	897.2985678	478.3987474	1184.216798	806.6900876	731.8897965
8.18_217.9982m/z	217.9982366	8.182716667	pos	685.0802935	773.5015396	729.5709948	684.4864308	788.4622894	573.0478448	1196.309007	793.1243795	818.5148807
8.20_210.0889m/z	210.0888513	8.19975	pos	764.8357058	672.7836064	536.0625863	712.3152784	711.4661012	803.7431616	1069.69176	675.9875666	709.3515877
8.20_309.1304m/z	309.1303778	8.19975	pos	5476.39644	6247.184145	5349.414197	6588.980455	6787.290276	6600.207144	5573.070512	4910.694313	3870.726255
8.21_152.5483m/z	152.5482845	8.21045	pos	78.79303286	0.001403199	30.08535996	61.91658393	45.78641977	67.615638	76.42352744	48.56063218	69.67340183
8.21_190.0033m/z	190.0032822	8.21045	pos	953.3704958	908.3932044	703.4007303	875.3107768	999.4614689	1126.627621	1284.870416	861.0560517	941.7449118
8.22_403.2321m/z	403.2320767	8.220666667	pos	6640.366488	5021.901384	5145.641815	6269.278689	6369.115078	6741.218965	6435.377107	5039.564171	4208.181697
8.23_170.9774m/z	170.9774285	8.232683333	pos	636.8478591	562.4363341	624.8492173	673.6481889	573.4120645	759.3340132	751.9042126	634.0302728	605.1074729
8.25_208.0624m/z	208.0623703	8.245133333	pos	66.69684531	91.69320164	48.28042562	130.1848443	105.9519029	115.2154094	152.4912618	50.11283726	70.26490465
8.26_125.9861m/z	125.986136	8.2588	pos	809.6584752	783.3128475	949.3932605	937.9245896	976.2587126	1227.343582	1086.283906	832.2951868	883.324551
8.26_215.9833m/z	215.9832613	8.2588	pos	5131.434612	4489.346399	4372.963882	4958.87524	5221.778943	5166.123877	6018.087241	4554.252642	4750.659201
8.28_340.3085n	341.3157793	8.280116667	pos	11490.30272	11274.65303	11057.69401	11149.28525	9891.536673	10070.14154	12087.08	10224.43542	11892.27151
8.29_115.5572m/z	115.557212	8.292383333	pos	50.79595622	57.97414283	60.47926573	79.99713914	59.0484438	58.71274619	76.68729539	44.54847726	129.5471005
8.29_243.9773m/z	243.9773488	8.292383333	pos	11028.6778	10516.00084	9407.738748	10236.85097	10787.72858	10164.90135	10605.09009	10094.23948	10035.15817
8.32_130.5215m/z	130.5215198	8.322633333	pos	1045.274581	856.4359193	747.6034071	653.1882744	828.0731687	700.428752	821.6637668	841.494707	971.745571
8.32_197.9923m/z	197.9922535	8.322633333	pos	778.5271354	817.1794841	724.9455368	547.6577904	741.321795	680.8675924	551.5420945	699.0341349	794.00037
8.34_125.9862m/z	125.9861575	8.3362	pos	759.0145835	1074.984781	852.050471	682.1185889	833.0252558	829.7591104	571.6747352	886.3036892	854.7773825
8.34_140.9510m/z	140.9510218	8.3362	pos	1708.751466	1531.022792	1642.947615	1567.050003	1595.11829	1584.173327	1563.21369	1648.931163	1833.105297
8.35_213.1460m/z	213.1459681	8.346716667	pos	804.2636895	780.520663	574.0740233	498.8866973	579.7368472	606.9162083	432.1604824	593.0351095	500.6545584
8.35_271.2740m/z	271.2740006	8.346716667	pos	1667.970476	41.13020124	201.2391226	0.001403199	68.94722524	214.5620886	0.001403199	2066.995907	0.001403199
8.36_420.8840m/z	420.8839866	8.357283333	pos	1300.706023	1146.010346	925.0014971	999.5304403	1113.296674	996.8526308	578.6031477	1103.874283	1626.392812
8.37_172.9768m/z	172.9768939	8.3679	pos	351.6142052	335.1397957	272.4109815	261.1990109	280.8877003	303.6053916	233.5779525	385.1579819	304.0278381
8.37_208.0391m/z	208.039051	8.3679	pos	15646.97315	14451.81796	13995.09557	14969.803	15877.29021	14738.49893	16386.71944	13948.90879	15217.01871
8.41_156.9850m/z	156.9850401	8.405166667	pos	27.01087591	70.53946952	52.07409476	41.26033204	89.53316562	62.24322503	77.00280425	47.45830659	92.57906164
8.41_241.1767m/z	241.1767474	8.405166667	pos	1281.850657	1014.529999	1294.954714	1258.584339	1322.868916	1298.445233	1336.720634	1306.902237	1329.689576
8.41_276.2802m/z	276.28021	8.405166667	pos	4104.598587	3385.320264	4143.26702	3706.773136	4379.511258	8883.25728	4754.367675	3011.824133	4824.986209
8.42_155.0700m/z	155.0699872	8.417466667	pos	658.9689115	500.099471	569.9326655	637.2045234	607.5360163	600.7466232	732.7615705	589.0177456	622.5711128
8.42_306.8941m/z	306.8941163	8.417466667	pos	3501.244869	2590.230508	3303.535639	3417.352014	3690.746493	3552.487461	4394.134402	3103.950974	3166.141484
8.42_308.8897m/z	308.8897486	8.417466667	pos	675.7466208	495.1542413	905.1428241	598.9949496	804.8206187	678.6828637	1217.202195	653.8041471	790.2207693
8.42_403.2320m/z	403.231954	8.417466667	pos	4482.37993	3303.69641	5179.343996	4554.6942	4289.093665	4715.095165	5798.557922	4521.287014	4417.861061
8.43_129.1273m/z	129.1273271	8.428066667	pos	311.4682208	245.7895944	380.9119391	397.1971032	309.8005121	328.5038939	527.8424957	370.394356	302.4127507
8.43_159.1165m/z	159.1165003	8.428066667	pos	677.192898	606.3313966	623.1511467	560.5504335	569.3153779	496.6981127	583.3303189	511.3858185	543.6946215
8.45_199.1691m/z	199.1691075	8.450466667	pos	1418.120246	1514.015271	1230.461087	1565.15518	1438.918177	1359.915353	1728.726359	1322.248007	1469.920236
8.47_140.9510m/z	140.9510041	8.466283333	pos	732.9740562	779.6837212	795.8886519	1067.338912	904.0346262	810.0920227	982.3890717	807.6296355	811.9360596
8.47_243.9773m/z	243.9772871	8.466283333	pos	5421.219304	5411.505533	4975.355829	5931.665139	6154.062454	5468.669495	6199.400562	5461.450082	5854.225135
8.48_294.9384m/z	294.9383809	8.4786	pos	2307.307896	2480.605558	2383.489733	3887.812911	3197.607211	2947.295564	3066.841241	2411.984923	3119.790304
8.48_306.8941m/z	306.8941206	8.4786	pos	1901.092603	2202.427935	2341.754522	3112.717393	3028.261186	2640.345794	3107.647636	2428.646896	2898.56972
8.50_221.1534m/z	221.1533995	8.497183333	pos	648.795413	868.1951655	850.3918189	899.992194	1034.448884	634.642275	673.3733381	651.7369958	628.0874681
8.50_403.2320m/z	403.2320133	8.497183333	pos	5628.467543	6091.945112	5325.186537	6919.254222	6820.692577	6287.050353	6637.617191	6174.288622	6024.60819
8.51_163.9880m/z	163.9880119	8.509533333	pos	139.0353197	150.6099583	173.4161501	240.9853937	213.6293998	117.1507297	206.1857207	134.963521	160.7055223
8.51_217.9791m/z	217.9790856	8.509533333	pos	1334.011561	1327.740391	1154.519731	1699.133103	1455.448982	1404.035802	1555.020023	1379.996693	1392.174374

8.52_148.9768m/z	148.9768311	8.517983333	pos
8.52_190.0033m/z	190.0033081	8.517983333	pos
8.54_217.9981m/z	217.9980731	8.53905	pos
8.58_113.0346m/z	113.0345534	8.58335	pos
8.59_168.9931m/z	168.9930743	8.593966667	pos
8.59_197.9922m/z	197.992238	8.593966667	pos
8.59_199.1690m/z	199.1690194	8.593966667	pos
8.60_547.2039m/z	547.2039409	8.602816667	pos
8.62_148.9768m/z	148.9767841	8.615133333	pos
8.62_305.2466m/z	305.2465713	8.615133333	pos
8.62_544.1953m/z	544.1953004	8.615133333	pos
8.63_243.9773m/z	243.9773102	8.625266667	pos
8.63_306.8943m/z	306.8942623	8.625266667	pos
8.64_403.2320m/z	403.2320265	8.637533333	pos
8.65_180.9895m/z	180.9895091	8.646416667	pos
8.65_208.0391m/z	208.039078	8.646416667	pos
8.67_251.8936m/z	251.8935996	8.672766667	pos
8.70_104.0305m/z	104.0305311	8.6957	pos
8.70_148.9768m/z	148.9768009	8.6957	pos
8.71_169.9973m/z	169.9972947	8.705566667	pos
8.72_155.0700m/z	155.0699674	8.719016667	pos
8.72_199.1692m/z	199.1692241	8.719016667	pos
8.77_127.9667m/z	127.9667294	8.768866667	pos
8.77_190.0033m/z	190.0033172	8.768866667	pos
8.77_192.4764m/z	192.4764262	8.768866667	pos
8.77_216.9224m/z	216.9224466	8.768866667	pos
8.78_304.1516n	327.1409041	8.782383333	pos
8.79_169.9972m/z	169.9972422	8.792966667	pos
8.79_284.9103m/z	284.9102676	8.792966667	pos
8.80_170.9775m/z	170.9774661	8.801366667	pos
8.82_131.0216m/z	131.0216005	8.817066667	pos
8.82_243.9774m/z	243.977407	8.817066667	pos
8.83_306.8942m/z	306.8942368	8.827616667	pos
8.83_402.2321m/z	403.2321336	8.827616667	pos
8.84_180.9896m/z	180.9895768	8.836483333	pos
8.84_271.2263m/z	271.2262824	8.836483333	pos
8.85_140.9511m/z	140.9510545	8.84705	pos
8.85_199.1691m/z	199.1690703	8.84705	pos
8.85_208.0391m/z	208.0391094	8.84705	pos
8.85_217.9790m/z	217.9789764	8.84705	pos
8.86_172.9899m/z	172.989891	8.855933333	pos
8.86_253.2157m/z	253.2157351	8.855933333	pos
8.88_215.0828m/z	215.0827795	8.878766667	pos
8.89_162.9830m/z	162.983041	8.887616667	pos
8.90_155.0701m/z	155.0700581	8.901566667	pos
8.90_172.9769m/z	172.9769141	8.901566667	pos
8.93_170.9774m/z	170.9774231	8.928616667	pos
8.94_213.1461m/z	213.1460895	8.939166667	pos
8.95_313.2612n	336.2503384	8.950966667	pos
8.96_217.9791m/z	217.9791573	8.96275	pos
8.98_169.9973m/z	169.9972679	8.982066667	pos
9.01_148.9768m/z	148.9768285	9.012583333	pos
9.01_338.2554m/z	338.2553762	9.012583333	pos
9.01_375.2793m/z	375.279343	9.012583333	pos
9.01_403.2321m/z	403.2321449	9.012583333	pos
9.01_428.3267m/z	428.326718	9.012583333	pos
9.01_489.2346m/z	489.23457	9.012583333	pos
9.01_506.2404m/z	506.24043	9.012583333	pos
9.01_547.2669m/z	547.2669235	9.012583333	pos
9.02_208.0391m/z	208.0390621	9.0248	pos
9.05_199.1690m/z	199.1690498	9.0492	pos
9.06_256.9154m/z	256.9154124	9.062583333	pos
9.06_261.1308m/z	261.1308098	9.062583333	pos
9.08_119.9571m/z	119.9570872	9.0816	pos
9.08_197.9922m/z	197.9922462	9.0816	pos
9.08_356.2789m/z	356.278859	9.0816	pos
9.10_140.9510m/z	140.9510348	9.102066667	pos
9.10_155.0700m/z	155.0700318	9.102066667	pos
9.11_306.8942m/z	306.8942149	9.11415	pos
9.12_168.9931m/z	168.9931165	9.124583333	pos
9.14_113.0346m/z	113.034591	9.13505	pos
9.14_130.9662m/z	130.966247	9.13505	pos
9.18_191.4786m/z	191.4785971	9.17725	pos
9.19_113.0346m/z	113.0345875	9.19115	pos
9.22_100.0142m/z	100.014179	9.215483333	pos
9.22_199.1690m/z	199.1690356	9.224183333	pos
9.22_205.9746m/z	205.9746574	9.224183333	pos
9.24_108.0230m/z	108.0229842	9.2429	pos
9.24_140.9511m/z	140.9510523	9.2429	pos
9.24_215.9831m/z	215.9831078	9.2429	pos
9.24_243.9413m/z	243.9412966	9.2429	pos
9.26_131.5292m/z	131.5291723	9.2563	pos
9.26_208.0391m/z	208.0391284	9.2563	pos
9.27_107.9670m/z	107.9669685	9.268383333	pos
9.27_114.5584m/z	114.5584113	9.268383333	pos
9.28_130.9662m/z	130.9662391	9.281766667	pos
9.28_323.8843m/z	323.8843121	9.281766667	pos
9.28_403.2318m/z	403.2317985	9.281766667	pos
9.30_193.0062m/z	193.0062039	9.3043	pos
9.30_197.1534m/z	197.1534395	9.3043	pos
9.30_308.8896m/z	308.8896118	9.3043	pos
9.33_100.9570m/z	100.956963	9.325183333	pos
9.33_142.9802m/z	142.9802339	9.325183333	pos
9.33_170.9774m/z	170.9773925	9.325183333	pos
9.34_140.9510m/z	140.9510185	9.337316667	pos
9.34_306.8941m/z	306.8941089	9.337316667	pos
9.35_352.8968m/z	352.8968063	9.3477	pos
9.36_157.0757m/z	157.0757437	9.359983333	pos
9.37_112.9668m/z	112.9668776	9.36895	pos
9.37_203.9709m/z	203.9709319	9.36895	pos
9.37_285.8986n	286.9058345	9.36895	pos
9.37_320.8630m/z	320.8630262	9.36895	pos
9.37_403.2321m/z	403.2321446	9.36895	pos
9.38_100.9569m/z	100.9569168	9.3777	pos
9.38_243.9414m/z	243.9413807	9.3777	pos
9.39_169.9972m/z	169.9972375	9.386383333	pos
9.40_127.9668m/z	127.9667721	9.399783333	pos

470.3090118	438.303723	222.0138621	472.2237068	497.1960621	348.7330826	408.9855332	458.2069588	423.9507065
828.5181339	772.4849145	309.5710473	727.5787213	688.5039183	526.3796072	777.6479551	695.5693435	827.6908806
786.9701267	687.0146696	534.1183405	582.1654277	841.2782443	834.9186057	650.5127792	819.6617544	792.990978
895.6608922	828.2632399	906.2543145	796.3391424	918.4524584	858.3113517	851.85788	935.7156792	893.7255438
2202.669045	2111.204157	3207.40157	2532.214862	2713.556624	2412.320486	3239.432584	2672.062443	2771.634583
1499.11243	1362.303672	1581.730267	1370.702251	1528.280141	1676.843484	1919.222235	1558.314837	1528.288916
897.6594411	682.0625348	971.9731807	720.862268	843.5181385	846.9427314	902.7494195	847.9083068	834.9166073
4044.561128	4989.675634	5883.943568	5855.854787	6221.813483	6422.807198	5422.70136	6123.121616	5390.367846
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1325.697113	961.0022142	1027.584329	630.6999032	527.3683526	593.8892509	763.6784143	732.8428604	648.0248397
1941.569533	2274.131883	2691.205138	2798.434838	2630.807388	2880.580416	2195.074009	2620.458612	2771.563778
5009.270147	4255.989621	4529.920928	4472.412317	4443.345895	4456.191432	5475.642663	4701.845061	5104.51797
2169.824433	2200.339731	2789.270881	2408.466336	2761.502012	3124.687853	3455.891474	2800.247012	2948.227822
2819.39254	2694.400513	2470.29789	2724.855259	2679.327156	2388.656926	3772.066401	2490.817621	2581.32053
1219.587066	863.0619283	621.5295667	904.9576048	782.1950919	861.6109604	1074.186235	895.4239648	970.9526989
5656.838114	4519.240107	4704.499796	4902.020609	4900.226704	5733.308968	5644.362526	5353.574531	5452.066945
871.3565231	792.8547884	611.7361018	827.920977	718.5095484	897.8696936	950.9784135	782.6707769	1025.408558
392.740173	289.8637877	296.8805607	300.3307199	246.7413281	545.2614242	320.0549016	381.0522983	432.3895321
487.9816732	441.9872951	433.9418261	545.7043489	534.6314049	808.7552603	420.3456868	513.8872394	694.6159225
1671.292141	1265.416669	1134.03314	1539.184114	1410.978154	2237.15863	1235.757954	1587.740062	1991.558844
321.3774947	297.1192022	249.9515654	301.5039334	377.391734	342.0586252	298.583647	326.7866956	321.0750346
766.396198	559.5004602	476.7120173	547.7082718	636.1398185	741.9175549	519.6014066	570.5429636	575.2883672
352.1063419	366.1263539	431.6953973	357.4581917	494.7890114	266.8294044	251.6441332	299.943161	358.3355513
2530.391847	2485.417579	2351.550819	2197.067445	2524.412837	2464.185128	2172.064387	2251.273382	2556.374799
260.3085921	298.4498882	355.0475742	311.2500239	353.9664642	324.2578238	358.9910985	324.1877337	308.8142895
1947.859492	2565.558474	2583.979154	2381.515942	3463.746615	1982.830959	1890.102049	2181.633235	2298.616188
31686.76052	36404.80276	39603.35826	2888.334835	3079.493469	2344.276895	26533.53849	31740.57683	32349.78631
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1302.325155	1412.223885	1736.372765	930.028765	1822.854459	1220.603919	1516.611661	1352.267368	1419.935331
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2983.599665	2466.160397	3022.033164	2685.98604	2692.536008	2779.994516	3226.966794	2660.002268	2868.277218
1474.881014	1306.953379	1611.32348	1299.343107	1387.877738	1471.565658	1572.929839	1529.239196	1625.41622
2088.090781	1935.107034	2061.812233	2050.104315	2048.448303	1980.611307	2173.129371	1976.773236	2052.357219
1381.529953	906.5032344	1209.640515	968.5690638	1041.205373	1123.327821	1375.959249	1060.793914	1112.721335
3775.503772	3231.760935	3447.47106	3444.548869	3206.287678	3410.65364	4205.255403	3406.525727	3689.564816
1332.564274	1010.809446	1314.378915	1160.523462	1059.726965	1309.825788	1461.549831	1260.698174	1265.934662
33.68312954	36.97905277	11.62531597	14.11940081	0.001403199	19.80194791	0.001403199	0.001403199	18.91902591
699.5942608	738.3895422	904.4285375	908.8045481	735.1123007	1080.985471	843.4834397	898.9993398	881.0658971
161.4980641	290.3626243	362.8814044	257.548851	346.9660597	243.6205174	206.8446282	333.5585522	223.4013565
3050.212157	2920.643955	3385.704536	3069.799355	3272.074779	3255.87202	3330.092289	3125.775914	3383.244096
839.0228991	874.7026566	745.2222458	849.1278007	722.7037054	855.8333871	870.0518391	793.2864898	912.9069057
478.9832555	482.5823643	402.4442188	522.9798227	510.074089	594.7511206	491.4920798	497.4285698	598.1995254
492.846644	528.3576183	338.6115104	519.5086041	487.2588174	503.7945441	536.5567126	648.5638872	533.4142954
785.0258538	934.434745	605.37629	582.7890457	474.4453293	626.8766868	543.4215293	688.9998739	570.1782575
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3376.414078	4134.148852	3724.516472	3685.133016	4170.326019	4072.007657	4329.312049	3932.384948	4835.582042
5134.759103	5665.830827	5756.546685	5884.114325	6253.949555	6203.007263	6023.071775	5878.223106	5916.324985
328.0366753	401.5309825	335.6206755	54.61597505	0.001403199	55.16138218	85.51247821	240.5611057	117.7786595
3466.20153	6154.981438	5643.513133	377.0932893	406.081582	301.1158665	1939.659609	2159.632105	1833.592131
4975.606042	7126.606147	5136.140478	5139.069805	6105.816857	4984.186134	5768.478788	4912.154652	5749.59933
823.3513331	1285.258293	1030.100904	0.001403199	0.001403199	0.001403199	164.1636483	313.0084953	192.4916846
4805.577208	7111.951252	7519.992688	96.99085249	71.46977466	255.0809149	1692.912864	2866.919037	2050.087756
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11303.6625	15185.60122	15648.18365	630.7955882	514.91973	633.7106545	3904.266334	5232.557114	4929.64378
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1278.986545	1072.396498	824.0347716	781.1334712	1117.992317	765.0299788	1481.600187	1175.160781	1274.705425
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639.8011585	561.3697167	571.281391	582.1045682	813.1212998	760.5339785	849.8224884	719.9585886	941.6142786
977.7004962	992.7343867	935.5249099	1149.674824	1096.653151	1086.203678	1197.630048	1059.63297	1213.906605
1731.177438	1655.109264	1431.32542	1563.911116	1767.356019	1530.065356	2000.717398	1706.937629	1712.953005
314.5835562	208.6379976	344.9185321	509.1844314	459.3299061	332.651736	582.4008526	567.3744088	592.5770537
955.486168	706.2932433	841.8645913	1083.424961	823.8097252	811.89886	996.9571161	1072.606925	1015.940915
627.944108	491.0431221	544.3750914	550.5910699	488.8391141	548.5029635	657.9354093	561.4295493	532.57035
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740.8394225	1199.445229	1283.310407	1088.190467	1148.87096	1574.858749	1022.811795	1165.33523	653.8356159
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313.2115789	225.6524037	308.1861217	323.8101292	193.0974605	289.0744943	199.0768269	271.3698072	312.2317651
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4319.932196	3557.464215	4658.02476	4196.288851	4641.067426	4329.396495	3735.815781	4068.948625	4787.656469
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381.1901403	339.580506	497.7359322	372.0826082	399.2033566	283.4086438	418.8576095	382.1663737	478.8359691
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2891.735126	2821.211016	3136.791274	3400.88931	3772.671336	2396.886326	4167.995614	3122.504616	3008.94254
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2439.005088	3485.941791	3436.287644	3401.862027	4490.760672	2706.16935	4699.254562	3200.657748	3199.4494
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906.8671952	1260.308256	898.9379087	1102.619187	1346.541319	1097.004678	1243.423172	1080.338608	1143.753082
273.3465239	316.9760185	166.7215769	251.8827815	325.7943721	370.9864487	380.3987534	275.0991148	290.2308884

9.43_114.5584m/z	114.55844	9.43395	pos							1689.595587	1584.750009	1375.028066	1365.839782	1688.781308	1470.928178	1670.648235	1428.661793	1508.239429
9.44_192.4763m/z	192.4763152	9.444333333	pos							173.8154718	450.5389007	207.6480164	470.4200359	307.6258453	515.8044807	362.6176045	481.9262536	419.687383
9.46_140.9510m/z	140.9510233	9.456	pos							311.19349	261.0957332	391.5221713	593.4795604	311.4376634	645.1946046	468.7302881	433.7700352	508.0795308
9.46_162.9830m/z	162.9830378	9.456	pos							2493.472082	1986.568233	2324.752245	2128.509674	2216.525165	2265.370978	2063.177299	2303.56263	2247.887171
9.46_163.9880m/z	163.988025	9.456	pos							606.3717971	475.153969	475.4448237	540.2923235	577.6550749	617.1000209	568.2135429	595.4533123	684.7804881
9.46_243.9414m/z	243.9413984	9.456	pos							1923.613859	1985.0454	2230.867018	2788.661912	1722.938998	2944.379495	2622.851303	2355.891304	2195.077567
9.47_332.2193m/z	332.2193388	9.466333333	pos							2409.945773	2272.190895	2858.27365	3325.864573	3042.117668	2872.570693	3321.990712	3060.864162	2592.942046
9.48_201.9754m/z	201.9754141	9.479683333	pos							6812.382069	6026.865429	5304.433501	6095.198261	6672.116089	7038.800905	6300.63572	6035.390597	6497.93559
9.49_100.9569m/z	100.9569092	9.488366667	pos							499.1025788	333.1267889	457.8960749	449.1760363	458.5634347	324.2765516	397.3593286	482.6619562	439.2713669
9.49_178.9904m/z	178.9904153	9.488366667	pos							61455.0745	59028.49829	59330.84208	62885.10357	64683.87541	65540.02667	65843.831	61472.0664	64567.67776
9.49_403.2320m/z	403.2320345	9.488366667	pos							9342.130238	6925.607228	6759.917108	5536.027138	7904.865103	5970.926175	6205.750794	6337.368231	7376.988553
9.50_192.0220m/z	192.022027	9.5017	pos							451.8215972	348.0153424	370.8358363	241.0695216	472.8948921	293.6140046	335.9138827	380.5465746	356.2966746
9.53_243.9414m/z	243.9414163	9.529466667	pos							2925.072665	2222.051441	1838.711411	1965.832358	2683.639477	2299.464092	2378.193905	2225.22329	2009.937765
9.53_286.9056m/z	286.9056023	9.529466667	pos							4422.689467	3185.835866	3428.999508	2781.3872	4203.012562	2797.73481	3166.64863	3495.865047	3570.457554
9.54_242.8471m/z	242.8470744	9.543266667	pos							1039.990917	857.1690548	894.2809995	1186.608793	1171.398308	816.7185347	1103.27959	1106.476307	708.3717953
9.54_252.8760m/z	252.8759565	9.543266667	pos							2571.775581	2467.241796	1734.063096	3032.854377	2291.996295	1825.518282	2635.751577	2549.480075	2165.776599
9.56_113.0346m/z	113.0345975	9.56185	pos							283.7732546	360.8331247	234.5890755	413.5694074	285.3066512	257.1848331	417.1798089	302.1891814	172.2714716
9.56_227.6321m/z	227.6320894	9.56185	pos							630.7777703	535.1463036	507.0057649	705.514523	605.6261458	336.091454	620.495174	641.1281433	481.2862271
9.57_215.9831m/z	215.983115	9.572233333	pos							13476.50805	12629.11072	10346.54758	12527.34141	11053.97353	12115.64861	11594.61814	12365.65214	10107.55188
9.58_152.5482m/z	152.5482476	9.5843	pos							253.9884075	134.7831958	199.2801345	112.6283654	192.210999	150.1185597	125.9977643	134.9539753	85.86083264
9.58_297.9422m/z	297.9421516	9.5843	pos							1852.290094	2195.238369	1154.571068	1930.601134	1700.732317	1303.841858	1664.476742	1518.480754	1257.195657
9.58_299.9377m/z	299.9376622	9.5843	pos							953.4883979	1147.371602	880.7590923	855.4662191	941.6368243	596.7446395	903.9231433	817.0727055	614.3691502
9.60_130.0347m/z	130.0347021	9.597966667	pos							340.9905078	402.9586996	459.6008766	474.5862671	359.5686723	320.8949823	400.7714941	456.5974347	326.1052476
9.60_162.9830m/z	162.9830365	9.597966667	pos							1389.798937	1439.111555	1297.204273	1691.244002	1365.189559	1357.657434	1608.283548	1505.93898	1034.974701
9.60_163.9881m/z	163.9880914	9.597966667	pos							299.8042488	370.497448	240.6573901	451.1897901	313.8478296	313.3304203	363.262511	329.3879043	295.4548739
9.62_114.5585m/z	114.5584817	9.618266667	pos							1207.310799	1099.105003	1111.402462	1078.794836	1070.497455	1065.409291	1232.385933	1048.291653	1098.005343
9.62_193.0062m/z	193.006172	9.618266667	pos							1408.779135	1514.816785	1317.156773	1827.810989	1394.329197	1648.455302	1527.677292	1422.682993	1168.241784
9.62_323.8842m/z	323.8842361	9.618266667	pos							5078.84508	5121.932421	4324.350753	4599.486799	5467.357216	5342.068742	4280.161203	4580.011901	5045.837124
9.64_403.2321m/z	403.2321333	9.642016667	pos							10962.70308	10207.25546	10339.48423	11722.20702	11764.09116	11892.43429	14016.31995	10681.15315	10740.60739
9.66_132.5269m/z	132.5269012	9.658933333	pos							0.001403199	7.907909868	19.062574	0.001403199	0.001403199	0.001403199	8.06932189	0.001403199	0.001403199
9.66_138.9799m/z	138.9799063	9.658933333	pos							8948.373223	7985.059726	7943.354965	8099.989265	9009.400938	9034.484842	8548.692504	8255.880178	8484.519943
9.67_217.9791m/z	217.9791089	9.669333333	pos							5374.970589	5108.545544	4942.15732	4531.624606	4659.326698	5156.941448	5057.320799	4777.353007	5057.582976
9.67_281.9131m/z	281.9131344	9.669333333	pos							7182.748419	7217.142941	6623.369152	6883.262368	6643.955735	7005.105392	7215.979083	7269.355511	6837.194636
9.68_1017.8270m/z	1017.827007	9.680983333	pos							154647.5035	17189.72217	2061.640736	340.9903959	1078.284038	140.0662346	1045.672757	540.8996815	997.1258793
9.68_169.9972m/z	169.9972256	9.680983333	pos							5744.339696	5575.432354	5479.097655	5980.395184	6060.889595	6039.843502	5489.706622	5833.759289	6015.82129
9.70_212.9856m/z	212.985627	9.69595	pos							98.81096299	185.401821	90.13330699	77.47671397	196.1079648	215.6223288	244.385765	91.4849472	101.7600936
9.71_112.9669m/z	112.9669051	9.709683333	pos							754.721014	548.5467279	778.5685799	778.6991607	953.9194823	731.0104328	1003.811168	760.4915817	935.4452664
9.71_328.9333m/z	328.933269	9.709683333	pos							408.9109955	303.2620211	505.7798351	305.7988479	246.7542901	512.8249649	102.4103959	440.2019005	695.2333433
9.73_297.9422m/z	297.94216	9.72875	pos							2155.885882	2367.742329	1147.583075	1517.257511	1088.568998	1160.11833	1431.56763	1494.770105	1213.764686
9.73_442.8686m/z	442.8685535	9.72875	pos							2132.33646	2824.976586	1208.097999	1778.20484	1692.73289	1332.771221	1225.289913	1893.779674	1463.249785
9.75_142.9909m/z	142.9909101	9.7507	pos							471.431748	598.0506129	330.3569212	501.9798683	434.7301691	410.956626	430.1144427	525.7749145	365.7921795
9.75_227.6319m/z	227.6319413	9.7507	pos							1762.407273	1894.927059	1252.320575	1679.515771	1812.861391	1741.611023	1629.38299	1514.970438	1978.912161
9.75_306.5632m/z	306.5632111	9.7507	pos							56.85091901	50.67755814	590.5193949	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199	0.001403199
9.75_308.8897m/z	308.8897159	9.7507	pos							1563.563947	2094.365096	1315.178234	1808.078902	1321.287712	1334.123678	1307.583064	1768.035656	1620.296904
9.75_375.2516n	398.2408804	9.7507	pos							72461.46088	81918.54544	70494.63015	84258.72725	71152.5774	72348.78606	60629.64556	60629.64556	75055.17713
9.77_130.0347m/z	130.0347033	9.7709	pos							327.9607662	400.2465604	201.1104405	305.8311901	274.3172856	247.0547754	267.4213027	270.3148295	201.3830058
9.77_205.1949m/z	205.1948986	9.7709	pos							1023.728253	1722.238889	1073.402415	1031.45269	1130.886826	1159.436609	949.944469	1142.997871	983.7159502
9.77_472.1363n	495.1254903	9.7709	pos							30607.23568	35099.19824	128732.6986	18436.93495	14108.04022	13204.98103	13633.30972	12977.46716	60857.52705
9.79_153.9931m/z	153.9931181	9.78575	pos							143625.9405	137664.267	132489.1564	139147.5763	146674.7038	141834.7648	141364.5617	137334.0086	142681.4377
9.80_111.5368m/z	111.5368401	9.79735	pos							0.001403199	11.52863005	43.04281068	81.19944931	106.1023319	86.1657104	28.82975078	27.57068872	55.22444862
9.80_113.0345m/z	113.0345258	9.79735	pos							440.2289577	718.3440367	322.7066252	453.7049261	321.4405088	514.6501704	356.1846766	418.3747895	380.6292982
9.80_162.9830m/z	162.9830299	9.79735	pos							2716.955881	3637.380479	2668.811967	2790.581295	3097.212746	3144.3931	3085.937243	3088.129735	3232.334865
9.81_360.7824m/z	360.7823816	9.806	pos							816.6739216	1254.884484	1035.229894	1110.379893	1175.676608	1201.436182	986.5798104	1182.968104	1289.173502
9.82_419.0189m/z	419.0189214	9.82105	pos							1442.477145	1253.363227	1432.869816	1879.417472	1906.093999	2115.212022	1598.350069	1533.051943	2021.481665
9.85_114.5585m/z	114.5584577	9.848266667	pos							706.1161931	441.1609256	537.1193833	558.3028718	667.4379122	599.4833449	476.5425455	574.6581934	566.9542723
9.88_100.9569m/z	100.9569017	9.87645	pos							869.5428167	436.2373872	839.2877206	575.0803817	923.6352666	592.9628911	829.0890843	745.5189888	722.3672628
9.88_126.9553m/z	126.9553481	9.87645	pos							40.77126052	44.55294891	20.17806936	19.28084623	20.97257243	0.001403199	46.36578276	0.001403199	0.001403199
9.88_130.0346m/z	130.0346444	9.87645	pos							418.2152634	212.4182111	364.2434935	216.1188097	394.9991274	244.0345773	279.6499053	296.4699841	281.4460132
9.88_131.5292m/z	131.5291668	9.87645	pos							53.39136878	77.11490733	24.09597691	46.07087021	35.77774637	17.01901673	35.35917099	119.6227474	56.6519493
9.88_163.9880m/z	163.9880156	9.87645	pos							728.3371662	507.2397863	644.2842935	656.1112276	801.6658387	725.6804055	588.964917	709.9854116	745.2769532
9.88_281.9128m/z	281.9128244	9.87645	pos							2523.769942	1492.003781	2396.025054	1818.497436	1641.823324	1615.090268	2069.315021	2355.6222	2202.928805
9.88_314.8738m/z	314.8738245	9.87645	pos							553.6882595	436.799772	636.0880255	492.78768	687.2078129	451.0853755	513.8002886	434.0878636	520.0777016
9.89_242.8471m/z	242.8470554	9.888483333	pos							1474.645194	898.0878798	1086.994721	660.217451	943.8734035	650.0648994	782.1500654	965.6309637	1020.618907
9.89_244.8443m/z	244.8442692	9.888483333	pos							378.7461092	83.45707011	335.1801517	184.7431411	288.3603249	189.8471657	224.8404105	282.7248134	317.0119387
9.89_307.2255m/z	307.2254643	9.888483333	pos							138.7589949	257.6075997	128.1768084	0.001403199	133.8066357	0.001403199	133.2897083	154.1014595	260.390587
9.90_111.0171m/z	111.0171499	9.90005	pos							279.1685111	968.9851819	604.93407	1183.000138	1213.801523	858.9534668	521.6574478	1503.224634	1319.542002
9.90_217.9791m/z	217.979077	9.90005	pos							3237.195647	1725.874125	2904.003687	1971.074713	2620.851112	2733.769287	2213.281618	2641.535784	2616.020159
9.91_111.5408m/z	111.5408329	9.908683333	pos							61.20868316	0.001403199	35.83614915	55.50531783	17.58412485	15.61710473	50.0388687	35.16335678	26.93937275
9.93_120.0255m/z	120.0254681	9.9276	pos							1987.338165	1483.522078	1620.773822	1804.514012	1568.730625	1708.716367	1513.875302	1506.582642	1923.79372
9.93_236.5705m/z	236.5705386	9.9276	pos							211.9308656	167.8502559	228.2135259	281.04721	53.6385823	0.001403199	54.25360034	0.001403199	144.3465479
9.93_256.5820m/z	256.5820243	9.9276	pos							6823.044676	4953.106152	7442.022433	8697.835983	4742.918162	5241.11633	4101.434287	3852.950961	7499.281762
9.93_257.0837m/z	257.0837365	9.9276	pos							1708.516163	1270.420444	2022.047791	2717.503221	1189.458138	1278.560641	1387.052723	824.7227873	1669.032096
9.93_277.5971m/z	277.597121	9.9276	pos							1934.13905	1623.75342	2181.509036	2539.144202	1682.23307	1641.090213	1409.630265	1063.077957	2513.173099
9.93_297.6086m/z	297.60862	9.9276	pos							182.845039	128.8916774	153.2990446	361.8816483	339.875113	204.9927022	257.2183517	152.5468636	394.8824454
9.93_416.2097n	439.1989757	9.9276	pos							60136.31453	47661.71977	67156.20195	80375.21853	43033.4072	45459.83818	43037.49704	36847.17718	65113.11086
9.93_443.1710m/z	443.1709515	9.9276	pos							194.4423101	176.2376239	381.562526	1250.672428	221.0955702	123.9870611	214.0028696	156.2053452	438.43743
9.93_828.4065n	851.3957419	9.9276	pos							41107.19626	21977.12849	47779.70257	91193.31709	26701.97821	26692.75807	18936.01661	15554.83246	60416.50053
9.94_277.0954m/z	277.0953988	9.942033333	pos							7743.479606	6478.020074	8296.409442	11096.96038	5009.851017	6295.017075	5513.928021	5016.909267	8317.368567
9.94_378.0843m/z	378.0843377	9.942033333	pos							741.6149253	873.2072719	825.7728732	1804.601122	704.1447441	639.386828	1203.784374	771.6365662	1309.512092
9.96_180.0441m/z	180.0441027	9.958533333	pos							1347.41498	1635.303264	1121.312598	1269.754541	1239.549864	1649.297646	1027.013067	1212.168922	1139.763149
9.99_130.0347m/z	130.034728	9.9885	pos							429.3520899	527.2521398	337.2065938	396.2467476	431.5195001	510.9412004	477.8244147	427.7778863	423.1432259
9.99_139.9834m/z	139.9833535	9.9885	pos							29.22567721	0.001403199	25.25489544	33.34263681	10.14868524	0.001403199	0.001403199	23.67043877	0.001403199
9.99_322.8870m/z	322.8870164	9.9885	pos							62.99365549	203.5755998	148.6160439	194.2931377	296.5095804	378.9821882	92.66757169	441.1706908	532.5467254
9.99_332.8191m/z	332.8190907	9.9885	pos							930.5909863	1103.3323	720.0703233	1011.86798	941.6429541	942.3857972	1064.937756	990.5437845	940.9419635

Supplementary file Table S4. Information of differential metabolites

ID	m/z	Retention time (min)	Ion mode	Metabolites	Compound ID	Super Class	Class	Sub Class	level	kegg	Score	Fragmentation Score	Adducts	Formula	Mass Error (ppm)	VIP	P-value	adj.P-value	log2(FC)	FC	average(LN)	average(CK)	LN1	LN2	LN3	CK1	CK2	CK3
6.69	421.0603m/z	421.060272		6.69475 neg	1-Methyl 2-galloylgalactarate	91922	Organic oxygen compounds	Organooxygen compounds			37.7		0 M+FA-H	C14H16O12	-5.602940506	19.2918717	1.8003E-05	0.0028021	-2.4325077	0.185243175	246856.818	1332609.516	219772.78	265174.662	255623.012	1249508.75	1394392.06	1353927.74
3.28	204.9813m/z	204.98127		3.280233333 neg	Pyroqallol-1-O-sulphate	HMDB0060016	Organic acids and derivatives	Organic sulfuric acids and derivatives			50.6	58.3	M-H	C6H6O6S	0.182427092	10.765532	0.008842625	0.00760009	-0.18446665	0.879974336	2657969.93	3020508.467	2540766.16	2769388.06	2663755.57	2945850.43	3065593.99	3050080.99
9.02	408.2878n	407.280525		9.01635 neg	Alkochelic acid	5491	Lipids and lipid-like molecules	Steroids and steroid derivatives		C17737	48.3	44.9	M-H, M+FA-H	C24H40O5	0.556417509	9.54672957	0.001486473	0.02538679	-1.1277428	0.457630375	23010.459	504797.04	216290.437	240334.407	236706.532	43643.568	547112.438	530825.024
13.07	810.5965m/z	810.596549		13.07185 pos	PC(16:0/20:1(11Z))	LMGP01011468	Lipids and lipid-like molecules	Glycerophospholipids			37.2		0 M+Na	C44H86NO8P	-2.256532355	9.25827417	0.027897165	0.13302305	-1.13578709	0.455086569	241951.587	531960.5759	312144.111	227646.374	186064.276	663121.398	536597.169	395263.16
0.76	151.1439m/z	151.143855		0.758666667 pos	Bis (2-hydroxypropyl) amine	44741	Unclassified	Unclassified			38.3		0 M+NH4	C6H15NO2	-1.871901467	8.09573226	0.000413697	0.01279428	2.052999824	4.14967924	256082.891	61711.49047	223255.472	282649.327	262343.873	53408.4616	63659.6513	68066.3585
14.64	854.7342n	877.722802		14.63885 pos	TG(16:0/18:2(9Z,12Z)/18:2(9Z,12Z))	HMDB0005390	Lipids and lipid-like molecules	Glycerolipids	**	C00422	37.7		0 M+NH4, M+Na	C55H98O6	-2.546063297	8.00179014	0.024784162	0.12428615	2.600339121	6.064291577	254278.403	41930.43822	150424.32	254566.726	357844.163	26129.8126	41558.1281	58103.37339
9.01	372.2689n	373.273144		9.012583333 neg	3alpha-Hydroxy-5beta-chola-7,9(11)-dien-24-oic acid	LMST04010330	Unclassified	Unclassified			52.1	66.4	M+H-H2O, M+H	C24H36O3	-1.610736918	7.99454351	0.005651719	0.05194163	-1.3021932	0.405509271	124968.739	332812.9545	127239.511	145603.244	132033.46	280663.488	364818.693	372956.683
7.43	584.3188n	607.307916		7.432366667 pos	Cholic acid glucuronide	HMDB0002577	Lipids and lipid-like molecules	Steroids and steroid derivatives			50.6	56.6	M+H-H2O, M+Na, M+H	C30H48O11	-1.475754588	7.68341224	0.000564574	0.0150214	-1.15348769	0.44953717	142363.47	316688.9851	126247.987	154520.339	146322.084	302219.081	300574.089	347273.786
0.78	193.1544m/z	193.15441		0.776966667 pos	altretamine	3923	Organic nitrogen compounds	Organonitrogen compounds			36.1		0 M+H-H2O	C9H18N6	-7.598292004	7.15375823	2.4471E-06	0.00135827	1.388475011	2.618017997	241295.354	92167.18712	234925.29	247541.587	241418.756	91077.0736	91295.8538	94128.634
0.82	194.9275m/z	194.927544		0.819566667 pos	Sulfate	HMDB0001448	Organic oxygen compounds	Homogeneous non-metal compounds	**	C00059	42.6	17.4	2M-H	H2O4S	0.315125954	6.85589386	0.003192697	0.03784423	0.53919707	1.453163536	459180.793	315987.0492	431275.248	476166.901	279739.939	325077.122	343143.954
0.68	156.0765m/z	156.076501		0.9788 pos	L-Histidine	21	Organic acids and derivatives	Organic acids and derivatives			57.6	96.9	M+H	C6H9N3O2	-1.622267271	6.52005052	2.1533E-05	0.00302935	0.493354584	1.407890064	426817.418	303161.07	429127.658	420123.476	433411.119	295624.524	307710.107	306088.493
5.22	405.1768m/z	405.176816		5.222166667 neg	1-O-(8R-hydroxy-8-methyl-3Z,9-decadienoyl)-beta-D-glucopyranose	HMDB0034064	Lipids and lipid-like molecules	Fatty Acyls			48.7	44.7	M+FA-H	C17H28O8	0.541646569	6.45192146	0.000673536	0.01640442	0.333277603	1.259872381	594714.356	472043.3317	591105.621	577291.236	615746.212	483737.573	469003.337	462489.085
8.07	405.2648m/z	405.264797		8.074883333 neg	(23R)-3alpha,7alpha,17alpha,23-Tetrahydroxy-5beta-cholan-24-oic Acid	LMST04010421	Unclassified	Unclassified			52.7	68.7	M-H2O-H	C24H40O6	0.352239726	6.33067568	0.000574309	0.01514166	-0.95468782	0.515953222	126734.375	245631.5213	111989.307	136297.047	131916.771	232710.936	263745.271	240438.357
2.00	216.1107m/z	217.114004		2.004416667 pos	γ-Glutamyl-γ-aminobutyraldehyde	63481	Unclassified	Unclassified			46.8	46.2	M+H, M+Na	C9H16N2O4	-1.291405511	6.2425366	7.1698E-05	0.00535821	-0.96145182	0.51298104	188226.496	242023.3476	119551.136	137808.821	127319.532	233754.579	249550.029	243505.435
5.85	433.2081m/z	433.208094		5.84575 neg	9,13-Dihydroxy-4-megastigmen-3-one 9-glucoside	HMDB0036318	Lipids and lipid-like molecules	Fatty Acyls			50.4	53.6	M+FA-H	C19H32O8	0.445073667	6.10699783	0.004468927	0.0454245	0.310700378	1.240309681	588446.117	474434.8334	607512.088	568518.575	592007.687	444419.706	482361.415	496523.38
6.28	352.0863m/z	352.086312		6.2811 neg	NAC-Diketide	69301	Unclassified	Unclassified			39.1		0 M+FA-H	C15H17NO4S	0.911651151	6.03228544	0.000362557	0.01209257	0.917815243	1.889252121	228468.098	120930.4439	212354.711	234866.028	238183.554	114621.003	117049.255	131121.074
12.08	772.6197m/z	772.619664		12.07935 pos	PC(14:0/22:0)	HMDB0007886	Lipids and lipid-like molecules	Glycerophospholipids	**	C00157	36.7		0 M+H2O	C44H88NO8P	-2.284130947	6.01669836	0.043541753	0.17345651	-1.2910549	0.425848967	95849.0982	223138.9332	129964.049	88103.1216	69800.1241	297469.991	211344.226	160902.57
0.80	138.0547m/z	138.054745		0.796983333 pos	Salicylamide	43329	Benzenoids	Phenols			40.9	13.9	M+H	C7H7NO2	-1.53186745	5.83290509	1.0597E-05	0.00252011	-0.83953425	0.558823947	125429.959	224453.443	125952.509	126877.341	123460.027	218730.677	223911.675	230717.978
3.26	231.1468n	232.154033		3.258783333 pos	Butyryl-L-carnitine	964	Lipids and lipid-like molecules	Fatty Acyls			65.1	44.9	M+H, M+Na	C11H21NO4	-1.306224871	5.82965725	0.000112614	0.00662604	0.528009347	1.441938213	325926.398	226033.5395	324986.052	331207.565	321585.577	214630.745	228531.369	234938.504
8.68	567.3179m/z	567.317871		8.68065 pos	Deoxycholic acid 3-glucuronide	LMST05010046	Lipids and lipid-like molecules	Steroids and steroid derivatives	**	C03033	52.4	65.2	M-H	C30H48O10	0.702483295	5.81468486	0.000190024	0.00877021	-0.97884248	0.507386668	102618.858	202249.8114	98305.5739	102502.301	107318.699	189772.309	214186.382	202790.743
0.78	118.0865m/z	118.086267		0.776966667 pos	L-Valine	35	Organic acids and derivatives	Carboxylic acids and derivatives		C00183	53.2	71.8	M+H	C5H11NO2	0.099931793	5.80335819	0.002919448	0.03630719	0.782652224	1.719635657	622436.815	521250.9567	639476.293	614816.51	616217.643	494266.489	537148.838	532336.542
4.81	187.0072m/z	187.007153		4.814166667 pos	p-Toluenesulfonic acid	HMDB0059933	Benzenoids	Benzene and substituted derivatives	***	C06677	45	30.9	M-H	C7H8O4S	0.532342117	5.76562274	0.000212963	0.00922276	-0.87012837	0.547098167	117931.117	215557.5075	111949.566	123423.85	118419.935	202268.317	219330.504	225073.702
6.78	745.3660m/z	745.366007		6.776866667 neg	Chalcomycin	Unclassified	Unclassified	Unclassified			39.5	0	M+FA-H	C35H56O14	1.139218365	5.69121981	0.001387861	0.0245783	-0.5984905	0.660444622	187107.733	283305.7102	195365.287	197057.222	168900.689	285816.042	299581.954	
4.28	213.0096m/z	213.009545		4.278183333 pos	Indoxylsulfuric acid	253	Organic acids and derivatives	Organic sulfuric acids and derivatives			56.2	84.8	M+NH4, 2M+H	C8H7NO4S	0.692021151	5.63419695	0.003047222	0.04702215	1.080904108	2.882604608	609753.304	407412.026	595781.017	605114.119	673409.212	394600.915	425265.993	
1.38	225.0631m/z	225.063121		1.380283333 neg	5-Acetylamino-6-formylamino-3-methyluracil	HMDB0011105	Organoheterocyclic compounds	Diazines	**	C16365	52	70.3	M-H	C8H10N4O4	0.852741347	5.41248041	0.003354486	0.03873375	0.512731658	1.426749105	300170.891	210388.0003	310562.434	300043.24	289906.999	235906.232	192594.84	202662.928
9.02	475.2680m/z	475.267994		9.01635 neg	Lucidenic acid G	HMDB0035599	Lipids and lipid-like molecules	Prenol lipids			40	9.26	M-H	C27H40O7	-4.478882489	5.32799447	0.001510546	0.0256939	-1.14254387	0.452960179	70592.8523	155847.8107	66348.889	74109.0829	71320.585	134418.585	166877.044	164247.803
7.35	470.0887n	451.070817		7.346316667 neg	(E)-Resveratrol 3-glucoside 4'-sulfate	HMDB0037073	Phenylpropanoids and polyketides	Stilbenes			41	14	M-H2O-H, M-H	C20H22O11S	0.798250293	5.26294309	0.001367384	0.02440004	-0.48538372	0.714307057	208564.064	291980.9648	191803.241	210629.211	223259.74	290085.958	301788.339	284068.597
5.79	310.2008n	331.200853		5.790983333 pos	Methylsalsalate	HMDB0036693	Lipids and lipid-like molecules	Fatty Acyls			51.8	64.1	M+NH4	C17H24O4	-1.547210994	5.1468826	0.024910893	0.09784152	-0.76781706	0.587884752	93849.0982	223138.9332	129964.049	88103.1216	69800.1241	297469.991	211344.226	160902.57
6.05	309.1936n	310.200876		6.0535 pos	1-(2E,5Z,7E)-decatrienoylcarnitine	LMFA07070016	Lipids and lipid-like molecules	Fatty Acyls			50	54.6	M+H, M+Na	C17H27NO4	-1.322987749	5.11502102	0.008302513	0.06523009	0.379759475	1.301124915	359320.839	276161.6778	335359.249	390943.788	351659.482	271105.342	285334.134	272045.557
5.30	549.1617m/z	549.161682		5.302883333 pos	Isoliquiritin apioside	HMDB0253655	Phenylpropanoids and polyketides	Flavonoids			44.8	28.2	M+H	C26H30O13	0.576966052	5.08148369	4.25576E-06	0.00169363	-2.44986011	0.183028458	18856.4193	92097.25881	17240.9908	14206.6795	19121.5876	93443.3123	88809.8802	94038.5842
4.41	179.0501m/z	179.050116		4.41115 pos	Hydrouric acid	1301	Benzenoids	Benzene and substituted derivatives	**	C01586	54.4	82.2	M+H, 2M-H	C5H4N4O3	0.272509782	5.01391512	0.016362684	0.05765756	-0.31123246	0.805952923	338328.546	419796.9625	341681.18	338761.576	334708.75	447411.823	442179.315	
4.52	287.0233m/z	287.0233		4.521733333 neg	4-Hydroxy-5-(dihydroxyphenyl)-valeric acid-O-sulphate	HMDB0059978	Benzenoids	Phenols			52.6	67.9	M+H2O-H	C11H14O8S	0.66257282	4.96934584	0.000640582	0.01595177	0.883198489	1.84445983	160435.321	86982.27252	149348.14	165986.88	165970.943	80598.8187	83071.9773	97276.0216
0.62	164.0665m/z	164.066545		0.616683333 pos	3-Oxo-3-ureidopropanoate	63408	Unclassified	Unclassified			36.2		0 M+NH4	C4H6N2O4	-0.25426927	4.73826733	9.32507E-05	0.00599648	0.43163916	1.348765145	254052.126	188359.0531	246728.72	254798.22	260629.437	189711.559	186409.197	188956.403
6.63	545.1305m/z	545.130538		6.63275 neg	Afromosin 7-O-(6''-malonylglucoside)	LMPK12050099	Lipids and lipid-like molecules	Polyketides			45.7	41.9	M-H	C27H26O13	0.867893053	4.7243055	2.91762E-06	0.00140496	-5.58270346	0.020865981	1385.31643	66391.14851	996.363687	1706.55353	1453.03207	65406.5265	69712.6282	64054.2908
4.29	195.0876m/z	195.087653		4.294383333 pos	Caffeine	1455	Organoheterocyclic compounds	Imidazopyrimidines	**	C07481	55.5	87.7	M+H	C8H10N4O2	-1.025191358	4.72387925	0.008065536	0.03273674	0.783071113	1.721453776	253141.159	356402.8087	264376.443	256179.072	330330.306	441119.375		
7.44	651.3006m/z	651.300565		7.440866667 pos	(+)-Galeon	87743	Phenylpropanoids and polyketides	Diarylheptanoids			36.3		0 2M-H	C20H22O4	6.473367759	4.67444871	0.001693103	0.02730193	-1.03428008	0.488259467	62268.3163	127531.2013	58941.1925	68395.98315	59467.7734	122495.058	116630.416	143468.13
4.11	306.0411n	287.023283		4.113883333 pos	4-hydroxy-5-(4-hydroxy-3-(sulfooxy)phenyl)pentanoic acid	HMDB0127746	Lipids and lipid-like molecules	Fatty Acyls			50	54.6	M-H2O-H, M+FA-H	C11H14O8S	0.606570723	4.59685075	1.65395E-07	0.00058142	-2.13652936	4.397029787	79542.6069	18090.07687	81008.1085	79279.2175	78340.4946	17889.7942	18045.7312	18334.7053
5.46	477.1769m/z	477.176959		5.457166667 pos	(7R',8R')-3-Methoxy-7,4',7,9''-tetrahydroxy-8,4''-oxyneolignan 4-xyloside	HMDB0040325	Organic oxygen compounds	Organooxygen compounds			44.3	24	M+H-H2O	C24H32O11	0.682735404	4.58524525	3.32476E-05	0.00338413	-1.9902335	0.357508566	95144.6455	15614.1814	94127.35	95083.1956	96220.8839	15135.055	16164.997	15764.462
7.45	372.2658n	373.273085		7.448183333 pos	(22E)-3beta-Hydroxy-5alpha-chola-7,22-dien-24-oic Acid	LMST04010287	Unclassified	Unclassified			47.1	41.6	M+H-H2O, M+H	C24H36O3	-1.763083638	4.58471864	0.000805159	0.01808009	-1.13070704	0.456691853	52360.0228	114650.661	46043.7509	57156.7481	53879.5695	108659.319	108662.182	126630.482
5.34	519.1504m/z	519.150415		5.3394 neg	Enterolactone 3'-glucuronide	HMDB0240377	Lignans, neolignans and related compounds	Lignan glycosides			45.5	31.7	M+FA-H	C24H26O10	-0.811084019	4.5775072	0.000206315	0.00909826	-3.70990424	0.076420089	5096.39958	66689.26485	4183.67725	5179.75433	5925.76717	58391.8556	66879.8023	74796.1367
5.40	285.1936n	286.20099		5.396716667 pos	2-Octenoylcarnitine	HMDB0013324	Lipids and lipid-like molecules	Fatty Acyls			50.2	55.5	M+H, M+Na	C15H27NO4	-1.384146005	4.52105728	0.010544682	0.07488499	0.331114307	1.25798464	318679.932	253325.7736	294908.605	335297.699	325833.493	240255.202	252863.577	266858.542
8.97	473.2529m/z	473.252894		8.974883333 pos	2-Acetyl-6-[3-(3-methyl-2E-pentenoyl)-2b,9a-dihydroxy-4Z,10(14)-copiapodien-1-one]	HMDB0037483	Lipids and lipid-like molecules	Steroids and steroid derivatives			39.6	6.57	M+FA-H	C29H36O5	-4.864015497	4.49052389	0.000553872	0.01435841	-0.98402683	0.543146407	74.8604132	1307.41797	64.3398818	79.7502964	79.4813975	1266.14161	1349.07	1305.126
2.38	188.9864m/z	188.986428		2.380333333 neg	Hydroquinone sulfate	HMDB0240263	Organic acids and derivatives	Organic sulfuric acids and derivatives			41.2	12.8	M-H	C6H6O5S	0.578086937	4.48091547	1.77751E-05	0.0028021	1.627538699	3.089854061	86737.5554	28071.73208	82478.2572	90176.7618	87557.6471	27344.104	29967.3166	29003.7746
11.75	810.5971m/z	810.597089		11.7471 pos	PC(14:1(9Z)/22:0)	HMDB0007919	Lipids and lipid-like molecules	Glycerophospholipids			37.9		0 M+Na	C44H86NO8P	-1.570588	4.47487894	0.034069019	0.14981219	-1.00230105	0.499203151	68614.8088	137448.669	89334.7098	64038.8659	52470.8506	170851.451	135849.272	105645.284
0.87	451.2705m/z	451.270521		0.870833333 pos	7-Ketodeoxycholic acid	HMDB0041827	Lipids and lipid-like molecules	Steroids and steroid derivatives			50.8	56.6	M+FA-H	C24H36O5	0.968662271	4.4368064	0.000455859	0.0113441	-1.19877124	0.435438566	78586.063	136478.827	70425.2475	85305.453	79913.4785	130194.964	142430.524	136957.962
7.18	357.2509n	358.258195		7.182883333 pos	(9Z)-3-hydroxydodecenoylcarnitine	LMFA07070024	Lipids and lipid-like molecules	Fatty Acyls			50.3	57.6	M+H, M+Na	C19H35NO5	-1.691657254	4.42147014	0.01413066	0.0891501	-0.27130507	0.828569678	306097.646	369428.974	280363.788	307812.66	330116.49	364761.337	364180.141	379345.444
12.36	814.6311m/z	814.631103		12.35646667 pos	PC(14:1(9Z)/24:1(15Z))	HMDB0007927	Lipids and lipid-like molecules	Glycerophospholipids			37.8		0 M+H	C49H88NO8P	-1.141103563	4.40458676	0.01664735	0.09794962	-0.74666131	0.595981187	92936.7431	155939.0551	111985.482	90023.84222	76800.9052	177081.284	155490.672	135245.21
0.76	342.1156n	365.107494		0.758666667 pos	Cytisine	916	Organic nitrogen compounds	Organonitrogen compounds		C07064	50.4	57.6	M+Na, M+K	C12H14N2O	-1.864728917	4.36038602	0.006125925	0.05442629	-0.54577201	0.686887858	219665.542	279753.7745	240335.683	220157.74	216144.169	275384.463	279764.106	284893.994
7.18	451.0706m/z	451.070854		7.17516667 pos	Torvanol A	HMDB0038789	Phenylpropanoids and polyketides	Flavonoids			41.4	15.8	M+H	C16H10O8	0.887364818	4.33951075	0.004285443	0.04457934	-0.4697747	0.722077671	147211.987	203872.7863	135218.367	161394.644	145022.949	191958.22	210840.16	208819.977
12.91	226.9511m/z	226.951131		12.9063333 pos	3-Chloro-2-methylidenelactone	HMDB0060368	Lipids and lipid-like molecules	Fatty Acyls			33.1	M+K	C7H5ClO4	1.791708206	4.3074007	0.018940206	0.10635965	0.105852334	1.076129973	846740.431	786838.442	855823.246	819043.614	865354.434	780009.934	779833.635	800671.757
7.20	408.2879n	407.280578		7.201166667 neg	1b,3a,12a-Trihydroxy-5b-cholanoic acid	HMDB0000326	Lipids and lipid-like molecules	Steroids and steroid derivatives			40.6	6.77	M-H, M+FA-H	C24H40O5	0.68668437	4.28658054	0.001636926	0.26722295	-0.63990244	0.641756345	98421.997	153363.4965	93447.8127	107734.776	94083.402	142276.911	159866.336	157947.243
8.31	517.1356m/z	517.135462		8.308666667 neg	Apigenin 5-O-(6''-malonylglucoside)	HMDB0038776	Organic oxygen compounds	Isoflavonoids			49.1	48.9	M-H	C24H20O13	0.601914154	4.23117294	0.00029324	0.00429546	-3.59415467	0.083116256	26200.3416	79103.42899	22345.3939	27096.8043	29164.734	92755.2567	86448.4656	71396.0108
4.95	320.1827m/z	320.182745		4.948983333 pos	N-(3-Oxododecanoyl)homoserine lactone	69239	Unclassified	Unclassified			38.9		0 M+Na	C16H27NO4	-1.629924129	4.23029361	0.020270674	0.11056941	-0.27484955	0.826536507	279978.56	338737.0761	257557.75	295487.242	286890.688	317198.729	348831.976	350180.523
1.45	160.0372n	319.067273		1.4461 neg	3-oxo-adipic acid	LMFA01170096	Lipids and lipid-like molecules	Fatty Acyls			42.9	21.5	M-H, 2M-H	C6H8O5	0.053989462	4.20282387	0.001337322	0.02410837	-1.54729767	0.342150351	27686.152	80918.08747	32508.1635	23341.7925	27208.5001	74521.1373	93153.4917	75079.634
0.78	146.0809m/z	146.080935		0.776966667 pos	L-trans-5-Hydroxy-2-piperidinecarboxylic acid	HMDB0029426	Organic acids and derivatives	Carboxylic acids and derivatives			54.2	75.7	M+H	C6H11NO3	-1.614302259	4.17383653	2.9532E-06	0.00140498	-1.44833224	0.36644479	29313.5932	79994.58947	28494.0877	29993.6997	29452.9923	77597.1376	80479.4048	81621.1662
4.39	331.0913m/z	331.091294		4.3893 neg	3α-Hydroxy-5β-chola-7,9(11)-dien-24-oic Acid	85300	Unclassified	Unclassified			55.6	84	M+H	C19H14N2O4	-7.919387226	4.12604325	0.00018466	0.00213019	0.163362914	1.120473284	326802.553	313799.2011	341634.477	316330.196	368962.383	317023.88	319517.708	305180.523
14.64	878.7344n	901.723657		14.63885 pos	TG(16:0/18:2(9Z,12Z)/20:4(5Z,8Z,11Z,14Z))	HMDB0005391	Lipids and lipid-like molecules	Glycerolipids	**	C00422	38.3		0 M+NH4, M+Na	C57H98O6	-2.237019436	4.07779849	0.002467674	0.03316134	0.540291044	1.454265865	160482.662	110353.0419	156333.001	156157.186	168957.799	99147.1357	111974.23	119937.76
2.28	148.0522n	166.086044		2.28185 pos	3,4-Dihydro-2H-1-benzopyran-2-one	HMDB0036626	Phenylpropanoids and polyketides	3,4-dihydrocoumarins			40.1	20.1	M+H, NH4, M+H-H2O	C9H8O2	-1.328476814	4.07516789	0.003261316	0.03817823	0.323047765	1.250970497	254357.621	203328.2335	248657.586	266153.633	248261.643	192443.784	210801.466	206739.449
2.26	381.0137m/z	381.013767		2.26065 neg	2,3-Dioxo-3-(tetra-7-sulfamoylbenzo[f]quinoxaline	69621	Unclassified	Unclassified			38.1	0	M-H	C12H8N6O6S	0.976573498	4.07587358	0.003396151	0.01304661	-1.11086726	0.463890909	31.6801572	2489.6492	1.9196954	2.0957457	1.9515.542	2364550.491	2.9228.804	2.9228.804
4.19	218.9970m/z	218.996962		4.189783333 neg	4-Hydroxybenzenesulfonic acid	34512	Unclassified	Unclassified			39	0	M+FA-H	C6H6O4S	0.45390928	3.95320001	0.04439053	0.17549861	-0.14180122	0.906386818	529499.653	584187.2835	556284.451	523309.271	508905.237	605136.269	561371.843	586053.74
0.78	377.0858m/z	377.085759		0.778533333 neg	5,7,4'-Trihydroxy-8,3'-dimethoxyflavanone	53149	Unclassified	Unclassified			37	0	M+FA-H	C17H16O7	-6.161846724	3.89155505	0.021641625	0.11509459	-0.3950451	0.760465602	159448.201	209671.8126	175417.656	149956.119	152970.829	189887.047	210688.275	228440.116
9.02	543.2556m/z	543.255623		9.01635 neg	Perindopril glucuronide	1796	Unclassified	Unclassified			39.4	0	M-H	C23H34N2O11	-0.570175861	3.8608558	0.001630411	0.02667854	-1.17902692	0.441648366	35684.0027	80344.48734	33302.0076	37198.9359	36951.0646	80778.1986	83054.1658	
8.94	395.2077m/z	395.207727		8.8368 pos	Androquinidole	HMDB0248395	Unclassified	Unclassified			40.9	8.45	M+FA-H	C23H30O5	0.570585215	3.85565339	0.00024225	0.00128485	-0.49386519	0.710119542	100791.285	40423.15758	107154.712	150896.7229	101438.777	41175.976	108849.382	147191.796
8.07	370.2504n	353.247079		8.074933333 pos	Antibiotic SB 202742	HMDB0041206	Benzenoids	Benzene and substituted derivatives			53.1	71	M+H-H2O, M+H	C24H34O3	-1.155725999	3.84660602	0.02019147	0.11036201	-0.75442979	0.592780631	71028.7328	119822.965	65854.0692	71190.0218	76042.1075	96410.1469	122889.333	140169.415
7.20	373.2731m/z	373.273131		7.20385 pos	3α-Hydroxy-5β-chola-7,9(11)-dien-24-oic Acid	42909	Unclassified	Unclassified			55.6	84	M+H	C24H36O3	-1.585052794	3.82955762	0.002707534	0.03053516	-0.8675574	0.548074061	53980.7988	98491.79636	46994.8903	58789.1305	56158.3575	87362.6036	106200.887	101911.899
7.47	360.1556m/z	361.155604		7.473983333 pos	Blumenolide C	HMDB0033537	Lipids and lipid-like molecules	Prenol lipids	*		40.7	6.8	M+FA-H	C17H24O6	0.537436737	3.78329784	0.003026088	0.03692253	0.746198061	1.678361753	75324.7667	45040.54747	73534.109	136134.041	131262.989	37533.1267	53074.1	44523.9923
5.28	550.1680n	573.157204		5.284233333 pos	Neoliquiritin Z''-apioside	HMDB0040544	Phenylpropanoids and polyketides	Flavonoids			53.9	73.4	M+H, M+Na	C26H30O13	-1.178776411	3.77575814	5.69789E-05	0.00488536	-2.72525313	0.151222725	7420.26546	49068.45471	6480.71036	7989.69628	7790.38973	45555.7641	48319.6022	53329.9978
5.22	428.1661n	427.158856		5.222166667 neg	rosavin	HMDB0257308	Unclassified	Unclassified			39.8	8.17	M-H, 2M-H	C20H28O10	-4.939279881	3.75800898	0.001017397	0.02051523	0.361045991	1.284356752	189282.5	147375.3301	188443.299	183687.332	195676.869	154099.771	142838.695	145187.525
8.28	129.0790n	411.125519		0.6788 pos	Allyxecloic acid	HMDB0033839	Organic acids and derivatives	Carboxylic acids and derivatives	***	C00408	51.4	63.1	M+H, M+NH4, M+H-H2O	C6H11NO4	-1.190233049	3.74246927	1.7903E-05	0.00127432	-1.87361573	0.272727401	8705.45633	37886.5613	8188.56128	8109.6528	9204.1454	47426.1854	46904.1354	47662.3757
5.85	455.1902m/z	455.190227		5.84575 neg	Flumethasone	HMDB0252336	Unclassified	Unclassified			47.4	44.2	M+FA-H	C22H28F2O5	3.764217594	3.65610067	0.003487554	0.03936069	0.345234339	1.270357312	191055.298	150394.9293	195772.769	184300.023	193093.103	140906.628	149999.569	160278.591
8.68	591.3131m/z	591.313052		8.6834 pos	(3a,5b,7a)-23-Carboxy-7-hydroxy-24-norcholan-3-yl-b-D-Glucopyranosiduronic	HMDB0002430	Lipids and lipid-like molecules	Steroids and steroid derivatives			49.9	54.1	M+Na	C30H48O10	-1.611904515	3.63284987	0.000624479	0.01579317	-1.03046725	0.489551571	37545.6843	76694.03288	31793.1959	40402.0419	40441.815	71073.5472	79299.2509	79709.3006
8.78	399.0950m/z	399.09499		0.778533333 neg	Bilforin	HMDB0002236	Organic oxygen compounds	Organooxygen compounds		C08996	44.5	33.6	M+FA-H	C16H18O8	4.815284609	3.6284039	0.00173087	0.02767817	0.436866606	1.353661111	151086.93	111613.5

4.86	379.1613m/z	379.161267	4.858383333	neg	Prenyl arabinosyl-(1->6)-glucoside	HMDB0041360	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		48.8	48.6	M-H	C16H28O10	0.780375182	2.88068193	0.018229678	0.10414419	0.273450951	1.208695593	159514.589	131972.5082	150206.378	169549.947	158787.442	125159.037	130439.627	140318.861
4.41	179.0580m/z	180.065278	4.4062	pos	Methyl n-formylanthranilate	88422	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*		42.2	22.2	M+H-H2O, M+H	C9H9NO3	-1.215022769	2.86381817	0.007399897	0.06125535	-0.39189697	0.762126843	81332.5846	106717.9111	75859.6538	89062.9074	79075.1927	100704.169	108217.149	111232.416
5.91	401.1455m/z	401.145539	5.908066667	neg	Zingerone glucoside	HMDB0040558	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			42.8	15	M+FA-H	C17H24O8	0.612882158	2.84560212	0.010793085	0.07603465	-0.52582488	0.694561872	58967.264	84898.50419	50360.1796	60581.7437	65959.8687	79617.514	91507.9449	83570.0536
5.85	423.0759m/z	423.075903	5.84575	neg	Enterolactone 3'-sulfate	HMDB0024050	Unclassified	Unclassified	Unclassified			49.8	59.8	M+FA-H	C18H18O7S	0.995961915	2.8430905	2.55052E-05	0.00337882	-5.51967749	0.021797742	525.770152	24120.39509	593.118702	467.49486	516.6996893	21989.6316	24944.7682	25426.7855
1.16	137.0456m/z	137.045583	1.157483333	neg	Hypoxanthine	HMDB0000157	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	***	C00262	39.7	6.1	M-H	C5H4N4O	-1.499528114	2.83652241	8.66802E-05	0.00583305	-0.88509857	0.541450529	27770.295	51288.7023	27334.9647	29619.002	26356.9183	50750.0136	53393.1983	49722.9001
7.29	593.3287m/z	593.328699	7.294266667	pos	Epoxymicin	45091	Unclassified	Unclassified	Unclassified			38.8	0	M+K	C28H50N4O7	-4.344914166	2.83628466	0.03787258	0.16057625	-0.63842424	0.642414233	50168.8684	78094.26674	41907.7503	57320.3142	51278.5409	63805.333	91350.9114	79126.5558
6.63	352.0863m/z	352.086274	6.63275	neg	(1R)-Hydroxy-(2R)-N-acetyl-L-cysteinyl-1,2-dihydronaphthalene	70328	Unclassified	Unclassified	Unclassified			40	38	M-FA-H	C19H17NO4S	0.789521113	2.83528634	0.00011491	0.00669528	0.822279425	1.768197498	54226.7219	30667.79698	51193.0306	55449.2306	56037.9044	30650.708	31312.9136	30039.7694
2.14	166.0848m/z	167.056114	2.1354	pos	9-Methylazathioprine	96280	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives			40	8.14	M+H, M+Na	C6H9N4O2	-1.43326675	2.79932662	0.000636235	0.01586857	0.52458341	1.439415811	76752.698	53322.11682	74290.6953	80485.5663	75481.8324	52394.8809	51313.7453	56257.7265
6.62	331.1401m/z	331.140113	6.61635	neg	Tryptophyl-Glutamine	HMDB0029081	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		39.5	6.73	M-H	C16H20N4O4	-3.208470741	2.77753886	0.002127145	0.03083556	0.709101564	1.63478574	60038.9837	36725.90374	53696.6433	63363.2319	63057.076	36011.3078	38556.3754	35610.028
3.24	315.0724m/z	315.072414	3.23635	neg	Phenylglucuronide	HMDB0059806	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		42.6	15.7	M-FA-H	C12H14O7	0.955035924	2.72133139	0.000147359	0.00760479	-0.57737799	0.670180686	44035.9664	65707.60293	41274.1844	46202.0203	44631.6944	66074.1821	64710.7464	66337.8802
5.41	337.1383m/z	337.138325	5.406433333	neg	Norepinephrine (noradrenaline)	63	Unclassified	Unclassified	Unclassified			37.4	0	2M-H	C8H11NO3	-6.460428137	2.70771328	0.028740802	0.13543365	0.410212367	1.328881413	102320.574	76997.52065	105367.969	112587.538	89006.2144	71692.5836	81884.2569	77415.7214
5.71	383.1537m/z	383.153654	5.709933333	neg	3b,16b-Dihydroxyandrosterone sulfate	5323	Unclassified	Unclassified	Unclassified			36	0	M-H	C19H28O6S	0.706196996	2.70400565	0.01546124	0.09437971	0.260381235	1.197795182	142912.581	119313.0373	132655.77	144135.634	151946.34	117761.99	117796.616	122530.206
0.82	601.1292m/z	601.129156	0.819566667	neg	1-Guanidino-1-deoxy-scyllo-inositol 4-phosphate	64554	Unclassified	Unclassified	Unclassified			38.3	0	2M-H	C7H16N3O8P	2.375907077	2.69684114	0.003373946	0.0388658	-0.96461233	0.512416087	23295.82	45462.70218	21307.4079	24660.8746	23919.1773	38879.999	47226.1143	50281.9933
2.26	402.9955m/z	402.995498	2.26065	neg	Uridine diphosphate (UDP)	97	Unclassified	Unclassified	Unclassified			40.7	7.81	M-H	C9H14N2O12P2	1.426624513	2.69681607	0.001543059	0.02601615	-0.32264766	0.799601088	86547.3771	108238.1933	83749.444	90528.2076	85364.4798	104671.981	108667.612	111374.987
3.29	227.9706m/z	227.968779	3.293883333	neg	Ammonium peroxydisulfate	92479	Unclassified	Unclassified	Unclassified			56.2	0	M+FA-H, 2M-H, M-H	H8N2O8S2	-7.153979098	2.69258641	0.002358631	0.03227886	-0.25543346	0.837735398	112559.841	134362.0445	107011.605	117665.306	113002.611	132981.847	134493.489	135010.797
5.65	401.1456m/z	401.145563	5.650833333	neg	Lamioside	LMPR0102070018	Lipids and lipid-like molecules	Prenol lipids	Isoprenoids		C11645	39.9	5.66	M-H2O-H	C18H28O11	0.578024854	2.68869796	0.041637118	0.15929907	-0.34100512	0.789491086	96428.2764	122139.7911	102444.08	83297.826	103542.923	119541.967	113847.396	133030.011
4.86	402.1498m/z	403.157029	4.8596	pos	Benzyl beta-primeveroside	95612	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			38.5	4.42	M+H, M+Na	C18H26O10	-7.073405536	2.68611544	0.000363689	0.01209257	0.293083773	1.200041063	128343.857	106949.5543	126123.052	131599.169	127309.349	105392.377	108653.759	106802.527
3.06	218.1035m/z	218.10349	3.05735	neg	Ipsainosinine	44848	Unclassified	Unclassified	Unclassified			39.7	0	M+FA-H	C8H15N3O3	0.539977844	2.66584817	0.000207519	0.00496826	0.645824154	1.564632875	58189.1003	37190.258	59147.2067	59427.1068	55992.5874	39555.5839	39456.0139	39951.1763
8.67	357.2782m/z	357.278154	8.672666667	neg	THA	LMFA01030822	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		47.4	43.5	M-H	C24H36O2	-1.831988911	2.6566612	0.000924417	0.01948289	-1.12444355	0.458678902	17831.1736	38875.06812	14785.4301	19291.7246	19416.366	35205.3681	41082.0677	40337.7686
5.45	597.0929m/z	597.092878	5.451166667	neg	Epitheaflagallin 3-O-gallate	89146	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives			36.3	0	M+FA-H	C27H20O13	7.759980343	2.64268635	3.34276E-05	0.0038111	-3.71420877	0.076192417	1680.25391	22052.77084	2283.229505	1357.79958	1399.73039	23470.5744	20256.9187	22430.8195
1.22	191.0169m/z	191.016875	1.22075	pos	Oxalosuccinic acid	3326	Organic acids and derivatives	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives	**	C05379	38.5	5.77	M+H	C6H6O7	-9.231098262	2.64173702	3.99466E-07	0.00089394	-2.66079645	0.159955199	3751.21776	24053.17543	4216.58766	3476.5667	3560.49891	23634.705	24416.7606	24108.0107
5.16	287.9796m/z	287.979616	5.157483333	neg	Acetyl tributyl citrate	HMDB0001915	Organic acids and derivatives	Organic phosphonic acids and derivatives	Bisphosphonates	*	C07752	41.9	15.3	M-H	C4H13NO7P2	-1.074134816	2.60722558	0.000581618	0.01028755	0.133481025	1.085080189	243876.747	223871.5431	244215.95	241596.67	245817.619	223584.905	227186.417	226243.307
6.03	353.0339m/z	353.033933	6.028183333	neg	cis-Resveratrol 4'-sulfate	HMDB0041714	Phenylpropanoids and polyketides	Stilbenes	Unclassified			48.9	51.9	M+FA-H	C14H12O6S	0.878324178	2.60698113	1.09923E-05	0.00252011	-4.15142652	0.056272485	1180.24916	20973.8235	1078.72266	1193.87655	1268.14828	20010.2003	20510.8826	22400.3876
5.33	543.1468m/z	543.14675	5.329033333	neg	5-Hydroxy-7,8,2',3'-tetramethoxyflavone 5-glucoside	LMPK12111294	Unclassified	Unclassified	Unclassified			39.4	0	M+Na	C25H28O12	-1.051215665	2.60569438	1.9082E-05	0.00283436	-4.82588284	0.035258555	723.614449	20523.08864	713.811841	856.565186	600.46632	19871.4864	21130.8329	21566.9466
5.85	523.1765m/z	523.176515	5.84575	neg	Sodium tetraacetate	41164	Unclassified	Unclassified	Unclassified		C11646	38.8	0	M+FA-H	C23H34O13	-8.272141988	2.60183795	0.002856886	0.01458232	-0.74758027	0.335572254	81548.1175	91088.56619	83318.4758	78610.7679	83015.3089	95760.6854	99099.1585	96439.7879
3.73	343.0673m/z	343.067274	3.730516667	neg	Isovanillic acid glucuronide	HMDB0240538	Unclassified	Unclassified	Unclassified			50.4	54.4	M-H	C14H16O10	0.592683993	2.59939924	0.001940283	0.02929453	-0.48115388	0.716404409	51289.4778	71592.91199	47339.0827	53101.4536	53427.8972	73866.0047	67620.1454	73292.5859
7.56	461.2397m/z	461.239683	7.556516667	neg	xi-Linalool 3-[rhamnosyl-(1->6)-glucoside]	HMDB0030422	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		40	5.16	M-H	C22H38O10	0.999288284	2.59679621	0.000480788	0.01385718	0.499664852	1.413885069	68469.4567	48426.46567	66962.1358	71378.1778	67068.0567	46147.3796	50501.5409	48630.4765
4.79	351.0957m/z	350.088414	4.792316667	neg	Indole-3-acetic-acid-O-glucuronide	HMDB0060001	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		49.6	52.8	M-H, 2M-H	C16H17NO8	0.780925824	2.58683163	0.022801402	0.11839664	-0.21228344	0.863169957	139757.201	161911.5677	132049.564	146328.542	140893.497	153191.726	168458.3	164084.677
7.18	373.1376m/z	373.13288	7.178516667	neg	Hydroxymaltol 5'-glucuronide	HMDB0060958	Unclassified	Unclassified	Unclassified	*		37.7	0	M+FA-H	C17H20O10	-3.368458889	2.58439655	0.004688837	0.02007519	0.009698262	0.645824154	1.564632875	58189.1003	37190.258	59147.2067	59427.1068	55992.5874	39555.5839	39456.0139	39951.1763
1.14	204.1228m/z	204.12279	1.137683333	pos	L-Acetylcarnitine	HMDB0000201	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	***	C02571	51	58.2	M+H	C9H17NO4	-1.201781096	2.57440815	0.005423045	0.05061189	0.528914888	1.442843563	67803.2188	46992.77212	65039.2775	74496.1249	63874.2539	50273.9596	44185.1006	46519.2962
8.68	589.2698m/z	589.29984	8.68065	neg	Boc-Phe(NMe)-Pro-Phe(NMe)-Gly-OMe	65475	Unclassified	Unclassified	Unclassified			36.8	0	M-H2O-H	C33H44N4O7	-5.455644779	2.57390363	0.00098133	0.0200564	-0.98684757	0.504579125	20151.7366	39937.7137	18358.1804	21014.481	21082.5485	35852.7472	42850.5203	41109.8736
5.13	223.0484m/z	223.06671	5.132616667	neg	4-Hydroxyphenylpropionylglycine	HMDB0094723	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**		52.7	65.9	M-H2O-H, M-H	C11H13NO4	0.418627795	2.56951648	0.018722243	0.10578341	0.255822621	1.638735279	54599.9399	33318.34045	45431.3697	51061.8062	54396.6439	33575.7557	37555.4346	36823.8131
4.90	536.1524m/z	559.141381	4.904516667	pos	Vaccinoside	HMDB0034733	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		38.8	0	M+H, M+Na	C25H28O13	-1.08675633	2.55902244	2.14625E-05	0.00302935	-4.56682949	0.042193674	841.250169	19937.82712	755.706724	996.25121	771.792572	18358.457	20287.7351	21167.2892
0.90	157.0737m/z	175.107483	0.898483333	pos	Ethadione	71882	Unclassified	Unclassified	Unclassified			40.7	7.8	M+H, M+NH4	C7H11NO3	-1.190473162	2.55060361	0.000178083	0.00847883	-0.56575557	0.675601498	39701.09	58764.06456	38446.1817	41126.3034	39530.785	56616.5847	58958.7333	60716.8757
5.22	495.1464m/z	495.146443	5.222166667	neg	Auriculoside	47465	Lipids and lipid-like molecules	Polyketides	Flavonoids			36.8	0	M+FA-H	C22H26O10	-9.679328746	2.53738169	0.002982316	0.0366141	0.407308984	1.326209766	79220.7051	59734.67177	79751.228	75965.7187	81945.1684	64431.2183	56071.2137	58701.5833
4.87	609.2274m/z	609.22736	4.874833333	neg	Isoquercitrin 6''-acetate	HMDB0040051	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C05554	38.6	0	M+FA-H	C29H30O14	2.250302396	2.53486586	0.001457828	0.02510548	-0.14612284	0.752823395	21557.2585	40226.3321	20836.2074	21360.5202	21978.8159	41943.0776	43736.7432	
4.88	173.0820m/z	173.081952	4.880083333	neg	Suberic acid	4243	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*	C08278	53.9	70.3	M-H	C8H14O4	0.114229274	2.52602541	0.001141975	0.02215836	-0.40291859	0.756326678	58995.7533	78003.0445	57292.1755	61030.7362	58664.3481	74095.949	79153.3114	80759.7531
4.95	500.1662n	545.164574	4.94705	neg	Ikarisoside A	LMPK12111710	Lipids and lipid-like molecules	Polyketides	Flavonoids			39	3.74	M-H, M+FA-H	C26H28O10	-4.013840909	2.52019199	1.84365E-05	0.0028021	-0.73038133	0.60274459	28128.6104	46667.54522	28750.3256	27505.0608	28130.4449	45383.3492	46869.7847	47749.5018
6.63	613.1176m/z	613.117804	6.63275	neg	Neobiorobin	HMDB0033006	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides			37.5	0	M+H	C27H32O15	-3.677435422	2.49250211	5.9713E-05	0.00491931	0.7922107	1.004551382	82.5110619	18289.33005	0.1014032	0.1014032	247.527679	17038.1542	20329.6435	17509.1904
2.20	285.0618m/z	285.061782	2.203283333	neg	Quinol glucuronide	HMDB0259508	Unclassified	Unclassified	Unclassified			46	32	M-H	C12H14O8	0.669222055	2.4722584	6.43941E-05	0.00506791	1.427307968	2.689444035	28610.4315	10638.0468	28070.1907	30570.4397	27190.6641	10709.213	10240.3315	10964.5959
7.44	787.2753m/z	787.275327	7.440866667	neg	Rotenone	44020	Phenylpropanoids and polyketides	Isoflavonoids	Rotenoids	*	C07593	38	0	2M-H	C23H22O6	-0.854037	2.46949812	0.001311029	0.02386246	-0.11102468	0.46320262	15645.953	33777.77304	15138.4879	17397.9578	14401.4131	32651.8992	30884.8206	37796.5993
3.03	264.9749m/z	264.97494	3.027516667	pos	Furfuryl 2-methyl-3-furyl disulfide	88332	Organoheterocyclic compounds	Heteroaromatic compounds	Unclassified	*		37.5	0	M+K	C10H10O2S2	-1.90498005	2.45439586	0.034956892	0.15243124	-0.25563852	0.837616333	107021.299	127788.8783	106191.837	106904.574	107967.487	115606.387	129433.6	138266.638
0.84	179.0561m/z	179.056148	0.841733333	neg	myo-Inositol	144	HMDB0000211	Organic oxygen compounds	Organooxygen compounds	**	C00137	51.5	58.4	M-H	C6H12O6	0.200241019	2.44957608	0.000367608	0.00532023	-0.14067861	0.817546949	93705.9178	73335.5122	90833.5473	87512.2807	92440.7857	80078.8702	80539.1588	79997.509
4.88	311.0775m/z	311.077535	4.880083333	neg	Hydroxytryptosol 3'-glucuronide	HMDB0240529	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			47	41.8	M+H2O-H	C14H18O9	1.890304594	2.44805683	0.000196302	0.00892522	0.772485234	1.708209632	42557.1205	24913.28918	40818.9993	44027.2286	42825.1337	23018.7068	26216.137	25505.0238
3.41	305.0863m/z	305.086299	3.414066667	pos	Dinitramine	72555	Unclassified	Unclassified	Unclassified			39.1	0	M+H+H2O	C11H13F3N4O4	2.166051029	2.44527833	0.001327758	0.02403553	-1.18847078	0.438767697	14006.7134	31922.84556	14026.755	14187.4829	13805.9024	36090.3134	31255.7333	28422.49
5.69	499.2806m/z	499.280217	5.692833333	neg	Ajugoside	LMFA04060002	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides			43.7	21.6	M+FA-H	C22H32O10	0.697302109	2.43446592	0.026673323	0.13316134	-0.46662606	0.728680911	38007.3109	65881.84545	43258.4041	41636.1462	48927.3825	64533.2966	68691.8671	66092.3416
4.64	271.0284m/z	271.028389	4.641416667	neg	5-(Hydroxyphenyl)-gamma-valerolactone-O-sulphate	HMDB0059993	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates			48.2	46.7	M-H	C11H10O6S	0.75678461	2.43276347	0.000428599	0.01296736	0.141929102	1.369288186	23995.9722	6366.181359	24722.9537	26403.5476	20861.4152	6561.281	6199.289535	6337.42663
0.86	217.1543m/z	217.1532	0.859583333	pos	Neotussilagine	HMDB0031820	Organoheterocyclic compounds	Pyrrolizidines	Unclassified			42.6	26.4	M+NH4	C10H17NO3	-1.749979154	2.43117272	0.023438706	0.1203175	-0.20774984	0.865886697	124717.483	144034.4135	122167.792	130681.326	121303.329	149288.746	135050.099	147764.396
1.22	321.0692m	344.058283	1.22075	pos	Beta-Citryl-L-glutamic acid	HMDB0013220	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			46.6	39	M+H, M+Na	C11H15NO10	-1.203187222	2.42212158	0.016784656	0.09437971	0.542951169	1.666365119	41499.7139	60463.02868	34444.8311	45657.9742	44586.3364	54538.86	62502.3389	64361.3512
6.75	211.1596m/z	234.146125	6.748833333	neg	Ebeokinone	68413	Unclassified	Unclassified	Unclassified			39.2	0.161	M+Na, M+K, M+H	C12H21NO2	-1.536326876	2.42201485	0.025397902	0.12933051	0.189924433	1.140714252	154206.314	135183.9985	160137.195	144761.928	157719.818	139715.765	137582.385	130053.845
7.51	318.2093m/z	318.209282	7.50885	pos	Glycopyrrolate	3132	Benzenoids	Benzene and substituted derivatives	Unclassified			44.6	37.5	M+H	C19H27NO3	9.180705082	2.37640769	0.001939309	0.02929453	-0.78195985	0.581576208	23539.4521	40475.26676	21293.8016	25301.4109	24023.1439	38667.1596	38247.4903	44511.1503
7.20	475.2680m/z	475.268049	7.201166667	neg	2-(2-Methylbutanoyl)-9-(3-methyl-2E-pentenoyl)-2b,9a-dihydroxy-4Z,10(14)-oc	HMDB0040994	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		39.1	4.16	M+FA-H	C29H38O5	-4.830498099	2.36844036	0.001354615	0.02427489	-0.62958523	0.646362214	30485.6761	47165.00358	28346.2061	34281.1964	28829.6259	45422.8358	48280.3216	47791.8533
4.34	373.1145m/z	373.114272	4.336566667	neg	Ethynylestradiol glucuronide	HMDB0033006	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			43.4	21.4	M+FA-H	C16H20O8	0.767973633	2.35388533	0.004486319	0.03193212	0.057976483	1.571976483	45182.1977	28742.28801	42136.636	47152.9769	46256.9781	28150.7657	28712.8519	29509.1092
5.68	433.1143m/z	433.114294	5.678766667	neg	4''-Hydroxyfenoprofen glucuronide	HMDB0060772	Benzenoids	Benzene and substituted derivatives	Diphenylethers	*		42.2	15	M-H	C21H22O10	0.62983243	2.34385029	6.15781E-07	0.00092499	-7.06889041	0.007448211	119.861126	16092.60691	0.0014032	71.6862183	287.895757	16344.656	15547.831	16385.3337
3.28	263.0111m/z	263.011052	3.280766667	pos	Methacrifos	72519	Unclassified	Unclassified	Unclassified			39.4	0	M+Na	C7H13O5PS	-1.247788555	2.34206068	0.000578592	0.01517868	-0.4037323	0.755900211	50465.9428	66762.75004	49022.1279	50762.461	51613.2396	63928.0723	68743.4314	67616.6115
0.78	262.1045m/z	262.104504	0.778533333	neg	Glutaminylalanine	HMDB0028790	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		42.6	13.4	M+FA-H	C8H15N3O4	0.2087009	2.34187738	0.001859968	0.02892573	0.802345346	1.743933884	38974.7363	22348.7465	36073.1039	41547.1962	39303.9098	19975.2565	21574.5007	25496.4973
7.74	369.1500m/z	369.156045	7.736233333	neg	AF Toxin II	HMDB0033504	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		39.5	2.4	M-H	C17H24O6	1.709031855	2.33739799	0.000316608	0.00437323	-0.36571707	0.807359392	73335.5122	90833.54073	67512.2807	72414.7857	80078.8702	86359.1588	91997.509	91993.8504
5.40	373.2459n	374.253156	5.396716667	pos	Dodecanedioylcarnitine	HMDB0013327	Lipids and lipid-like molecules	Fatty Acyls	Carboxylic acids and derivatives	*		48.8	50.5	M+H, M+Na	C19H35NO6	-1.49672917	2.33249028	0.004867124	0.04749372	-0.49625357	0.7089454	40678.1825	57378.442	36460.3153	43260.4121	42313.8201	54327.5835	56503.4876	61304.255
9.02	679.2304m/z	679.23044	9.01635	neg	Lactodifucoteatroase	58473	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		38.9	0	M+FA-H	C24H42O19	0.328356414	2.32993466	0.002377313	0.03245455	-1.22017064	0.429231946	12375.8854	28832.62884	11113.1172	13431.2483	12583.2907	24686.1141	32650.7664	29161.006
9.19	814.6317m/z	814.631071	13.49236667	pos	PC(20:5(5Z,8Z,11Z,14Z,17Z))	LMFA07040002	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	**	C00157	38	0	M+H	C44H82NO8P	-1.182082969	2.32244851	0.011728891	0.05081647	0.508167467	1.194722994	19405.1495	12803.4631	19100.5495	12803.4631	13966.8203	12214.7807	12545.7845	
3.91	257.0695n	258.076806	3.911966667	pos	1,3,5-Trihydroxy-10-methylacridone	95860	Organoheterocyclic compounds	Quinolines and derivatives	Benzoquinolines			40.2	11.8	M+H, M+Na	C14H11NO4	2.808855857	2.31260555	5.53151E-05	0.00486128	1.839007389	3.577637931	21742.2403	6077.261243	20137.0042	22958.9477	22130.7691	5624.14367	6296.88397	6310.75608
2.63	233.0126m/z	233.012603	2.634083333	neg	Hydroxytyrosol 4'-sulfate	HMDB0240532	Organic acids and derivatives	Organic oxygen compounds	Arylsulfates			45	29.6	M+H	C8H10O6S	0.300401909	2.29748282	0.000628234	0.01580205	0.454251886	1.370072166	58008.1444	42339.48099	56908.3546	58192.8264	58923.2522	39862.9293	42107.5816	45047.9321
13.49	666.6296n	649.626284	13.49236667	pos	Campesterol stearate	91434	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid esters	*		37.8	0	M+H+H2O, M+H	C46H82O2	-2.863875665	2.29731451	0.009667232	0.07189159	0.743731252	1.389314435	59061.1894	42511.03131	57492.9047	59021.0126	56572.7381	42204.8437	45755.4772	
6.84	435.2239m/z	435.22386	6.842166667	neg	7,8-Dihydro-8a,8a-dihydroxy-alpha-ionol 9-glucoside	HMDB0041578	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		40.6	4.68	M-FA-H	C19H34O8	0.741669159	2.29137769	0.024170624	0.12237321	0.228347805	1.169869735	12301.1931	105150.1101	127664.318	128379.314	112992.163	104791.492	106411.259	109247.579
4.93	479.1904m/z	479.190406	4.927016667	pos	Enterodiol glucuronide	HMDB0240503	Unclassified	Unclassified	Unclassified			52.2	65.2	M+H	C24H30O10	-1.605772246	2.29104443	0.000114415	0.00668487	-0.75144905	0.594006633	22482.2592	37848.49851	21316.0529	23578.1467	22552.578	36277.4354	38703.2061	38564.854
5.30	617.1487m/z	617.148665	5.302883333	neg	Rhamnazin 3-[6''-(3-hydroxy-3-methylglutaryl)glucoside]	LMPK12112636	Lipids and lipid-like molecules	Polyketides	Flavonoids			49.4	56.7	M-H2O-H	C29H32O16	-3.975806101	2.29043618	3.14201E-06	0.00144096	-3.5215626	0.087077114	1457.20892	16734.69471	1670.05979	991.099777	1710.46718	17144.2734	16062.1876	16997.6232
4.59	457.1873m/z	457.187256	8.087016667	neg	2-Methoxyestrone 3-glucuronide	HMDB0004482	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	**	C11132	45.6	38.4	M-H2O-H	C25H32O9	0.975732235	2.28704635	0.000672404	0.00290982	0.646581073	1.209.2.6	28687.8211	32215.976	30328.9618	42777.0499	42677.2466	32215.976	30328.9618	42777.0499
4.93	284.1407n	267.137429	4.927016667	pos	16-Oxoestrone	LMST02010048	Lipids and lipid-like molecules	Steroids and steroid derivatives	Estrane steroids	*	C14441	42.6	21.6	M+H-H2O, M+H	C18H20O3	-1.857259797	2.28526607	0.000221254	0.00936659	-0.69834991	0.616276674	24630.8872	39967.25545	22987.5918	26023.6631	24881.4069	38326.0724	40828.2631	40747.4308
5.78	557.1624m/z	557.162362	5.775866667	pos	5,7-Dihydroxy-6-C-methylflavanone 7-xylosyl-(1->3)-xyloside	52623	Unclassified	Unclassified	Unclassified			39.1	0	M+Na	C26H30O12	-1.095916419	2.27083384	6.60795E-05	0.00508515	-4.40181954	0.047306442	748.196745	15815.95901	861.948769	686.445503	696.199562	14899.3836	14991.3567	17557.1364
13.72	771.5196m/z	771.515582	13.72123333	pos	MGDG(16:1(9Z)/16:1(9Z))	LMGP04010211	Lipids and lipid-like molecules	Glycerolipids	Glycerophosphoglycerols	*		36.9	0	M+NH4	C46H70O10P	-4.108646725	2.26859213	0.032425598

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ID	m/z	Retention time (min)	Ion mode	Metabolites	Compound ID	Super Class	Class	Sub Class	level	kegg	Score	Fragmentation Score	Adducts	Mass Error (ppm)	VIP	P-value	adj.P-value	log2(FC)	FC	average(HN)	average(CK)	HN1	HN2	HN3	CK1	CK2	CK3
3.28_204.981741	204.981741	3.282233333	neg	Pyrrosetin-1-O-sulphate	HMDB0060016	Organic acids and derivatives	Organic sulfuric acids and derivatives	Organic sulfuric acids and derivatives	*		59.6	58.3	M-H	C8H6O6S		0.182427292	0.224525741	4.006775-07	0.00012819	-2.378946531	0.192246969	580991.8133	302058.467	603150.4824	569451.8993	569473.0582	294580.4128	3065593.986	3090080.986
4.28_213.0087	213.0087	4.27815333	neg	Indoxylsulfuric acid	253	Organic acids and derivatives	Organic sulfuric acids and derivatives	Anilinesulfates	*		56.2	84.8	M-H_2H2O	C8H7NO4S		0.692031151	13.18191292	2.737385-05	0.00027822	-3.366524763	0.09421946	58595.77852	31420.3285	63675.59785	57224.49681	59512.32839	31749.2116	594600.9147	594250.8591
4.41_264.1104	264.11041	4.4062	pos	N(2)-chenodeoxycholyl-L-glutamine	HMDB0062645	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C05597	42.6	18.3	M+Na, M+K, M+H, M+H-H2O	C31H18N2O4		-2.19616811	13.13032464	0.000688315	0.004769361	-0.672452486	0.627439175	145685.03	2321912.766	152291.219	138438.822	144494F.25	2157146.012	2356584.116	2412008.171
0.76_113.0595n	114.066273	0.758666667	pos	Creatinine	HMDB0000562	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00791	44.3	26.5	M+H, M+K	C4H7N3O		0.432927897	11.57044171	0.001678975	0.00882648	0.324881804	1.252561864	337738.117	269189.961	344484.708	327185.438	268350.898	283335.605	298133.388	298133.388
0.82_194.927n	194.927544	0.819566667	neg	4-methoxy-2-oxobutanoic acid	HMDB0001446	Homogeneous non-metal compounds	Non-metal oxoacids	Non-metal sulfates	**	C00509	42.6	17.4	[M-H-2H2O]-	C5H6O5		0.315125643	10.21361949	2.354224E-05	0.00073824	-1.397585947	2.634826674	83257.792	315987.0049	84503.1389	84637.6326	80564.4365	279759.9389	325077.1222	343143.9538
4.39_266.1119	4.3863	4.38633333	neg	Phenylacetylglutamine	HMDB0006344	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C04148	57.9	93.9	M-H, 2M-H, M-H2O-H	C13H16N2O4		0.028046749	9.914479585	0.00011519	0.001681912	-0.648503743	0.636412029	86169.8335	135079.614	88058.1803	85431.2344	84585.3958	129934.567	140173.866	136349.995
4.19_218.9979mz	218.998951	4.189783333	neg	4-Hydroxybenzenesulfonic acid	345 12	Unclassified	Unclassified	Unclassified	*		39	0	M-H-FA	C6H6O4S		0.45309028	9.71913423	5.59137E-06	0.000389562	-2.308080102	0.201928983	117964.3438	584187.2839	114771.9275	107025.7739	131496.33	605136.289	561331.6432	586553.7366
9.02_406.2878n	9.01635	9.02	neg	Alkocholic acid	5491	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	**	C17737	48.3	44.9	M-H, M+FA-H	C24H40O5		0.354177133	9.353207261	0.000194031	0.002246893	-3.288830077	0.102350955	51851.16426	504797.04	50806.15871	52945.86209	51293.83597	547112.4376	463453.658	545170.5734
0.93_146.0219n	191.0196885	0.925866667	neg	Oxosuberic acid	119	Lipids and lipid-like molecules	Fatty Acids and Conjugates	Keto acids and derivatives	**	C00026	52	61	M-H, M+FA-H	C8H6O5		0.418160227	9.031810955	0.001770946	0.00912826	0.992182707	1.868991361	899986.3309	479410.6012	910328.1777	929922.2747	847668.5402	389361.3497	484495.8807	564170.5733
12.98_835.6642mz	12.98333333	12.98333333	neg	SM(d18:1/24:1(15Z))	LMSP01021207	Lipids and lipid-like molecules	Sphingolipids	Phosphosphingolipids	**	C00550	37.4	0.3	C47H95N2O6P	C29H52NO7P		-2.259432316	8.982357951	0.000393699	0.003394161	-1.785135666	0.294615631	168616.5648	377105.57	164646.4107	169067.4998	169615.7834	585894.3298	561861.7174	586355.19
13.07_810.5985mz	810.5985488	13.07185	pos	PC(16:0/20:1(11Z))	LMGP01011468	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	*		37.2	0	M+Na	C44H88NO8P		-2.256532355	8.856891553	0.000161729	0.022645616	-2.176501408	0.221286225	117650.2252	531660.5759	139793.4924	116560.9592	96190.22407	663121.9383	536597.1894	395265.16
14.84_854.7342n	854.734	14.83685	pos	2-Octenoic-carnitine	5	Lipids and lipid-like molecules	Fatty Acids and Conjugates	Fatty acyl carnitines	**	C03622	55.5	55.5	M+Na, M+K	C15H27NO4		0.139414605	8.752174122	0.000155025	0.018603915	-1.115082165	0.461210827	35707.5198	419364.4522	36324.8776	35090.1621	35225.7736	503564.4615	334826.4426	419343.2029
0.84_227.1285n	227.128	0.84	neg	Butenyl-L-carnitine	5	Lipids and lipid-like molecules	Fatty Acids and Conjugates	Fatty acyl carnitines	**	C02862	52.4	65.1	M-H	C11H21NO4		0.107139356	8.734413221	0.000154502	0.001822945	-1.107123595	0.461210827	35707.5198	419364.4522	36324.8776	35090.1621	35225.7736	503564.4615	334826.4426	419343.2029
0.84_212.1557mz	212.155735	0.84	neg	Salsoline-Propionic-Acid	LMSP01030489	Organic oxygen compounds	Organooxygen compounds	Ethers	*		46.2	55.3	M+H-H2O, M+H	C11H13O2		-0.158693984	7.583039991	2.404484E-05	0.000747552	-1.026022039	2.309249307	501670.6445	217656.6323	528218.2512	492073.0615	484520.6807	214022.1883	216787.119	222076.7615
0.86_234.1818mz	234.181836	0.86	neg	Acetyl-lysine	HMDB0094038	Lipids and lipid-like molecules	Prenol lipids	Farnesenes	*		46.8	64.1	M-H	C13H25NO3		0.059092264	7.575439644	0.000127216	0.000825313	-0.969564499	1.959842408	324626.8639	241221.1176	339218.8779	310034.8359	324684.9606	212984.6852	219841.6579	239864.0852
10.75_788.5424mz	788.542013	10.7481333	pos	PG(16:1(9Z)/20:3(5Z,8Z,11Z))	HMDB0010593	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoinositols	*		49.6	0	C42H75O13P			0.015312852	6.931853195	0.524184575	0.328415752	0.328641257	3.042135407	1.05E+06	344750.2047	323373.3075	286674.624	701465.9313	559760.6858	559760.6858
5.71_508.3539mz	5.750363	5.750363333	neg	Acetylarachidonoyl-carnitine	HMDB0061653	Lipids and lipid-like molecules	Fatty Acids and Conjugates	Fatty acyl carnitines	*		51.6	64.1	M-H-H2O	C27H43NO4		0.154419768	6.754274596	0.000723291	0.004914228	-0.837031945	0.559048316	90648.1854	230312.6382	93446.1253	87850.1584	90848.1454	230312.6382	230312.6382	230312.6382
7.43_584.3188n	607.307916	7.432366667	pos	Cholic acid oxocinoate	HMDB0002577	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal oxocinoates	*		50.6	56.6	M+H-H2O, M+Na, M+K	C39H48O11		-1.475754588	7.246575906	7.118395E-05	0.001301042	-2.494997138	0.177390771	561773.0336	316868.9851	580321.6743	573913.0346	531093.35076	302219.0809	300574.0888	347273.7938
0.79_116.0853mz	0.779666667	0.779666667	pos	L-Valine	35	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00183	53.2	71.8	M+H	C5H11NO2		0.059931793	7.239453747	0.000127216	0.000838315	-0.744204384	0.597439175	1.49E+06	2.52E+06	1.49E+06	1.49E+06	1.49E+06	2.52E+06	2.52E+06	2.52E+06
4.41_179.0583n	176.0510155	4.41115	neg	Hippuric acid	1301	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	**	C01586	54.4	82.2	M-H, 2H-H	C9H9NO3		0.227250762	7.047809583	8.709135-05	0.001458643	-1.279900405	0.411813865	172877.2414	419786.9825	175356.5331	170268.6304	173008.3625	394704.7497	447411.8227	417240.3151
2.26_547.0137mz	2.263333	2.263333333	neg	2,3-Dioxo-6-nitro-7-sulfamoylbenzo[f]quinoxaline-1-carboxylic acid	69621	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		38.1	0	M-H	C11H5N5O8S		-2.976034688	6.950687596	2.568746-06	0.000285901	-0.158430799	0.901678157	29875.57093	249956.6492	29839.19687	29911.94497	29875.57093	249956.6492	249956.6492	249956.6492
6.05_309.1939n	310.2008757	6.0535	pos	GE,SZ,TE(1-decatrienoic)carnitine	LMFA07070016	Lipids and lipid-like molecules	Fatty Acids and Conjugates	Fatty esters	*		50	54.6	M+H, M-H	C17H29NO4		-1.322987749	6.822686558	1.94568E-06	0.000234707	0.835964994	1.784937211	492853.9296	276161.6778	494341.4215	496032.8328	488187.5345	271105.3421	285334.1339	272045.3573
0.93_138.0893n	5.52541897	0.93	neg	Isoleucine-alpha-keto-gamma-methylvalerate	HMDB0035319	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		49.7	0.2	M-H	C7H12O3		-0.446175133	6.796418834	0.000204568	0.002459545	-1.042218834	-1.425183795	131721.2284	302919.5809	132319.7924	131123.7304	132045.6188	303293.0357	302245.1358	302745.1358
5.56_541.2657n	541.265741	5.56185	neg	Cheetolobolaxin N	88035	Alkaloids and derivatives	Cytochalasans	Cheetolobolaxins	*		36.6	0	M-H, C2H4O2-H	C31H38N2O5		-9.321353293	6.579179639	0.00146059	0.02610039	0.527533281	1.441482476	743870.881	516052.893	677882.1575	802851.388	750869.0874	569820.9977	478962.7138	499434.9675
5.74_745.3880mz	745.388092	6.779666667	neg	Thiocolchicoside	7113	Unclassified	Unclassified	Unclassified	*		39.5	1.9	C33H42NO14	C33H42NO14		-1.192218385	6.563533396	2.193368E-05	0.000710844	-1.84061645	0.278622476	78935.33788	283305.7102	82097.56359	77170.4763	80535.5094	285618.2745	280819.6249	283581.9538
8.07_405.2646n	405.2647973	8.074883333	neg	(23R)-Salsha,7alsha,17alsha,23-Tetrahydroxy-5beta-cholan-24-oic acid	LMST04010421	Unclassified	Unclassified	Unclassified	*		52.7	68.7	M-H2O-H	C24H40O6		0.352230726	6.411996677	2.7956E-05	0.00097001	-2.548702338	0.175083164	41949.7283	249561.5213	44439.99586	41457.64625	39951.96879	232710.9358	263745.2709	240438.357
0.83_345.1656n	345.165642	0.83	neg	3-Hydroxyhippuric acid	HMDB0013228	Lipids and lipid-like molecules	Lipids and lipid-like molecules	Fatty Acids and Conjugates	*		45.9	38.5	M-H	C18H27NO3		0.435583487	6.335979453	1.85074E-05	0.000344887	-1.302735206	0.406134827	13388.9868	33219.82778	13381.1837	13396.7899	13381.1837	33219.82778	33219.82778	33219.82778
0.75_243.0333n3	243.033393	5.7632	neg	4-phenylbutanoic acid-O-sulphate	HMDB0059983	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	**		49.6	0	M-H	C10H12O5S		0.128104902	6.090843621	0.000445192	0.003460158	-0.715852883	0.607580205	288946.2571	475568.7988	292601.6817	301779.7214	282457.3883	445016.1828	500560.6096	498690.9269
4.72_312.2974n	312.297427	4.09033333	neg	Phenol-sulfate	HMDB0060054	Organic acids and derivatives	Organic sulfuric acids and derivatives	Phenol sulfates	**	C02180	56	90.1	M-H	C6H6O4S		0.128624485	6.085239855	0.000144501	0.000746151	-0.944603288	0.519451181	1376.09305	2849.8736	1376.09305	1376.09305	1376.09305	2849.8736	2849.8736	2849.8736
8.68_357.1179mz	357.317805	8.68065	neg	Deoxycholic acid 3-glucuronide	LMST05010046	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal oxocinoates	**	C03033	52.4	65.2	M-H	C30H46O10		0.102483295	5.951048474	1.77153E-05	0.000695929	-2.905672991	0.133445865	28389.42725	202249.6114	29714.68254	27730.16346	23616.41574	189772.3091	214186.3825	202790.7427
0.91_516.3468mz	0.741216667	0.741216667	neg	beta-D-fructose 2,6-bisphosphate	HMDB0062400	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C00085	38.9	1.96	M-H2O-H	C12H24O12P2-H		0.196146426	5.879429466	0.000852	0.003988013	-0.553224477	0.676503533	29768.5253	94419.7546	29722.2407	29814.8099	28784.3245	95634.2407	93032.7075	93379.9301
4.28_279.9889mz	279.989729	4.27815333	neg	2-Methyl-4-amino-5-hydroxymethylpyrimidine diphosphate	3426	Unclassified	Unclassified	Unclassified	*		39.8	0	M-H2O-H	C6H11N3O7P2		1.378133309	5.753845392	7.47579E-07	0.000190424	-3.765181784	0.073729287	12998.8613	178319.1457	13866.23491	12551.34963	12562.05835	172900.2324	179307.3857	178700.3623
0.84_224.1023n	6.8861	6.886	neg	N-Decanoylvanillin	4	Lipids and lipid-like molecules	Fatty Acids and Conjugates	Fatty amides	*		53.5	73.3	M+H, M+Na, M+K	C18H27NO3		-1.791262172	5.733308967	0.001441125	0.015336967	-0.401137563	0.757916857	1.49E+06	4277134.2	1.49E+06	1.49E+06	1.49E+06	4277134.2	4277134.2	4277134.2
12.08_772.6197mz	772.619636	12.07935	pos	PC(14:0/22:0)	LMGP02076886	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	**	C00157	36.7	0	M-H+H2O	C44H88NO8P		-2.284133947	5.719240611	0.011717292	0.036942744	-2.278850045	0.206001853	49380.42196	223336.9332	56451.16138	49092.41176	42797.69274	231973.2984	237469.9913	211344.2384
0.84_177.0789n	177.078979	4.94705	neg	(HK*,8R*)-5-Methoxe-7,4',7,8,9*-pentahydroxy-6-4'-nonenoldonan	LMPK04040325	Lipids and lipid-like molecules	Prenol lipids	Unclassified	*		44.3	0	M-H	C10H18O3		-0.446175133	5.719240611	0.011717292	0.036942744	-2.278850045	0.206001853	49380.42196	223336.9332	56451.16138	49092.41176	42797.69274	231973.2984	237469.9913	211344.2384
11.65_746.6033mz	746.603263	11.6507167	neg	PA(P-20:0/19:1(9Z))	82316	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphates	*		37.4	0	M-H	C43H81O7P		-3.645386424	5.595328376	0.020163365	0.050725466	-2.307019406	0.202794362	44411.59645	218986.1586	33631.26382	43225.84855	56375.44719	305520.5061	204960.5646	146483.3879
0.79_234.1641n	234.164118	1.10748333	neg	Ile-Hexanone	3866	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	*	C07513	39.6	1.96	M-H-H2O	C12H23NO3		-0.266544888	5.589503373	0.000127216	0.000838315	-0.744204384	0.597439175	1.49E+06	2.52E+06	1.49E+06	1.49E+06	1.49E+06	2.52E+06	2.52E+06	2.52E+06
10.69_756.5577mz	756.557582	10.69025	pos	PC(16:0/20:3(5Z,8Z,11Z))	61854	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	*		37.2	0	M-H+H2O	C44H88NO8P		-2.284133947	5.719240611	0.011717292	0.036942744	-2.278850045	0.206001853	49380.42196	223336.9332	56451.16138	49092.41176	42797.69274	231973.2984	237469.9913	211344.2384
0.84_197.0703n	0.5373333	0.537333333	neg	2,2,6,7-tetramethyloctyl(4,3,0)nona-1(9),4-dien-5-one	5	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		45.4	0.2	M-H	C12H22O2		-0.446175133	5.719240611	0.011717292	0.036942744	-2.278850045	0.206001853	49380.42196	223336.9332	56451.16138	49092.41176	42797.69274	231973.2984	237469.9913	211344.2384
0.84_216.1157n	216.115735	0.84	neg	3-Methoxy-4-hydroxyphenylglycol	HMDB0004826	Lipids and lipid-like molecules	Fatty Acids and Conjugates	Fatty acyl carnitines	*		46.4	64.1	M-H	C9H12O4		-0.446175133	5.719240611	0.011717292	0.036942744	-2.278850045	0.206001853	49380.42196	223336.9332	56451.16138	49092.41176	42797.69274	231973.2984	237469.9913	211344.2384
0.78_377.0859mz	377.085794	0.778833333	neg	4-Hydroxy-2-oxo-7-phenylheptanoic acid	63149	Unclassified	Unclassified	Unclassified	*		57	0	M-H	C13H15O4		-0.446175133	5.719240611	0.011717292	0.036942744	-2.278850045	0.206001853	49380.42196	223336.9332	56451.16138	49092.41176	42797.69274	231973.2984	237469.9913	211344.2384
14.52_907.7394mz	907.739317	14.51666667	neg	22-O-Glu-Camptosil	103412	Lipids and lipid-like molecules	Prenol Lipids	Sterol Lipids	*		64	0	M-H	C48H76O19		-0.446175133	5.719240611	0.011717292	0.036942744	-2.278850045	0.206001853	49380.42196	223336.9332	56451.16138	49092.41176	42797.69274	231973.2984	237469.9913	211344.2384
0.88_203.1154n	204.122783	0.8802	pos	DL-Acetylcarnitine	HMDB0240773	Lipids and lipid-like molecules	Fatty Acids and Conjugates	Fatty acyl carnitines	**	C02571	47	43	M-H, M+FA-H	C9H17NO4		-1.862635432	5.321568139	0.002203832	0.010564109	1.033994937	2.133935059	275293.4646	122609.3565	279148.8527	271437.8765	268496.6948	116753.5253	128086.5819	127084.3024
0.83_175.0395n	175.039497	0.91533	neg	Pyrrole-2,5-dicarboxylic acid	HMDB0004319	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	*		40	0	M-H	C6H5NO4		-0.478682429	5.319810687	0.002203832	0.010564109	1.033994937	2.133935059	275293.4646	122609.3565	279148.8527	271437.8765	268496.6948	116753.5253	128086.5819	127084.3024
10.83_786.5396657	786.529657	10.83215	neg	PE(18:3(6Z,9Z,12Z,15Z)/18:0)	85149	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoethanolamines	**	C00350	56.6	0	M-H	C41H76NO8P		0.012268563	5.309056751	0.000442192	0.002985564	-1.212121293	0.431636181	112482.0126	263594.4947	121413.4547	116561.6898	99450.89219	308377.4238	255566.3863	217839.6741
0.84_228.1644n	228.164359	0.88484333	neg	Oxoarnetaze	42	Benzenoids	Benzene and substituted derivatives	Phenols	**	C07144	42	13.7	M-H	C12H23NO3		-1.492187364	5.284407224	0.002275781	0.012947625	-1.219503302	0.429612745	79440.49445	24534.6341	80650.2341	78230.74549	78705.94	24534.6341	24534.6341	24534.6341
4.95_320.1827mz	320.182746	4.949583333	pos	N(3)-Dendrobanoxinol*homosserine lactone	69239	Unclassified	Unclassified	Unclassified	*		38.9	0	M-H	C19H27NO4		-1.629924129	5.138729875	0.000430656	0.003079421	-0.713090931	0.610012188	209833.7444	338737.0761	213525.538	198441.8088	203133.8854	337198.7292	340851.9759	350180.5234
0.83_216.1952n	393.1351345	0.83	neg	Glucosyl-6-methoxy-2,6-dimethyl-2,4,7-octadienoate	LMPK03050622	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**		36.4	36.4	M-H, M+Na, M+NH4	C17H28O8		-1.234176354	5.108983955	0.000208568	0.002459545	-1.042218834	-1.425183795	131721.2284	302919.5809	132319.7924	131123.7304	132045.6188	303293.0357	302245.1358	302745.1358
0.68_156.0765mz	156.076514	0.6788	pos	L-Histidine	21	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00135	57.6	96.9	M+H	C6H9N3O2		-1.622267271	5.085493535	0.000311411	0.002392572	0.510862955	1.424091907	431974.7456	303161.0412	411186.638	442487.3254	442280.2741	295824.5235	303770.107	309088.4932
0.72_457.3196n	457.319596	7.91733	neg	Androsterone glucuronide	HMDB0004295	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glucuronides	**	C11135	50.3	53.3	M-H	C25H38O8		-2.293196268	5.085493535	0.000311411	0.002392572	0.510862955	1.424091907	431974.7456	303161.0412	411186.638	442487.3254	442280.2741	295824.5235	303770.107	309088.4932
0.76_342.1156n	365.1047942	0.75866667	pos	Lactulose	916	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C07064	50.4	57.6	M-NH3, M+K	C12H22O11		-1.864728917	4.996029735	3.24495E-05	0.000885588	-0.846735525	0.558358445	155870.1003	279157.7745	162326.1824	144722.1752	160391.9434	275364.4635	279704.8661	282363.994
0.84_197.0703n	197.097153	4.87416667	neg	a-Tubulinaseulfuric acid	HMDB0059933	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	**	C08677	45	30.9	M-H	C7H6O5		0.533421117	4.979061218	0.000139455	0.001671198	-0.842072664	0.556358445	155870.1003	279157.7745	162326.1824	144722.1752	160391.9434	275364.4635	279704.8661	282363.994
0.85_215.1527n	55.12103769	4.4062	pos	Dutasteride	HMDB0015258	Lipids and lipid-like molecules	Steroids and steroid derivatives	Androstane steroids	*		39.5	0	M-H, M+FA-H	C27H35F6NO2		0.015424185	4.960798	0.004333365	0.017497874	-1.467079868	0.360291954	73275.40439	201698.3958	80739.25121	67743.02409	73323.93787	159238.8008	214815.7945	231040.552
0.84_292.0959n	5.105699722	5.1045	neg	Pyrrosetin-2-O-glucuronide	HMDB0060017	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**		51.6	60.5	M-H, M+FA-H	C16H19NO12S		0.154343427	4.941937931	0.000853971	0.004539291	-1.320835966	0.398429424	4316.40987	13947.51	4300.5971	4332.4227	4316.40987	13947.51	13947.51	13947.51
0.83_264.9749n41	264.9749491	3.027315667	pos	Furfuryl 2-methyl-3-furyl disulfide	88332	Organic oxygen compounds	Organooxygen compounds	Heteroaromatic compounds	*		39.5	0	M-H	C10H10O2S2		-1.90498005	4.824301635	6.2838E-05	0.001209427	-3.337076883	0.096671291	12351.5824	127768.8783	12682.18058	11928.77839	12143.78824	115806.3888	139433.6104	138268.6376
0.83_195.0879n	196.087643	4.23438333	neg	Caffeine	1455	Organic oxygen compounds	Organooxygen compounds	Heteroaromatic compounds	**	C07481	55.5	0	M-H	C8H10N4O2		0.333953676	4.914040067	1.79E-05	0.000259566	-3.368164209	0.092238264	24417.2282	118585.6304	24611.9396	24222.5168	24417.2282	118585.6304	118585.6304	118585.6304
0.76_162.1122mz	162.112191	0.75866667	neg	L-Carnitine	34532	Organic nitrogen compounds	Organonitrogen compounds	Quaternary ammonium salts	**	C00318	54.7	77.6	M+H	C7H15NO3		-1.866632448	4.763613641	1.26423E-05	0.000146592	0.048239192	1.679314166	277633.7125	165283.5986	278030.7583	273308.564	281661.8173	170565.5003	158612.0086	166952.2669
0.76_215.2324mz	0.778533333	0.778533333	neg	2-C-Methyl-D-erythritol 4-phosphate	1203	Unclassified	Unclassified	Unclassified	*		39.3	1.3	M-H	C5H13O7P		-1.344619181	4.741910401	0.000708726	0.004539291	-1.320835966	0.398429424	4316.40987	13947.51	4300.5971	4332.4227	4316.40987	13947.51	13947.51	13947.51
3.29_227.9706n	227.968792	3.23088333	neg	Ammonium oxercarbuxilate	92479	Unclassified	Unclassified	Unclassified	*		56	0	M-H, 2M-H	H6NO2S2		-1.753979686	4.713582724	1.6981E-06	0.831466-05	-2.435490753	0.164959671	24838.12337	134382.0445	25028.22213	24439.30986	25050.29931	132981.8471	134403.4894	135610.7971
0.84_161.2705n	161.270474	0.84	neg	Ethocholanone-alpha-acetonide	HMDB0004494	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	*	C11136	50.3	6.34	M-H	C10H18O2		0.533953676	4.713582724	1.6981E-06	0.831466-05	-2.435490753	0.164959671	24838.12337	134382.0445	25028.22213	24439.30986	25050.29931	132981.8471	134403.4894	135610.7971
0.47_274.2564n	473.252364	8.074883333	neg	2-Ansetrol-9(3-methyl-2E-pentenoic)-2b-3a-dihydroxy-4Z,19:14)-[4]dodecanolide	HMDB0037243	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*		39.6	6.57	M-FA-H	C24H38O5		-4.864215647	4.604963921	1.864E-05	0.000672261	-2.343851431	0.196595756	257482.7755	130714.9791	274124.4992	256447.0552	259647.7518	124341.0374	136941.9419	130360.9163
0.84_183.0809n45	183.0809445	7.446666667	pos	11-Ketoxin	87743	Organic oxygen compounds	Organooxygen compounds	Cyclic dicarbonyls	*		38.3	0	M-H	C10H12O3		-1.292139668	4.602135	0.000217644	0.002392572	-0.510862955	0.701678723	2294938.08	1275312.203	2344553.417	2245322.743	2344444.076	1275312.203	1275312.203	1275312.203
11.33_435.3094mz	435.30307	11.32543333	pos	Enoxolonol	3516	Lipids and lipid-like molecules	Steroids and steroid derivatives	Enolactone steroids	*	C01604	49.6	0	M+K	C23H40O4		-0.779399081	4.577941834	0.000213031	0.001702504	-1.477491165	0.339112843	593713.7808	165528.5655	608689.6108	584632.3243	388151.5972	173818.1188	158579.6218	163587.9559
8.14_614.5312mz	614.531204	8.14	neg	3-Hydroxyhippuric acid	HMDB0013228	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoinositols	*		49.7	0	M-H	C27H51O13P		-0.446175133	5.719240611	0.011717292	0.036942744	-2.278850045	0.206001853	49380.42196	223336.9332	56451.16138	49092.41176	42797.69274	231973.2984	237469.9913	211344.2384
1.71_810.5977mz	810.597789	11.7471	pos	PC(14:1(9Z)/22:0)	HMDB0007919	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	**		37.4	0	M+Na	C44H88NO8P		-2.256532355	8.856891553	0.000161729	0.022645616	-2.176501408	0.221286225	117650.2252	531660.5759	139793.4924	116560.9592	96190.22407	663121.9383	536597.1894	395265.16
0.84_197.0703n	1.3863E+08	0.84	neg	2-Hydroxyisocaproic-d-formylamino-3-methylvaleril	HMDB0011106	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C16365	45.9	0.5	M-H	C6H12O3		-0.446175133	5.719240611	0.011717292	0.036942744	-2.278850045	0.206001853	49380.42196	223336.9332	56451.16138	49092.41176	42797.69274	231973.2984	237469.9913	211344.2384
0.84_197.0703n	1.47943333	1.479433333	neg	N-Methyl-4-pyridone-carboxamide	1502	Unclassified	Unclassified	Unclassified	*		43.1	25.4	M-H	C7H6N2O2		-1.367386147	4.743411	4.53218E-06	0.000389562	-2.308080102	0.201928983	117964.3438	584187.2839	114771.9275	107025.7739	131496.33	605136.289	561331.6432	586553.7366
2.46_402.9955mz	402.995479

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1.14	198.0754n	197.0680811	1.1382	neo	6-amino-5N-methylformylamino1-1-methuracil	HMDB0059771	Organic nitrogen compounds	Organonitrogen compounds	N-arylamides	CHYI0N4O3	0.339765386	1.984813062	0.019455578	0.054281386	0.568100928	1.50336864	65588.85221	43896.97106	64675.57669	58805.83112	74365.1488	51284.85952	40638.52594	39567.52772
0.76	126.0218nV	126.0218441	0.78866667	pos	Taurine	31	Organic acids and derivatives	Organic sulfonic acids and derivatives	Organosulfonic acids and derivatives	C00245	51.1	64.2	M+H	C2H7NO3S	-0.770972781	1.979364655	1.593676	0.000802947	1.510917598	2.849912268	29899.29521	10491.30373	304.1216991	28852.36299	30426.37097	11543.54013	9518.775234	10411.59784
1.29	141.1152n	141.1152	1.26533333	pos	Cordrivolone	HMDB0033364	Oxoacetaldehydes compounds	Oxoacetaldehydes compounds	Unclassified	Unclassified	39.7	2.12	M+H-NH3	C8H15NO	-1.365645777	1.977330735	1.459186	0.000599642	-3.231296089	0.106494822	2304.55892	2164.29883	2269.131954	2406.539482	2216.00821	2070.675721	22041.19775	22744.19775
5.85	455.1902n	455.1902274	5.84575	neo	Flumethasone	HMDB0022336	Unclassified	Unclassified	Unclassified	Unclassified	47.4	44.2	M-FAR	C22H28F2O5	3.764217594	1.975735313	0.01813215	0.051139802	-0.223760292	0.856335555	128787.7733	150394.9293	128943.9115	128750.6302	128668.7782	140906.6279	140999.5688	160278.5913
2.36	357.0831nV	357.0830364	2.378	neo	Vanillic acid 4-O-glucuronide	HMDB0029024	Unclassified	Unclassified	Unclassified	Unclassified	43.4	22.8	M+Na	C14H16O10	-1.415477357	1.973862443	9.42436E-07	0.000172117	-2.662522423	0.155788703	3543.633637	2479.632984	3330.194281	3268.992147	4011.175303	22403.98922	22491.75311	23352.1645
3.41	305.0883nV	305.088299	3.41406667	pos	Dinitramine	29301	Unclassified	Unclassified	Unclassified	Unclassified	39.1	0	M+H-H2O	C11H13N3O4	0.119139434	1.978858869	0.000997756	0.006024855	-1.3829071	0.383443356	12246.68887	31922.84556	11533.87588	12543.68762	12644.4369	36590.31335	31255.73333	28422.49001
7.30	751.3149n	751.3139351	7.29525	neo	9E061	69700	Unclassified	Unclassified	Unclassified	Unclassified	57.2	28.6	[M-H]	C29H52N2O5	0.112303727	1.969692108	0.000130797	0.001181401	-2.731612707	0.150053719	3423.611444	22798.58653	2968.328387	3756.006858	3335.490508	20267.34574	23214.41661	24737.02923
3.06	286.0910nV	286.0909607	3.05735	neo	Tetrashydin B	86564	Unclassified	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	37.2	2	0 M-H	C12H17NO7	-7.88451166	1.969192298	0.000109231	0.001648343	1.193830324	2.22041858	39336.64903	15779.31389	35029.35995	38992.60213	33177.98593	15327.82093	15104.35321	17116.06752
6.03	354.1029nV	354.1019923	6.0186	neo	Ethacrynic acid M1	2585	Unclassified	Unclassified	Unclassified	Unclassified	38.7	2	0 M-H	C13H12Cl2O4	0.849433451	1.95074794	0.000366308	0.002344678	-1.233404192	0.425312891	14366.85333	14366.85333	14366.85333	14898.92907	13931.13769	13497.82618	13497.82618	13497.82618
6.12	385.1507nV	385.150736	6.12345333	neo	4-Deacetylneosolaniol	HMDB0036158	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	C19748	39.2	0.779	M+FAH	C19H24O7	0.979104045	1.965166156	0.00651359	0.023583409	0.344894766	1.270583238	95257.19483	75002.2121	91039.8997	99781.27028	94950.39451	69268.91248	78572.21245	79165.01137
4.86	445.1441n	445.1441044	4.85836364	neo	a-3-Hydroxy-5-phenobenzamide acid O-beta-D-Glucuronoside	LMFA07050135	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	C00049	52.9	74.5	M+FAH	C19H21NO9	-1.345943725	1.959477855	0.004422631	0.023616988	-0.459911784	0.323163688	78260.78553	78753.31332	78753.31332	81126.03574	79149.35683	79731.70904	82773.24597	82773.24597
3.85	156.0365nV	156.0365472	3.84583333	pos	Ureidosorbine	63361	Unclassified	Unclassified	Unclassified	Unclassified	36	0	M-H	C7H7NO3	4.400096103	1.957429768	0.559853417	0.094378382	0.192430478	1.142687156	18078.345	15820818.61	18043.1627	18022.02977	17317.7636	14626.2072	16109.2562	15981.7256
4.76	419.2184nV	419.2184019	4.75	neo	Ala-Ala-Ala-Ala	29	Unclassified	Unclassified	Unclassified	Unclassified	38.7	2	0 M-H	C12H24N4O6	0.924226497	1.959547866	0.00396258	0.015028435	-1.232404192	0.42531991	14366.85333	14643.59423	14366.85333	14898.92907	13931.13769	13497.82618	13497.82618	13497.82618
4.64	263.0870nV	263.087006	4.41115	neo	Oseltamivir	83386	Unclassified	Unclassified	Unclassified	Unclassified	37.4	2	0 M-H	C14H24O4	6.700618884	1.950428835	0.002682821	0.002887791	-1.147602442	0.45137473	15625.83326	34618.25007	16280.84971	14037.87342	19058.68672	37450.18674	36407.16876	35385.5887
3.63	496.1662nV	496.1662	3.62833333	neo	Uridine 5'-diphosphate-N-acetylglucosamine	LMFA01050296	Nucleosides, nucleotides, and analogues	Pyrimidine nucleosides	Unclassified	C00290	51.6	61.9	M+FAH	C17H25N3O17P2	0.978422295	1.949453633	0.000579414	0.002387144	-1.237242305	0.422611284	92261.1	72274.33	94183.26226	94183.26226	94183.26226	94183.26226	94183.26226	94183.26226
3.63	496.1662nV	496.166239	3.43111667	pos	Uridine 5'-diphosphate-N-acetylglucosamine	LMFA01050296	Nucleosides, nucleotides, and analogues	Pyrimidine nucleosides	Unclassified	Unclassified	46.6	46.3	M+H	C17H25N3O17P2	-1.005665109	1.942921002	0.002944191	0.010144841	-1.224632253	0.430875955	14899.125	14899.125	14899.125	15446.55899	15446.55899	36922.4498	37264.05677	31623.51993
5.01	460.1501nV	460.1501	5.01417667	neo	Kaempferol 3-rutinoside-7-glucoside	LMPK11111843	Organic oxygen compounds	Organooxygen compounds	Flavonoids	Unclassified	52.1	64.2	M+H	C33H40O20	0.941563183	1.941558135	1.41E-06	0.000172117	-2.662522423	0.155788703	3543.633637	2479.632984	3330.194281	3268.992147	4011.175303	22403.98922	22491.75311	23352.1645
5.01	462.0752n	462.0752	5.01543333	pos	Ethyl beta-D-glucuronoside	HMDB0029968	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	Unclassified	39.1	0	M+H	C8H16O6	-1.126286011	1.937429606	1.22358E-05	0.000186797	-1.588753154	0.332282829	92141.89237	27736.40724	9314.102486	9221.270859	9109.084367	26960.67881	28178.23536	28370.99776
5.01	462.0752n	462.0752	5.01543333	pos	5,6,7,8-Tetrahydroxyflavone 7-glucuronide	LMFA12110277	Unclassified	Unclassified	Unclassified	Unclassified	39.1	0	M+H	C21H18O12	-1.273705867	1.931155922	2.19831E-05	0.000373101	-2.405680754	0.311398889	22894.08857	4308.510484	24042.54864	24042.54864	24042.54864	24042.54864	24042.54864	24042.54864
9.25	397.1876nV	397.1886961	9.24521667	neo	Idebenone Metabolite (QS-10)	758	Unclassified	Unclassified	Unclassified	Unclassified	49.1	0	M-FAH	C19H28O6	0.580915444	1.931288509	2.09091E-06	0.000245701	0.640596781	1.569973606	51391.94042	32965.23452	51622.82014	50866.34138	51666.65975	52326.24751	32387.95873	33581.49731
5.26	268.1419n	268.1419	5.01343667	pos	Dihydrotestosterone	1126	Unclassified	Unclassified	Unclassified	Unclassified	41.2	0	M-H	C19H28O2	-1.528421345	1.930452236	0.000735444	0.003772644	-0.944466289	0.359728136	48035.98	20254.76437	48035.98	48035.98	48035.98	48035.98	48035.98	48035.98
13.15	799.5445nV	799.5445056	13.1512167	pos	PG(18:0/18:1(12Z))	HMDB0116603	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols	C04014	38.6	0	M-FAH	C42H81O15P	-1.867874572	1.92982719	0.004634181	0.018941162	-0.758449053	0.552881607	28305.07875	47741.53625	31854.47775	28375.49067	24865.28808	52749.37539	47525.74745	42949.48589
4.95	446.0782nV	446.0781732	4.9417	neo	Geniesein 5-O-glucuronide	HMDB0041736	Phenylpropanoids and polyketides	Isoflavonoids	Isoflavonoid O-glucuronides	Unclassified	55.6	64.1	M+H	C21H18O11	1.226464317	1.928566208	1.58282E-05	0.000810936	0.564572258	1.982939172	19551.13231	19551.13231	19551.13231	19551.13231	19551.13231	19551.13231	19551.13231	19551.13231
6.50	435.1983nV	435.1983439	6.4952	pos	5-(2,3-Dihydro-3-methylbutyl)-4-(3,4-epoxy-4-methylbutanamido)-8(1H)-one	HMDB0033082	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	Unclassified	41	11.2	M-H2O	C23H32O8	-1.442965841	1.919324446	0.000638152	0.004568801	-1.14512432	0.452157294	15334.88637	33915.38655	14616.21103	15143.02047	16045.36739	32638.64843	37396.92331	33417.58541
4.66	358.1371nV	358.137118	4.99231667	neo	L-L-Cystolaurokorsinol	HMDB0034276	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	Unclassified	45.1	5.92	M-FAH	C15H21NO7S	0.871478487	1.918857553	0.000228313	0.001810074	-1.658477851	0.426543403	47660.7272	26033.75214	47660.7272	47660.7272	47660.7272	47660.7272	47660.7272	47660.7272
4.88	383.1347nV	383.1347473	4.88008333	neo	15-Acetyl-4-deoxoninalol	HMDB0033444	Nucleosides, nucleotides, and analogues	Purine nucleosides	Unclassified	Unclassified	41.6	11.7	M-FAH	C17H22O7	-0.625493613	1.916339488	4.28202E-07	0.000139893	0.705910341	1.630198346	46932.57463	28728.88522	48618.88688	47172.52547	46706.29655	28250.31238	28917.72014	29016.61523
5.76	93.1169nV	93.1169	5.77859667	pos	Unedifidin	13	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	C05791	45.4	33.4	M+H	C5H12O3	-1.342943626	1.915453833	0.034823578	0.083151508	-0.328783809	0.902074431	82774.23581	93885.31355	83705.81142	83705.81142	83705.81142	79773.74499	83705.81142	83705.81142
8.61	499.2709nV	499.2709905	8.60666667	neo	9-Hydroxy-10-O-D-glucuronoside-12Z-octadecenoide	HMDB0060121	Lipids and lipid-like molecules	Saccharolipids	Unclassified	Unclassified	48.9	47.8	M-H	C24H42O10	0.75344944	1.912987456	0.009845078	0.032199855	0.173886953	1.128695303	174884.5794	155026.422	180843.9289	167270.8278	176539.8785	154281.9657	158003.2077	152794.0425
3.90	352.0425n	352.0425	3.91035913	neo	4-(2-(5-Carboxy-2-hydroxy-3-methylphenoxy)-2-oxoethyl)benzoic-2-oxide	HMDB0032626	Unclassified	Unclassified	Unclassified	Unclassified	37.6	4.1	M+H2O-H	C17H14O7	-1.413089757	1.910291165	0.000619547	0.002615405	-1.162911825	0.454243807	35344.38641	16888.97832	35344.38641	35344.38641	35344.38641	35344.38641	35344.38641	35344.38641
4.14	622.1164n	622.1163619	4.13611667	pos	Apigenin 7-glucuronosyl-(1->2)-glucuronide	LMFK12110359	Lipids and lipid-like molecules	Polyketides	Flavonoids	Unclassified	52.3	68.5	M+H	C27H26O17	-1.035000898	1.904320059	2.01471E-05	0.000589725	2.613236242	0.116749597	21494.79565	35124.90758	22924.10042	20620.99036	20939.29618	3958.183134	3801.980459	3778.852702
4.67	387.1664n	387.1664	4.5107	neo	Jasmidine glucoside	HMDB0032870	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	Unclassified	43.1	23.9	M+H	C16H26O8	0.968614158	1.903862487	0.000892215	0.003892215	0.028084341	0.975661747	90241.67252	84096.30762	90241.67252	90241.67252	90241.67252	90241.67252	90241.67252	90241.67252
6.94	607.3079nV	607.3079333	6.9443	pos	04E1-3alpha,15alpha-Diacetoxy-23-oxo-7,9(11),24-tanostatien-21-oic	90684	Lipids and lipid-like molecules	Prenol lipids	Triterpenoids	Unclassified	36.9	0	M-H	C34H48O7	8.36535175	1.901218351	1.34772E-05	0.000577767	-1.355183793	0.391793726	11498.22551	29347.65381	12500.91721	11269.28262	10724.47671	28524.87128	28943.98998	30081.09208
3.81	176.0321n	176.0321063	0.88463333	neo	Glucosinic-2-3-lactone	HMDB0035355	Organic nitrogen compounds	Organonitrogen compounds	Furofurans	Isoxanthides	43.1	17.6	M+H-NH3	C7H9NO3	-0.029035349	1.901804048	0.000602213	0.002607213	-0.529819113	0.388072123	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365
3.43	121.0284nV	121.0284198	3.43111667	pos	Sesamol	HMDB0033812	Organic oxygen compounds	Benzodioxoles	Unclassified	C10832	40.8	5.83	M+H-H2O	C7H6O3	0.101594477	1.860990393	0.002170426	0.010021405	-1.140381048	0.453639764	14737.07591	32468.28164	14140.87887	14617.46303	15455.56582	31484.74524	30136.97859	28943.12168
4.64	622.2151n	622.2151	4.64225	neo	Tenesthilic acid	HMDB0033832	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	C06337	43.9	23	M+H-H2O	C28H34O12	-0.018676657	1.859146185	0.000136447	0.000615468	-0.164433249	0.558600284	25861.4513	19597.15467	25861.4513	25861.4513	25861.4513	25861.4513	25861.4513	25861.4513
15.07	296.2579nV	296.2579947	15.0659667	pos	10,12,14-octadecatrienoic acid	LMFA01030154	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates	Unclassified	45.5	32.5	M+NH4	C18H30O2	-1.800948032	1.858600354	0.001963587	0.005760447	0.13777792	1.100219212	208128.1811	189171.2863	201027.1778	213247.2304	208110.135	189217.0018	194187.4336	194187.4336
2.36	281.0913nV	281.0912818	2.35478667	neo	2'-Deamino-2'-oxoniline	2	Unclassified	Unclassified	Unclassified	Unclassified	37.1	5.92	M-H	C11H16N2O7	-7.63935336	1.857988552	0.000203383	0.001188002	-1.604495991	0.502319611	26993.73106	26993.73106	26993.73106	26993.73106	26993.73106	26993.73106	26993.73106	26993.73106
6.46	200.1294nV	200.1293813	6.47743333	neo	2,2,6,6-tetramethyl-4-oxiperidinone	HMDB0031179	Organic oxygen compounds	Organooxygen compounds	Phenylpropanes	Unclassified	54.8	75.7	M-FAH	C9H17NO	1.059318336	1.855686174	0.001337402	0.005138285	0.719597993	1.646723112	44627.07454	27221.98664	47455.33024	43594.81709	43430.87628	29231.66947	29364.75714	30729.5533
4.67	217.0912nV	217.0912346	4.66761667	neo	4,4'-Bisfenidifine	70164	Unclassified	Unclassified	Unclassified	Unclassified	35.2	16.2	M-H	C12H14O2	4.627552427	1.851781975	0.000887358	0.003551545	0.509453322	1.379534889	20496.17274	20496.17274	20496.17274	20496.17274	20496.17274	20496.17274	20496.17274	20496.17274
2.07	327.0949nV	327.094755	2.07036667	neo	meta-O-Desilalted flecainide lactam	HMDB0060832	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	Unclassified	49.4	13	M+H2O-H	C19H17F3N2O4	-1.417609947	1.851709214	0.000231734	0.002248528	0.736929568	1.666525464	42646.07879	25988.27986	46962.63849	43553.38157	43722.21631	23857.1372	27031.87963	25875.62275
3.50	617.1487nV	617.1486945	3.50	neo	Tunisil glucuronide	HMDB0029766	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	Unclassified	49.5	51.6	M+H2O-H	C24H30O18	0.879156447	1.849917728	0.000136447	0.000615468	-0.224648427	0.212758224	25861.4513	19597.15467	25861.4513	25861.4513	25861.4513	25861.4513	25861.4513	25861.4513
5.30	617.1487nV	617.1486945	5.30268333	neo	Rhamnazin 3-(6''-(3-hydroxy-3-methylglutaryl)glucoside)	LMPK12112636	Lipids and lipid-like molecules	Polyketides	Flavonoids	Unclassified	56.7	49.4	M+H2O-H	C29H32O16	-1.597589101	1.838926991	1.07173E-06	0.000118638	-3.277975666	0.02322167	53.31365995	16734.69407	0.001403199	161.1387735	0.001493199	17144.27341	16092.18757	16997.62516
3.79	434.1611nV	434.1611	3.79328333	neo	Mulberrisin F	HMDB0036275	Phenylpropanoids and polyketides	Flavonoids	Flavonoid O-glycosides	Unclassified	38.3	3.97	M+H	C20H26O7	0.870159669	1.838579786	0.000653184	0.002551148	0.354200577	1.376529264	46403.05511	46403.05511	46403.05511	46403.05511	46403.05511	46403.05511	46403.05511	46403.05511
2.46	290.1594nV	290.1594097	2.44421667	pos	3-Methoxitatyvarotine	HMDB0033552	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	Unclassified	44.7	28	M+H	C13H23NO6	-1.197986946	1.835171674	9.52147E-05	0.00152722	1.013330773	2.01836822	33193.77331	16444.23466	33263.43662	32033.37769	34264.60543	16027.39368	17851.85578	16553.47822
4.66	281.1080nV	281.1080	4.65643333	pos	5-Hydroxy-7-methoxyflavanone-5-neosperidoside	HMDB0030239	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	Unclassified	54.1	14	M-FAH	C21H28O12	-1.542624757	1.829549779	0.000302231	0.001291845	-1.596257004	0.460286246	14899.125	14899.125	14899.125	15446.55899	15446.55899	36922.4498	37264.05677	31623.51993
7.92	601.2249nV	601.224761	7.91555	neo	5,4'-Dihydroxy-6,C-(neosperidosyl)-8-(rutinosyl-1->2)-chamnocide	52591	Unclassified	Unclassified	Unclassified	Unclassified	37	0	M-H	C27H34O15	-0.549089397	1.828185041	5.173E-05	0.001093465	0.378573394	1.300555653	71891.97778	55291.46203	71414.80536	71315.52777	72915.80023	54296.18108	54833.64112	56739.58389
3.71	166.1086n	166.1086	3.70	neo	Na-Acetyl-L-lysine	HMDB0029283	Organic nitrogen compounds	Organonitrogen compounds	Amino acids, peptides, and analogues	C02727	53.6	72.9	M+H	C8H16N2O3	-1.192615303	1.826289697	0.000207105	0.000910705	-0.044241565	0.182421552	13478.67897	15578.8311	13728515	15997.0071	15199597.18	15635.5146	13063.12184	13720.05615
6.44	343.1404nV	343.140462	6.44271667	neo	Indotinal glucoside	LMPR0102070024	Lipids and lipid-like molecules	Prenol lipids	Isoprenoids	C11653	41.2	19.4	M-H	C16H24O8	0.559498285	1.822539325	0.014901009	0.000615468	-0.164433249	0.558600284	25861.4513	19597.15467	25861.4513	25861.4513	25861.4513	25861.4513	25861.4513	25861.4513
2.21	226.0959n	226.0959	2.21502583	neo	Chromonar	76	Organic nitrogen compounds	Organooxygen compounds	Benzodioxoles	Unclassified	47	0.779	M+H	C11H13NO4	-1.658781826	1.822493665	0.000602213	0.002607213	-0.529819113	0.388072123	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365
5.64	547.1462nV	547.1462793	6.53981667	neo	5,7,4'-Trihydroxyflavanone 4'-O-rutinoside	LMPK12140252	Unclassified	Unclassified	Unclassified	Unclassified	44.2	23.9	M-H2O-H	C27H32O14	0.999747334	1.82537444	0.001105871	0.004619035	0.702034221	1.626795894	43526.02211	26756.8864	39758.22355	45901.48868	44624.33491	25804.56056	27603.51866	26862.58799
2.64	274.0948nV	274.0948	0.89039667	neo	Cloboxi	Daidzea	Unclassified	Unclassified	Unclassified	C08909	36.4	0	[M+H-H2O]+	C18H14N2O2	0.283578004	1.820495249	0.000679102	0.002839241	-0.364417766	0.664972486	89440.24486	84348.77161	89440.24486	89440.24486	89440.24486	89440.24486	89440.24486	89440.24486
0.84	361.0809nV	361.0809543	0.84173333	neo	Phosphinothrin	63589	Unclassified	Unclassified	Unclassified	Unclassified	37.5	0	2M-H	C14H21O4P	-7.341280325	1.820388602	0.002552432	0.010188584	-0.838886031	0.535607326	21646.39169	38718.29944	21683.47966	21622.21659	21633.47652	37482.71485	35068.58612	35068.58612
0.76	391.1352nV	391.1352755	0.75866667	neo	2,2-Dimethyl-3-(4-methoxphenyl)-4-ethyl-2H-1-benzopyran-7-ol	63588	Unclassified	Unclassified	Unclassified	Unclassified	37.6	0	2M-H	C22H24O5	7.5466E-07	1.819788662	0.002552432	0.010188584	-0.838886031	0.535607326	21646.39169	38718.29944	21683.47966	21622.21659	21633.47652	37482.71485	35068.58612	35068.58612
4.91	399.1961nV	399.1961243	4.61186333	neo	Fluorenobutine 17-acetate	70218	Unclassified	Unclassified	Unclassified	Unclassified	37.4	0	2M-H	C23H32O5	1.783403731	1.816852227	0.000243564	0.001044869	-0.454665512	0.373424776	46962.73629	53624.31361	49885.15231	49447.57387	50275.37564	53624.31361	49885.15231	49447.57387
4.66	455.2083nV	455.2083	4.65666667	neo	Ala-Ala-Ala-Ala	29	Unclassified	Unclassified	Unclassified	Unclassified	38.7	2	0 M-H	C12H24N4O6	0.924226497	1.815450245	0.000396258	0.001704447	-1.232404192	0.42531991	14366.85333	14643.59423	14366.85333	14898.92907	13931.13769	13497.82618	13497.82618	13497.82618
4.68	495.2084nV	495.2083975	4.68	neo	L-Isoleucine	6	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	C00407	46.5	39.2	M+H	C6H13NO2	-1.139597178	1.810041401	0.000334238	0.001504307	-0.503057135	-1.64179687	57539.68191	33915.38655	14616.21103	15143.02047	16045.36739	32638.64843	37396.92331	33417.58541
4.28	284.1504nV	284.1504433	4.27815333	neo	Petasinine	53413	Organic oxygen compounds	Organooxygen compounds	Pyrrolidines	Unclassified	51.3	59.1	M-FAH	C13H21NO3	1.405531954	1.791823537	4.30569E-05	0.000196245	0.539468634	1.398419788	16486.00152	32389.97861	17210.08721	16127.81265	16120.30472	31006.75598	33553.61066	33609.56881
3.96	417.2135nV	417.2133881	7.58625	pos	5-Hydroxy-7-methoxyflavanone-5-neosperidoside	HMDB0030239	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	Unclassified	52.9	68.5	M-H	C22H26O11	0.520975545	1.789229063	0.000602213	0.002607213	-0.529819113	0.388072123	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365	28377.13365
13.81	799.5445nV	799.5445761	13.81325	pos	PG(18:0/18:1(9Z))	LMGP04010037	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols	Unclassified	39.1	0	M-H	C42H81O15P	-1.905698387	1.785947633	0.002851469	0.012001941	-0.899119995	0.570729882	21952.16824	39443.21516	24793.16235	21638.0243	19425.13207	40105.22444	40737.46229	34466.93875
3.78	159.1003nV	159.1003	1.93678667	pos	4-(5-Isobutenoic)-3-(3-methylbutanamido)-1H-indol-3-ol/methyl-3-one	3060	Unclassified	Unclassified	Unclassified	Unclassified	36.1	0	M-H	C7H12O2S2E5	1.927717561	1.778626357	3.54522E-07	0.000107105	0.443964611	1.202770135	5445.944837	5445.944837	5445.944837	5445.944837	5445.944837	5445.944837	5445.944837	5445.944837
2.07	245.1143nV	245.1143366	2.07036667	neo	Glutamylaline	LMPR0102883832	Unclassified	Unclassified	Unclassified	Unclassified	49.7	51.4	M-H	C11H18N2O5	0.163842702	1.773652297	0.000239117	0.000725127	0.997953013	1.971823353	31759.65463	16166.74444	29668.87776	33085.56899	32526.51984	14765.84409	16589.19567	16965.14357
5.76	557.1564nV	557.1564	5.75	neo	5,7-Dihydroxy-8-C-methylflavanone 7-xylosyl-(1->3)-xyloside	52533	Unclassified	Unclassified	Unclassified	Unclassified	52.9	67.4	M-H	C27H34O15	-1.059549119	1.770967948	3.90323E-05	0.000615468	-0.164433249	0.558600284	25861.4513	19597.15467	25861.4513	25861.4513	25861.4513	25861.4513	25861.4513	25861.4513
5.53	611.0583nV	611.0582925	5.52541667	neo	UDP-alpha-D-galactos-1,4-furanone	60033	Unclassified	Unclassified	Unclassified	Unclassified	37.4	0	M-H	C15H24N2O17P2	0.954987709	1.767272822	0.000703328	0.004538977	-1.340742073	0.394917521	10295.45295	26076.50565	9491.220046	11958.89587	9436.268331	28867.62264	25368.19944	23993.73686
5.30	579.1499nV	579.1499	5.61673333	neo	(E)-2-O-Coumaroyl-beta-D-glucopyranose	HMDB0038380	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	Unclassified	41.9	1.951	M-H	C15H18O8	1.185115824	1.765497799	0.002279032	0.009719782	-0.440852279	0.312453746	12245.72446	41977.2752	11977.2752	12245.72446	27779.45335	42622.49599	42639.34422	30164.43626
5.31	219.1013nV	219.1013288	5.30655	neo	iR1-Bisfalin A	HMDB0040358	Benzenoids	Benzene and substituted derivatives	Acetophenones	Unclassified	52.2	66.2	M+H	C13H14O3	-1.109403636	1.764022355	6.80658E-07	0.000156048	-4.979385162	0.01169974	502.9858082	15867.19234	430.7948377	490.1362766	588.0263309	15396.69802	15845.7511	16359.72129
4.66	453.1360nV	453.1360575	4.66	neo	Melanedin A	31	Unclassified	Unclassified	Unclassified	Unclassified	37.7	0	M-H	C21H26O9	-1.163326426	1.763477307	0.000215107	0.000972647	-0.225402987	0.204708469	40015.12267	40015.12267	40015.12267	40015.12267	40015.12267	40015.12267	40015.12267	40015.12267
6.84	179.056nV	179.0561477	0.84173333	neo	muco-Inositol	144	Organic oxygen compounds	Organooxygen compounds	Alcohols and polyols	C00137	51.5	59.4	M-H	C6H12O6	0.200241019	1.757084451	0.042205345	0.006745903	-0.259566278	0.835093541	92937.22749	11289.60308	92333.90997	95160.43442	91337.3411	102835.4116	103766.6902	123196.7006
4.84	265.144n	265.144	4.88233333	neo	Mefenidin	68637	Unclassified	Unclassified	Unclassified	Unclassified	36.2	0	M-H2O-H	C15H21NO3	-1.396703224	1.744417635	0.000215107	0.000972647	-0.225402987	0.204708469	40015.12267	40015.12267	40015.12267	40015.12267	40015.12267	40015.12267	40015.12267	40015.12267
2.42	99.0687n	122.0576595	2.42161667	pos	5-Valerolactam	62467	Organic oxygen compounds	Organooxygen compounds	Fluorenes	Fluorenones	49.5	51.5	M+H	C5H9NO	2.742393729	1.75642142	2.94715E-05	0.000615468	-2.145636039	0

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0.74	192.0744n	175.0710964	0.73955	oos	Servilseirine	HMDB0029048	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		42.7	18.2	M+H-H2O; M+Na; M+K	C6H12N2O5	-1.23306573	1.00173663	7.82137E-05	0.001363375	0.280685875	1.214772265	28267.98063	23270.18936	28495.68523	27670.42166	28637.85501	23271.85736	23300.59563	23236.11511
6.60	406.2879n	407.2880071	6.6024	neo	omega-muricholic acid	LMST04010065	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	*	C17727	37.9	0	M-H; M+FA-H	C24H40O5	0.75707878	1.00170924	1.23078E-05	0.000564954	-8.15719851	0.003502992	17.44623005	4980.379363	52.33083376	0.001403199	0.001403199	4668.485997	5316.488039	4956.184052
3.80	326.0883n	326.0883515	3.80375	oos	DHBDA-Gc	HMDB0037261	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		41.2	13.9	M+H+H2O	C14H17NO9	-1.72372887	1.00089211	1.9718E-05	0.000688348	-3.038551278	0.12170402	686.6159449	5641.886972	877.8636025	576.5794261	605.604936	5361.685484	6058.454257	5554.920276
8.50	334.2347n	334.2346976	8.497183333	oos	N-3-oxo-hexadeco-11(Z)-enoyl-L-Homoserine lactone	45315	Unclassified	Unclassified	Unclassified	*		36.9	0	M+H+H2O	C20H33NO4	-8.54681669S9	1.000761431	0.000490134	0.03129059	0.122196812	1.088390969	65598.19402	60270.80294	64675.36099	67259.78406	64859.43791	61817.10501	59330.55629	59655.74751
7.34	316.2477n	316.2477924	7.3446	oos	Decanoylcarnitine	HMDB0000651	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	***		51.4	62.2	M+H	C17H33NO4	-1.403817465	1.000079421	0.00153587	0.008280821	0.398557778	1.318189485	21942.94655	15863.52383	20393.59453	21274.9744	21469.27972	16872.34808	15927.84453	14990.57834

ID	m/z	Retention time (min)	Ion mode	Metabolites	Compound ID	Super Class	Class	Sub Class	level	kegg	Score	Fragmentation Score	Adducts	Formula	Mass Error (ppm)	VIP	P-value	adj.P-value	log2(FC)	FC	average(HN)	average(LN)	HN1	HN2	HN3	LN1	LN2	LN3
3.28	204.9813/z	204.9812701	3.280233333	neg	Pyroqallol-1-O-sulphate	HMDB0060016	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		50.6	58.3	M-H	C6H6O6S	0.182427092	24.61876445	6.45184E-06	0.000478455	-2.194480184	0.218471927	580691.8133	2657969.932	603150.4824	569451.8993	569473.0582	2540766.164	2769388.06	2663755.572
6.69	421.0603/z	421.0602718	6.69475	neg	1-Methyl 2-qalloylqalactarate	91922	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			37.7	0	M+FA-H	C14H16O12	-5.602940506	18.65960015	1.32678E-06	0.000225325	2.54340388	5.829628222	1439083.473	246856.818	1467918.863	1453157.8	1396173.755	219772.7802	265174.6615	255623.0122
4.41	264.1104/z	287.0996471	4.4062	pos	N(2)-phenylacetyl-L-glutaminate	HMDB0062645	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		C05597	42.6	18.3	M+Na, M+K, M+H, M+H-H2O	C13H16N2O4	-2.19816811	11.96211711	0.001076013	0.008952771	-0.760411335	0.590327995	1456859.03	2467880.64	1529191.219	1396438.622	1444947.25	2274387.989	2666535.992	2462717.939
0.76	113.0590/z	114.0662372	0.758666667	pos	Creatinine	HMDB0000562	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***	C00791	44.3	26.5	M+H, M+K	C4H7N3O	0.432927687	15.66211226	0.001321541	0.010199031	0.427145839	1.344570907	3373387.117	2506894.92	3403823.116	3444484.798	3271853.438	2269314.34	2341776.412	2515594.008
4.28	213.0097/z	212.0024497	4.278183333	neg	Indoxylsulfuric acid	253	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		56.2	84.8	M-H, 2M-H	C8H7NO4S	0.692021131	14.79969611	7.86598E-06	0.000513651	-3.780242427	0.072783618	58936.77862	809753.3544	63673.55765	57224.44981	55912.32839	768364.9263	855781.0175	805114.1193
4.39	264.1110/z	263.1037232	4.3893	neg	Phenylacetylglutamine	HMDB0006344	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	***	C04148	57.9	90.9	M-H, 2M-H, M-H2O-H	C13H16N2O4	-0.028048749	14.03022514	0.000860291	0.007838762	-0.847933923	0.55557981	861950.8335	1551443.767	885556.1803	854312.3244	845983.9958	1427805.186	1689978.386	1536547.731
4.19	218.9970/z	218.9969615	4.189783333	neg	4-Hydroxybenzenesulfonic acid	34512	Unclassified	Unclassified	Unclassified			39	0	M+FA-H	C6H6O4S	0.45390928	10.95217608	1.26056E-05	0.000634788	-2.166278886	0.222784554	117964.3438	529499.6532	114771.9275	107625.7739	131495.33	556284.4509	523309.2714	508905.2372
0.82	194.9275/z	194.9275444	0.819566667	neg	Sulfate	HMDB0001448	Organic acids and derivatives	Organic sulfuric acids and derivatives	Non-metal oxoanionic compounds	**	C00059	42.6	17.4	2M-H	H2O4S	0.315125643	10.42162011	3.36716E-05	0.001123737	0.858401477	1.813028341	832507.792	459180.7934	845031.3365	846527.6026	805964.4365	434781.2753	466594.2038	476166.9011
0.93	146.0216/z	191.0198685	0.925866667	neg	Oxoglutaric acid	119	Organic acids and derivatives	Keto acids and derivatives	Gamma-keto acids and derivatives	**	C00026	52	61	M-H, M+FA-H	C5H6O5	0.418166227	9.507167872	0.002219591	0.01448951	0.641999334	1.56049024	895966.3309	574156.9592	910328.1777	929902.2747	847668.5402	496383.3445	612087.1789	614000.3543
0.84	144.1017/z	144.1017035	0.8386	pos	4-heptynoic acid	LMFA01030489	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			45.2	35.3	M+NH4	C7H10O2	-1.598993884	9.337715069	3.82468E-05	0.001209447	1.313029955	2.484628151	501670.6445	201909.7482	526218.2512	493773.0015	485020.8807	186660.1692	215927.7092	203141.3662
5.76	245.0333/z	243.0332993	5.778333333	neg	4-phenylbutanoic acid-O-sulphate	HMDB0060983	Lipids and lipid-like molecules	Benzenoids	Benzene and substituted derivatives			45.4	30	M-H	C10H12O5S	0.128104008	8.773631156	0.000109898	0.000876291	-0.952785434	0.516641187	288946.7581	559278.4011	289601.6617	301779.7214	282457.3883	600388.9867	578872.5143	498573.7024
5.40	285.1936/z	286.20089	5.396716667	neg	2-Octenoylcarnitine	HMDB0013324	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters	*		50.2	55.5	M+H, M+Na	C15H27NO4	-1.384146005	8.705630505	0.000225086	0.003465345	0.866565208	1.823316747	581054.4571	318679.9321	612226.1862	554684.9915	576252.1935	294908.605	335297.6987	325833.4928
0.76	151.1439/z	151.1438551	0.758666667	pos	Bis (2-hydroxypropyl) amine	44741	Unclassified	Unclassified	Unclassified			38.3	0	M+NH4	C6H15NO2	-1.871901467	8.576391901	0.000129204	0.00246876	-6.865534735	0.008575671	2196.082608	256082.8909	1791.730557	2469.8242	2326.693066	223255.4724	282649.3274	262343.8728
12.98	835.6642m/z	835.6642352	12.98333333	pos	SM(d18:1/24:1(15Z))	HMDB0012107	Lipids and lipid-like molecules	Sphingolipids	Phosphosphingolipids	**	C00550	37.4	0	M+Na	C47H93N2O6P	-2.597420216	8.548297097	0.020157601	0.068752284	-1.426186287	0.372113262	188016.5649	451519.9594	233466.4521	160967.4586	109615.7839	573652.3029	437339.9238	343567.6516
5.56	541.2657/z	541.2657411	5.57185	pos	Chaetoglobosin N	88035	Alkaloids and derivatives	Alkaloids and derivatives	Chaetoglobosins			36.6	0	M-H	C32H38N2O5	-9.32135293	8.474728017	0.005385668	0.025832592	0.626722159	1.544052876	743870.881	481765.1599	877862.1575	802851.388	750869.0974	504422.3146	520719.9105	420153.2547
0.78	193.1544/z	193.1544095	0.776966667	pos	altretamine	3923	Organic nitrogen compounds	Organonitrogen compounds	Amines			36.1	0	M+H+2O	C9H18N6	-7.598292004	7.902104087	6.49512E-07	0.000159297	-3.130191727	0.114213752	27559.24767	241295.3539	29368.6879	24956.28248	28352.77264	234925.7192	247541.587	241418.7557
3.26	231.1468/z	232.1540327	3.258783333	pos	Butyryl-L-carnitine	964	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*	C02862	52.4	65.1	M+H, M+Na	C11H21NO4	-1.306224871	7.847773369	3.70389E-05	0.001185471	0.722423278	1.649951112	537762.6229	325926.3981	533577.1436	557185.3378	522525.3875	324986.0522	331207.5649	321585.5773
0.86	254.9816/z	254.9816395	0.86335	neg	Ascorbic acid 3-sulfate	HMDB0240641	Organoheterocyclic compounds	Organooxygen compounds	Dihydrofurans			48.9	48.6	M-H	C6H8O9S	0.050992854	7.649782074	0.002246757	0.014576625	0.724814824	1.652688493	527428.8629	319133.8629	553953.4736	504464.9608	523868.1543	269466.4022	358784.6132	329150.5734
5.79	310.2086/z	310.2085327	5.790983333	neg	Acetylbisdemethoxycurcumin	HMDB0036893	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*		51.8	64.1	M+NH4	C17H24O4	-1.547207794	7.543454148	0.000695011	0.005855753	0.522249843	1.436193206	654683.7816	455845.5942	692512.6653	641125.8901	630412.7893	439050.2307	461524.8964	466964.6556
5.36	345.1556/z	345.1556421	5.361783333	neg	(1R,3S,4S,6R)-6,9-Dihydroxyfenchone 6-O-b-D-glucoside	HMDB0033222	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		45.9	33.2	M+H	C16H26O8	0.435583056	7.397910429	6.61977E-05	0.00168222	-1.287157895	0.409757456	130868.5867	319380.6114	121351.0357	138791.8237	132462.9006	315444.2101	304962.7212	337734.9027
5.85	433.2081/z	433.2080936	5.84575	neg	9,13-Dihydroxy-4-megastigmen-3-one 9-glucoside	HMDB0036318	Lipids and lipid-like molecules	Prenol lipids	Fatty Acyls	*		50.4	53.6	M+FA-H	C19H32O8	0.445073667	7.391270278	0.000104398	0.002191722	-0.557238639	0.679601698	399908.9798	588446.1167	396903.7542	400951.8953	401871.2899	607512.0878	565818.575	592007.6873
9.02	408.2876/z	407.2805251	9.01635	neg	Allocholic acid	5491	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroids and steroid derivatives	*	C17737	48.3	44.9	M-H, M+FA-H	C24H40O5	0.556417509	7.229140276	1.76708E-05	0.000778104	-2.161085394	0.223587991	51651.16426	231010.4585	50806.15871	52946.68209	51200.65397	216290.437	240034.4068	236706.5318
1.16	229.1544/z	229.1543616	1.157483333	pos	Methoxamine	HMDB0014861	Benzenoids	Benzene and substituted derivatives	Methoxybenzenes		C07513	39.6	1.88	M+NH4	C11H17NO3	-1.454615557	7.146529981	0.03233394	0.097373678	0.193253631	1.143339321	1640818.973	1435111.12	1716092.23	1574755.917	1631608.772	1361516.16	1527930.795	1415886.404
2.26	381.0137m/z	381.0136579	2.26065	neg	2,3-Dioxo-6-nitro-7-sulfamoylbenzo[f]quinoxaline	69621	Unclassified	Unclassified	Unclassified			38.1	0	M+FA-H	C12H8N4O6S	-2.976034588	7.052031143	6.00471E-06	0.000468047	-2.795567864	0.14402909	28675.57093	199095.6886	29938.74647	28297.0227	27790.94363	191896.9538	209574.5704	195815.5416
5.53	339.1087m/z	339.1086909	5.525416667	neg	trans-isoeugenol-O-glucuronide	HMDB0060021	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		49.7	52.4	M-H	C16H20O8	0.440173133	6.969633855	0.00150014	0.011133685	-1.203620779	0.434184227	131721.0284	303375.8951	116019.7858	151205.7504	127937.5492	279872.9775	287912.8451	342341.8626
4.15	178.0510/z	178.0510155	4.1413	neg	Hippuric acid	1301	Organic acids and derivatives	Benzenoids	Benzene and substituted derivatives	*	C01586	54.4	82.2	M+H, 2M-H	C9H9NO3	0.272599778	6.960260626	4.30861E-06	0.000261339	-0.868676952	0.510974446	1239747.214	338328.5456	1272872.414	1338324.562	1206163.304	173008.5625	314544.8832	361861.1787
4.00	172.9914/z	172.9914257	4.002233333	neg	Phenol sulphate	HMDB0060015	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	***	C02180	56	90.8	M-H	C6H6O4S	0.128824485	6.817143456	3.26466E-05	0.001098216	-1.694820723	0.308893042	71376.09365	231070.5779	73576.74837	69812.46795	70739.06463	216549.9843	242558.9318	234102.8175
6.90	313.2247/z	314.2320238	6.8951	pos	9-Decenoylcarnitine	LMFA07070048	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		53.5	73.3	M+H, M+Na	C17H31NO4	-1.791262172	6.802480576	0.004363745	0.022905192	0.531394195	1.445325258	543051.0523	375729.3033	575192.8047	545015.1901	508945.1621	335236.1433	383437.3353	408514.4314
0.78	118.0863/z	118.0862667	0.776966667	pos	L-Valine	35	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00183	53.2	71.8	M+H	C5H11NO2	0.099931793	6.598313424	0.001115509	0.009156829	0.316538254	1.245338771	776390.0375	623436.8155	803052.3064	746456.9305	779660.8755	639476.2928	614616.5102	616217.6434
4.41	528.2212/z	551.2103769	4.4057	pos	Dutasteride	HMDB0015258	Lipids and lipid-like molecules	Steroids and steroid derivatives	Androstane steroids			39.5	0	M+Na, M+K, M+H	C27H30F6N2O2	0.016424985	6.551522211	0.003573568	0.019890427	-1.634976057	0.321976956	192753.4449	227576.6544	80758.23217	127533.9787	184356.6437	227239.5674	270408.3921	208963.7024
4.29	279.9898/z	279.9897939	4.278183333	neg	2-Methyl-4-amino-5-hydroxymethylpyrimidine diphosphate	3426	Unclassified	Unclassified	Unclassified			38.8	0	M+H2O-H	C6H11N3O7P2	1.378133209	6.550778392	1.73264E-06	0.000248714	-3.620913876	0.081282361	12999.8813	159934.8381	13866.23991	12551.34563	12582.05835	154097.5251	165811.4207	159895.5685
10.75	788.5424m/z	788.5424013	10.74813333	pos	PG(16:1(9Z)/20:3(5Z,8Z,11Z))	HMDB0010593	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols	*		37.5	0	M+NH4	C42H75O10P	-1.569627596	6.491606992	0.016365814	0.09909737	-0.580177524	0.668881466	326041.0572	487442.2054	369075.2407	322373.3075	286674.6234	551570.9471	467010.825	443744.8441
0.80	234.0546/z	279.0528521	0.800366667	neg	cis-3-(6-Hydroxy-7-methoxy-5-benzofuranyl)acrylic acid	1203	Unclassified	Unclassified	Unclassified			37.2	0	M+FA-H, 2M-H	C12H10O5	7.800665069	6.465915815	0.001691047	0.012062075	-0.563812989	0.676511804	309278.2823	457166.1288	285127.9497	332854.495	309852.4022	484904.9816	447737.5897	438855.815
0.71	473.1563/z	473.1563049	0.741216667	neg	beta-D-Mannosyl-(1->4)-beta-D-mannosyl-(1->4)-2,6-bisacetamido	HMDB0034539	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C00665	38.9	1.09	M+FA-H, 2M-H	C20H34N2O11	3.190143685	6.334782129	0.000766051	0.006556133	0.072529987	1.051074446	1239736.904	1129561.587	1283624.247	1260444.379	1218332.782	1021144.177	1238019.757	1128709.804
5.22	405.1768m/z	405.1768158	5.222166667	neg	1-O-(8R-hydroxy-8-methyl-3Z,9-decadienoyl)-beta-D-glucopyr	LMFA13010039	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides			48.7	44.7	M+FA-H	C17H28O8	0.541646569	6.330516712	0.000426724	0.000553604	-0.385952812	0.765273415	455119.0866	594714.3564	468108.4905	449736.7716	447511.9978	591105.6213	577291.2356	615746.2121
7.47	369.1557m/z	369.1556656	7.473983333	neg	Blumealactone C	HMDB0035357	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*		40.7	6.8	M+FA-H	C17H24O6	0.537543887	5.462991391	3.06212E-05	0.001064747	0.840793882	1.791035436	232200.0661	129645.713	234991.0835	227522.7352	234086.3795	121540.1093	136134.0407	131262.9889
4.52	287.0233m/z	287.0233001	4.521733333	neg	4-Hydroxy-5-(dihydroxyphenyl)-valeric acid-O-sulphate	HMDB0059978	Benzenoids	Phenols	Benzenediols	*	C07144	42	13.7	M+NH4	C11H17NO3	-1.492187027	6.282347647	0.000524343	0.005769144	0.276122995	1.210936316	790401.2499	652719.0896	792386.2021	808501	770316.5475	637472.8552	662965.6427	657718.7709
7.18	357.2509/z	358.2581953	7.182833333	pos	(9Z)-3-hydroxydodecenoylcarnitine	LMFA07070024	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters			50.3	57.6	M+H, M+Na	C19H35NO5	-1.691657256	6.224037296	0.003415824	0.019320609	0.540241913	1.454522285	446104.6282	306097.6462	479168.8622	432021.7243	424303.2983	280363.7877	307812.6603	330116.4905
3.09	345.1936/z	345.1936391	3.08208757	neg	(2E,5Z,7E)-decadienoylcarnitine	LMFA07070016	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters	*		50	54.6	M+H, M+Na	C17H27NO4	-1.322997749	6.150892837	0.001316818	0.010164937	0.455588752	1.371450483	350283.8394	241561.4215	496032.8328	488187.5345	335358.6497	309043.7873	373677.4316	
4.39	549.1971m/z	549.197051	4.3893	neg	Tracheloside	HMDB0030557	Lignans, neolignans and related compounds	Lignan glycosides		*		40.5	6.34	M-H	C27H34O12	-1.270532078	5.945505726	0.000295314	0.004079089	-1.422839249	0.372977563	72946.2986	195578.2488	76206.53988	71445.88563	71186.47028	175099.9005	207070.4876	204564.3582
4.39	331.0913m/z	331.0912942	4.3893	neg	3',4'-Dihydroxid	85300	Organoheterocyclic compounds	Azolidines	Imidazolidines	*		37.5	0	M+FA-H	C15H14N2O4	-7.919199621	5.85500812	3.85651E-05	0.001215866	-0.562437782	0.677156976	247204.519	365062.353	251884.5429	247346.2027	242382.8114	354594.4769	371630.1986	368962.3834
0.78	162.1121/z	162.1121691	0.758666667	pos	L-Carnitine	34532	Organic oxygen compounds	Organooxygen compounds	Quaternary ammonium salts	**	C00318	54.7	77.6	M+H	C7H15NO3	-1.866632448	5.662236104	1.08189E-05	0.000590127	-0.727219001	0.604901525	276133.0537	278661.8564	281661.8173	169646.913	270023.4067	269519.2	288167.3474	
3.94	302.0640/z	301.0566972	3.9351	pos	Pyroqallol-2-O-glucuronide	HMDB0060017	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		51.6	60.5	M-H, 2M-H	C12H14O9	0.634343121	5.636167703	2.41256E-06	0.000293302	-4.187750369	0.054873356	6316.420877	115109.0675	6444.97756	5937.848805	6566.436265	109930.7518	119228.2215	116168.2293
4.79	351.0957/z	350.0884143	4.792316667	neg	Indole-3-acetic-acid-O-glucuronide	HMDB0060001	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		49.6	52.8	M-H, 2M-H	C16H17NO8	0.780925824	5.627831322	1.97032E-05	0.000810659	0.830405989	1.778185691	248514.2549	139757.201	251882.5431	248890.0916	244770.1302	132049.5639	146328.5416	140893.4973
6.78	745.3660m/z	745.3660072	6.776666667	neg	Chalcomycin	71013	Unclassified	Unclassified	Unclassified			39.5	0	M+FA-H	C35H56O14	1.139218365	5.577989226	0.000401209	0.00487741	-1.245125966	0.421871062	78935.33788	187107.7327	82097.35639	71170.14783	83538.5094	195365.2668	197057.222	168900.6895
13.07	810.5965/z	810.5965488	13.07183	pos	PC(16:0/20:1(11Z))	LMGP01011468	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphocholines	*		37.2	0	M+Na	C44H86NO8P	-2.256532351	5.544560009	0.033750313	0.105888545	-1.040241321	0.486255232	1544.965098	24191.58743	1597.93	1491.257	1544.965098	24191.58743	23796.8757	
7.47	369.1557m/z	369.1556656	7.473983333	neg	Blumealactone C	HMDB0035357	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*		40.7	6.8	M+FA-H	C17H24O6	0.537543887	5.462991391	3.06212E-05	0.001064747	0.840793882	1.791035436	232200.0661	129645.713	234991.0835	227522.7352	234086.3795	121540.1093	136134.0407	131262.9889
4.52	287.0233m/z	287.0233001	4.521733333	neg	4-Hydroxy-5-(dihydroxyphenyl)-valeric acid-O-sulphate	HMDB0059978	Benzenoids	Phenols	Benzenediols	*		52.6	67.9	M-H2O-H	C11H14O8S	0.66257282	5.462160141	5.61602E-05	0.001549989	-1.474083703	0.359961945	57750.61011	160435.3209	60281.27941	57366.007	55604.54391	149348.1402	165986.8798	165970.9427
7.09	367.1402m/z	367.140208	7.086816667	neg	2-Hydroxyphenylacetic acid glucuronide	HMDB0240440	Unclassified	Unclassified	Unclassified			40.6	7.21	M+FA-H	C17H22O6	1.138188607	5.433918482	0.000567643	0.006045754	0.573670092	1.488304878	314194.0961	211108.692	320624.5545	320974.2633	300983.4703	197895.9135	225369.658	210060.5044
0.89	203.1154/z	204.1227854	0.884716667	neg	DL-Acetylcarnitine	HMDB0240773	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters	**	C02571	43	18.3	M+FA-H, 2M-H	C9H17NO4	-1.862853443	5.384719907	1.26479E-05	0.000729028	0.038348809	1.817472803	154227.1814	49741.9681	317145.2604	254221.7814	254568.1248	154944.8392	184423.1677	
9.01	372.2658/z	373.2731335	9.012583333	pos	3alpha-Hydroxy-5beta-chola-7,9(11)-dien-24-oic Acid	LMST04010330	Unclassified	Unclassified	Unclassified			52.1	66.4	M+H-H2O, M+H	C24H36O3	-1.610736918	5.372416679	5.64774E-05	0.001549989	-1.920369863	0.264186772	35654.31351	134958.7386	36720.65622	34767.53938	35474.74493	127239.5112	145603.2442	132033.4604
5.33	346.1623/z	369.1515345	5.329033333	pos	Glucosyl 6-hydroxy-2,6-dimethyl-2E,7-octadienoate	HMDB0035822	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		46.2	36.4	M+H, M+Na, M+NH4	C16H26O8	-1.231470034	5.334186927	0.000105072	0.002192066	-1.198174831	0.435826301	75807.26696	173939.1742	78554.51715	74540.1555	74327.1282	162437.0852	183898.3465	175482.0909
3.03	264.9784/z	264.9784981	3.027916667	pos	2-furfuryl 2-methyl-furyl disulfide	88332	Organoheterocyclic compounds	Organooxygen compounds	Heteroaromatic compounds	*		37.5	0	M+H	C10H12O2S2	-1.904966705	5.265128794	0.011911E-06	0.000159527	-3.154312815	0.112851584	12981.5864	107021.2993	12961.6417	13001.5311	12743.78824	106191.8857	107850.7871	
4.95	477.1770m/z	477.1769595	4.94705	pos	(7R*,8R*)-3-Methoxy-3',4',7,9,9'-pentahydroxy-8,4'-oxyneolign	HMDB0040325	Lignans, neolignans and related compounds	Lignan glycosides				44.3	24	M-H2O-H	C24H32O11	0.682735328	5.255302522	1.0238E-08	1.96309E-05	-7.175061996	0.006919761	658.3769354	95144.46552	559.5341947	679.4385182	736.1580934	94127.34998	95085.13564	96220.88393
0.78	377.0858m/z	377.0857594	0.778533333	neg	5,7,4'-Trihydroxy-8,3'-dimethoxyflavanone	53149	Unclassified	Unclassified	Unclassified			37	0	M+FA-H	C17H16O7	-6.161846724	5.24055199	0.00029019	0.00403473	-1.313637291	0.402305317	64146.8591	159448.2012	64293.84771	63423.55236	64723.17724	175417.6561	149956.1187	152970.8289
14.52	907.7338m/z	907.733817	14.51608333	pos	22-O-Glc-Campesterol	103412	Lipids and lipid-like molecules	Sterol Lipids	Sterols	*		37.4	0	M+Na	C56H100O7	-2.610080177	5.105939454	0.049217606	0.132672145	-3.946365988	0.064866347	7599.332926	117153.7051	10836.52999	8939.044313	3022.424478	181861.5112	123056.9745	46549.62972
3.29	227.2279/z	227.2278792	3.293833333	pos	Ammonium peroxydisulfate	92479	Unclassified	Unclassified	Unclassified			36.2	0	M+FA-H, 2M-H, M-H	H8N2O8S2	-7.153997898	5.058163203	9.16132E-06	0.000552203	-1.780964111	0.120665548	24835.12337	112599.8406	25028.22213	24435.93866	25050.20931	107015.8046	117665.3062	113004.1111
1.48	153.0656/z	153.065643	1.479433333	pos	N-Methyl-4-pyridone-3-carboxamide	1502	Unclassified	Unclassified	Unclassified			43.1	25.4	M+H	C7H8N2O2	-1.387388141	5.019997801	1.28646E-05	0.000638547	1.264444582	2.402347049	148099.9038	61648.00537	153610.662	145997.7673	144691.2822	58416.84117	64663.3046	61863.87035
7.43	584.3188m/z	607.3079165	7.432366667	pos	Cholic acid glucuronide	HMDB0002577	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid glycosides	*		50.6	56.6	M+H-H2O, M+Na, M+H	C30H48O11	-1.475754588	4.972448985	0.000542196	0.005886902	-1.341509452	0.394607573	56177.70336	142363.47	58032.72473	57391.0346	53109.35076	126247.9868	154520.3388	146322.0844
8.07	405.2648m/z	405.2647973	8.074883333	neg	(23R)-3alpha,7alpha,11alpha,23-Tetrahydroxy-5beta-cholan-2	LMST04010421	Unclassified	Unclassified	Unclassified			52.7	68.7	M-H2O-H	C24H40O6	0.352239726	4.939860353	0.000366626	0.004619615	-1.595074517	0.33100513	41949.7283	126734.3749	44439.56986	41457.64625	39951.96879	111989.3075	136297.0466	131916.7707
2.38	181.9864m/z	188.9864277	2.380333333	neg	Hydroquinone sulfate	HMDB0240263	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		41.2	12.8	M-H	C6H6O5S	0.578086937	4.932639693	3.30968E-05	0.001024766	-3.533270044	0.043055739	7302.212661	86737.55538	7332.477187	7271.825134	8247.215717	90176.76184	83256.34271	
5.24	199.0072m/z	199.0071767	5.244033333	neg	4-Vinylphenol sulfate	HMDB0027775	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		50.5	58.8	M-H	C8H8O4S	0.616744442	4.88385186	8.59194E-05	0.001954921	-3.686897952	0.07764851	6925.544134	89190.94711	6933.159812	6917.928557	7113.531819	91538.63601	79435.85399	96598.35132
10.69	790.5577m/z	790.5576682	10.68925	pos	PG(16:0/20:3(5Z,8Z,11Z))	61854	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols	*		37.2	0	M+NH4	C42H77O10P	-2.061542431	4.855296306	0.027181577	0.085812578	-0.255806819	0.837518626	482464.1529	576063.7885	505091.7397	475951.368	466349.351	625044.8753	559451.982	543694.5084
1.92	204.9813m/z	204.9813008	1.924916667	pos	Pyroqallol-2-O-sulphate	HMDB0060018	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		47	41.2	M+H	C6H6O6S	0.33145368	4.83013563	1.27681E-05	0.000638547	-2.150382035	0.225229559	23262.44632	103272.5448	22998.25004	23691.42378	23097.66515	101065.988	109311.4273	99440.21906
11.33	435.3054m/z	435.305357	11.32583333	pos	Tigogenin	3516	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid glycosides	**	C01694	36.9	0	M+K	C29H44O4	7.558862895	4.695981322	0.017143893	0.061116879	-1.278515916	0.412219336	59371.57836	144429.0954	60842.32343	58815.51972	176431.1936	140631.8759	115529.2938	
8.68	567.3179m/z	567.3178705	8.68065	neg	Deoxycholic acid 3-glucuronide	LMST05010046	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid glycosides	**	C03033	52.4	65.2	M-H	C30H48O10	0.702483295	4.693021449	2.0073E-05	0.000814193	-1.926829607	0.263006506	26989.42725	102618.8579	29714.68254	27737.18346	23516.41574	98035.57394	102502.3008	107318.6989
2.26	402.9955m/z	402.9954979	2.26065	neg	Uridine diphosphate (UDP)	97	Unclassified	Unclassified	Unclassified			40.7	7.81	M-H	C9H11N2O12P2	1.428624513	4.665600372	3.47386E-06	0.000340794	-2.852235843	0.138481404	11985.20226	86547.37714	12251.9983	11488.0168

9.00	567.3179m/z	567.3179213	9.004166667	neg	6α-Glucuronosyihydoexycholate	43177	Unclassified	Unclassified	Unclassified		38.3		0	M-H	C30H48O10	0.791722943	2.011112684	2.69908E-06	0.000307608	-3.087606479	0.117635346	1847.128657	15702.15685	1670.71076	1793.292684	2077.382528	15098.14842	15739.63061	16268.69153
4.93	447.0914m/z	447.0914371	4.927016667	pos	Baicalin	49507	Phenylpropanoids and polyketides	Macrolides and analogues	Unclassified		C10025	54.9	79.3	M+H	C21H18O11	-1.682941586	2.006663269	3.72653E-05	0.00119091	23.23361951	9863166.88	13839.98835	0.001403199	15168.89748	13521.33207	12829.73551	0.001403199	0.001403199	0.001403199
5.65	469.1330m/z	469.1330134	5.650833333	neg	Plumieride	HMDB0256647	Unclassified	Unclassified	Unclassified			40.3	13.8	M-H	C21H26O12	-4.544250278	2.004514202	0.001404041	0.010659639	-1.233730005	0.42521665	10505.3902	24705.97093	11321.84955	10133.03921	10061.28185	26264.99111	21201.49558	26651.4261
0.82	220.9965m/z	220.996463	0.818116667	pos	2,4-Dinitrotoluene	HMDB0245464	Unclassified	Unclassified	Unclassified			37.6	0	M+K	C7H6N2O4	3.01153261	2.002348682	7.86616E-05	0.0018621	0.72227216	1.649778294	35093.57472	21271.69139	35056.06061	36326.80297	33897.86058	20386.07333	21905.02901	21523.97182
9.01	426.3206m/z	426.3206054	9.012353333	pos	Cholic acid	HMDB0000619	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	***	C00695	55.9	86.3	M+NH4	C24H40O5	-1.946050533	2.000022765	4.86151E-05	0.001428121	1.366615518	0.255852544	4731.120209	18491.58949	5293.012099	4265.794588	4634.553048	17300.95422	19633.19941	18540.61483
5.35	391.1333m/z	391.1332755	5.351683333	pos	2,2-Dimethyl-3-(4-methoxyphenyl)-4-ethyl-2H-1-benzopyran-7-	70549	Unclassified	Unclassified	Unclassified			36.4	0	M+K	C22H24O4	7.5480122	1.990599493	6.66187E-06	0.000482026	-1.300820664	0.405895243	9279.556996	22861.95063	9418.012766	9317.532429	9103.125793	22002.81296	23367.46994	23215.56899
6.50	435.1983m/z	435.1983439	6.4952	pos	5-(2,3-Dihydroxy-3-methylbutyl)-4-(3,4-epoxy-4-methylpentanc	HMDB0030082	Organic oxygen compounds	Organic oxygen compounds	Unclassified			41.2	11.2	M+Na	C21H32O8	-1.442965841	1.987351439	0.000182826	0.003029196	-0.918761685	0.528962852	15334.86637	28990.441	14816.21103	15143.02047	16045.36759	27304.40653	30613.52953	29053.38694
6.63	319.1400m/z	319.1399845	6.63275	neg	Valproic acid glucuronide	HMDB0000901	Organic oxygen compounds	Organic oxygen compounds	Carbohydrates and carbohydrate conjugates			46.4	36.6	M-H	C14H24O8	0.447312973	1.986688558	0.000226487	0.003472549	-1.436602968	0.369436171	8008.151692	21676.68548	8195.089068	8017.823363	7811.542644	19523.82477	22702.9125	22803.31917
6.46	408.2879m/z	407.2806642	6.458366667	neg	Lapacholic Acid	LMST04010085	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives			45.2	32.5	M-H, M+FA-H	C24H40O5	0.897124983	1.985943615	0.00041167	0.005002289	-1.077186027	0.475729691	12453.10202	26176.84425	14002.12255	10963.38712	12393.7964	24510.9174	27680.89745	26338.7179
4.41	263.0287m/z	263.028706	4.41115	neg	Oxalureate	63388	Unclassified	Unclassified	Unclassified				0	2M-H	C3H4N2O4	6.700818884	1.981133889	7.99123E-06	0.000518618	-0.899362433	0.537239604	15625.80328	29085.35252	16280.84971	14937.87342	15658.68672	28649.25634	29491.2565	29115.54474
6.30	528.2649m/z	528.2649105	6.302033333	neg	N-[(3a,5b,7a)-3-hydroxy-24-oxo-7-(sulfooxy)cholan-24-yl]-Glyc	HMDB0002496	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	*	C15559	37.6	0	M-H	C26H43NO8S	2.359147252	1.975426454	0.002497626	0.015652802	-1.684985233	0.311006097	6289.629418	20223.49236	7176.058351	6595.679163	5097.15074	17741.60596	18823.32285	24105.54827
5.74	413.1437m/z	413.143749	5.744566667	neg	4-Hydroxy-3-prenylbenzoic acid glucoside	HMDB0039891	Organic oxygen compounds	Organic oxygen compounds	Carbohydrates and carbohydrate conjugates			38	0	M+FA-H	C18H26O8	-4.268894057	1.974764926	5.02996E-05	0.001461323	-1.25179081	0.418175937	9634.527866	23039.42891	9539.028662	10944.87881	9419.275837	22096.98819	22706.92813	23514.3704
2.48	290.1594m/z	290.1594097	2.484216667	neg	3-Methylglutarylcarnitine	HMDB0000552	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		44.7	28	M+H	C13H23NO6	-1.397998048	1.973635328	0.000188256	0.003086041	0.751190229	1.683180889	33193.77331	19720.85919	33283.43662	32033.27789	34264.60543	18148.77532	20444.16477	20569.6375
2.58	367.0631m/z	367.0630804	2.578	pos	Vanillic acid 4-O-glucuronide	HMDB0060024	Organic oxygen compounds	Organic oxygen compounds	Carbohydrates and carbohydrate conjugates	*		43.4	22.8	M+Na	C14H16O10	-1.415477357	1.971886347	0.000219232	0.003397536	-2.263218745	0.208306715	3543.633827	17011.61587	3330.194281	3288.992147	4011.715053	15212.05697	17037.74144	18785.04921
0.90	173.0092m/z	173.0091686	0.904683333	neg	5-Hydroxy-2-furoic acid	HMDB0059784	Organoheterocyclic compounds	Furans	Furoic acid and derivatives			47	35.8	M+FA-H	C5H4O4	0.055726043	1.970777751	0.000360843	0.00457111	0.682441046	1.604852879	35821.73768	22320.88571	35452.89126	36824.85412	35187.46768	20160.98464	23114.9589	23686.71358
3.73	366.0564m/z	365.0491325	3.730516667	neg	5-formamido-1-(5-phospho-D-ribosyl)imidazole-4-carboxamide	HMDB0062708	Nucleosides, nucleotides, and analogues	Imidazole ribonucleosides and ribonucleotides	1-ribosyl-imidazolecarboxamides			41	10.4	M-H, M+FA-H	C10H15N4O9P	-3.430518917	1.969171369	3.24278E-05	0.001097357	-1.459825235	0.363537167	7659.84476	26932.78334	8291.780964	6709.855147	20066.02392	21517.40771	21214.9184
4.25	174.0712n	192.1050592	4.249833333	pos	4,4'-Thiobis-2-butanone	92123	Organic oxygen compounds	Organic oxygen compounds	Carbonyl compounds			41.2	9.48	M+H, NH4	C8H14O2S	-1.304233115	1.967566853	0.000958058	0.008406546	0.622325603	1.539354599	38760.46042	25179.68273	41189.92339	37402.56131	37688.89656	23231.76183	26226.03296	26081.25342
4.97	284.1852m/z	284.1851729	4.970833333	pos	Adhumulinic acid	HMDB0030137	Organic oxygen compounds	Organic oxygen compounds	Carbonyl compounds	*		47.7	44.2	M+NH4	C15H22O4	-1.735169309	1.967329314	0.000326148	0.004308876	0.845399712	1.796762486	30297.67154	16862.36872	32351.75323	29285.0183	29256.24308	16012.69287	17909.1578	16665.25548
7.55	579.2792m/z	579.279157	7.547766667	neg	Corchoroside A	HMDB0033846	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroid lactones	*		43.3	24.9	M+FA-H	C29H42O9	-3.60986084	1.966944895	0.000199847	0.003202546	0.469442482	1.384574307	48232.2731	34835.45294	48501.58506	48737.67972	47457.55453	33179.28221	36467.90853	34859.16807
5.04	267.1352m/z	267.1351887	5.037216667	neg	3-Hydroxymethylglycinexylidide	HMDB0060678	Organic oxygen compounds	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C16572	42.8	30.2	M+FA-H	C12H18N2O2	0.711101157	1.955784751	0.000822398	0.007624627	0.823217884	1.763498907	31148.43529	17604.47018	28302.31003	32056.98415	33086.0117	18243.64056	17045.63814	17524.13186
1.20	162.0581m/z	162.0580694	1.199716667	pos	trans-S-(1-Propenyl)-L-cysteine	HMDB0029440	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		39	0	M+H	C6H11NO2S	-1.59337463	1.964099543	5.0639E-05	0.001467141	-3.559218321	0.084833722	1229.819089	14496.81863	1122.153065	1304.897462	1262.406739	13561.45304	15904.55058	14024.45227
4.28	284.1504m/z	284.1504433	4.278183333	neg	Petasinine	HMDB0030516	Organoheterocyclic compounds	Pyrrolizidines	Unclassified			51.3	59.1	M+FA-H	C13H21NO3	0.405319954	1.962711115	0.000247195	0.003646978	-0.855508199	0.55267061	16486.00152	29829.70546	17210.08721	16127.61265	16120.30472	28413.4949	31805.07853	29270.54297
4.39	261.0881m/z	261.0881157	4.3893	neg	Phenylalanylaspartic acid	HMDB0028991	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			46.4	33.1	M+H2O-H	C13H16N2O5	0.125575567	1.960706106	0.004672157	0.024033482	-0.614414879	0.653194759	26255.21868	40195.0847	29563.28234	23883.02496	25319.34874	37087.15884	43147.22125	40350.67401
6.48	469.2084m/z	469.2083647	6.477433333	neg	Beta-Angelicynol-6-O-tiglyl-15-hydroxy-1alpha,10R-dimethoxy-3-oxo-1	HMDB0039013	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*		40.6	9.19	M+FA-H	C25H32O8	1.035971178	1.960016885	1.01776E-05	0.000574611	-1.437998612	0.369078957	7109.424945	22883.40546	7225.321371	7547.945018	20225.10353	21105.0638	21334.57764	
0.84	174.1122m/z	174.1122396	0.8386	pos	Isovalerylalanine	5715	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		41.5	14	M+H	C8H15NO3	-1.329639991	1.956243267	2.29871E-05	0.000891258	1.502707505	2.833740216	20315.06579	7168.993713	20738.26286	20976.08656	19230.84795	7063.109071	7564.376115	6879.495952
7.08	387.1664m/z	387.1663947	7.076316667	neg	W 140	64665	Unclassified	Unclassified	Unclassified			37.9	0	M+FA-H	C16H27N2O4P	-7.75088162	1.953104095	0.000245583	0.003637115	0.902719992	1.869587498	28437.04132	15210.32921	28467.99669	30178.71286	26664.41442	14606.23274	15774.68449	15250.0704
1.16	137.0458m/z	137.0458832	1.157483333	pos	Hypoxanthine	HMDB0000157	Organic oxygen compounds	Organoheterocyclic compounds	Purines and purine derivatives	***	C00262	39.7	6.1	M+H	C5H4N4O	-1.495529119	1.951185146	0.000466792	0.003004545	0.384931487	1.142732107	14755.54156	27770.29498	41082.25415	38609.14877	42428.416	27334.88469	29619.0196	29585.91831
7.18	435.1462m/z	435.1461674	7.178516667	neg	Chidamide	64835	Unclassified	Unclassified	Unclassified			38.5	0	M+FA-H	C22H19FN4O2	-3.177056297	1.948316053	0.030821249	0.093956032	0.233111771	1.175367385	102211.302	86961.15211	101110.1099	100824.1446	104699.6515	79368.273	94927.71655	86587.46679
7.34	417.2134m/z	417.2134196	7.33585	neg	Blumenol C glucoside	HMDB0040668	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		45.6	32.2	M+FA-H	C19H32O7	1.110598595	1.948068826	0.00352102	0.01996381	0.433883142	1.35086466	52609.65451	38945.1705	51347.5043	55613.48968	50867.96956	35694.00996	40536.98919	40604.51235
3.80	195.0532m	194.0459171	3.801716667	neg	L-Dopaquinone	HMDB0039119	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			53	75.4	M-H, M+FA-H	C9H9NO4	0.18314937	1.94452087	5.82548E-06	0.000457595	-2.114779483	0.230880865	3891.150852	16853.50882	4488.129983	3865.340166	3339.982406	16462.58124	16793.95743	17303.96378
5.56	426.1496m/z	409.1463023	5.56402	pos	Ditobloxin	HMDB0003556	Organic oxygen compounds	Organic oxygen compounds	Organic oxygenchalcogen compounds	**	C01674	41	12.1	M+H+H2O, M+H	C15H26N2O12	2.384879781	1.941389365	0.000565343	0.003204856	0.41434591	1.332694323	52646.2754	39503.63824	51126.19388	52017.61193	54795.01792	39741.36612	39162.53164	40607.02304
6.53	571.1413m/z	571.1412935	6.533083333	pos	Puerarin xyloside	71530	Unclassified	Unclassified	Unclassified			38.9	0	M+Na	C26H28O13	-1.675037591	1.93793864	5.82206E-05	0.001570867	1.527074389	2.882008097	19800.17198	6870.269378	20768.65458	19920.65916	18711.2022	6318.159483	7676.353302	6616.295349
1.94	539.1938m/z	539.1938383	1.938766667	pos	4-[[5-(acetylamino)-1-(hydroxymethyl)-1H-indol-3-yl]methyl]-3-(	3060	Unclassified	Unclassified	Unclassified			36.1	0	M+NH4	C27H27N3O6S	-3.921754251	1.935856221	0.000214494	0.003338825	-8.232001189	0.003325988	43.27961162	13012.55677	0.001403199	0.001403199	129.8360285	11177.56256	14669.85317	13190.25458
7.52	467.1518m/z	467.1517676	7.5231	pos	Pyridinoline	5814	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			38.6	0	M+K	C18H28N4O8	-4.91458486	1.935240967	0.005031786	0.025296421	-0.354428289	1.278475779	62465.70995	48859.51768	65385.93924	61404.82013	60606.3705	45103.39907	51544.44971	49930.70427
5.20	397.1151m/z	381.1015445	5.205	pos	Etherotoil sulfate	HMDB0061856	Unclassified	Unclassified	Unclassified			46.8	0	M+H	C18H22O5S	0.515369	1.931385444	0.018418E-07	0.000158022	-3.210106524	0.028343564	1050.728915	1001.886093	1141.611669	1350.538139	1378.378847	1016.618304	1235.631	1231.872
8.34	359.1714m/z	359.1714462	8.338466667	neg	(-)-trans-Carveol glucoside	HMDB0029848	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		42.5	16	M+FA-H	C16H26O6	0.970179707	1.933427487	0.000197192	0.003183557	0.670730462	1.59187876	34786.39899	21852.41732	35814.3944	34229.51141	34315.29116	20164.46675	22738.35396	22654.43124
9.24	395.2078m/z	395.2077739	9.2377	pos	NPD 3	LMFA03010142	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids	*		47.6	24.9	M+K	C20H30O5	0.705264719	1.926976529	0.000788252	0.007412314	-0.608133861	0.656045662	24779.19597	37770.53549	25042.52564	25141.22323	24153.83905	35428.59696	40215.88369	37667.12581
4.39	321.0625m/z	321.0624865	4.3893	neg	Aesculin	HMDB0030820	Phenylpropanoids and polyketides	Coumarins and derivatives	Coumarin glycosides	*	C09264	38.5	1.23	M+2D+H	C15H16O9	2.633326679	1.922463993	4.4403E-05	0.001339838	-0.565624974	0.67565329	28489.82362	39206.23789	27558.74502	25337.15254	26573.57331	39132.11259	39540.85085	38965.75022
13.15	799.5445m/z	799.5442056	13.15121667	pos	PI(18:0/18:1(11Z))	HMDB0010603	Lipids and lipid-like molecules	Glycerophospholipids	Unclassified			38.6	0	M+H	C45H81O19P	-1.867874572	1.918058145	0.000586588	0.003387546	0.564869962	0.690163947	28305.07875	18700.40578	27664.47721	28135.49067	28455.28808	45503.06924	49995.14416	49113.6038
4.86	439.1072m/z	439.1071737	4.858383333	neg	Hallactone B	67431	Unclassified	Unclassified	Unclassified			37.6	0	M-H	C20H24O9S	0.787968512	1.91555578	1.7635E-05	0.000778104	0.491467064	1.071429331	13375.80084	784.6310333	13931.7522	12337.56939	13858.08093	783.098203	886.757442	684.0374548
7.94	302.1731n	347.1713378	7.9373	neg	Gamma-glutamyl-Arginine	86035	Unclassified	Unclassified	Unclassified			37.4	0	M+H, M+FA-H	C11H22N6O4	9.43784676	1.909598289	0.001666042	0.01194837	0.491524631	1.406929869	44662.16888	31766.99626	46570.41694	41704.23861	45711.85108	30124.54761	32761.04348	32415.39768
1.59	220.0846n	221.0917737	1.589283333	pos	4-Hydroxy-L-tryptophan	364	Organic acids and derivatives	Indoles and derivatives	Tryptamines and derivatives	**	C00643	55.3	79.6	M+H, M+2Na-H	C11H12N2O3	-1.455894979	1.902805985	0.005725252	0.027677841	1.303699132	1.237125217	68932.52656	55719.92687	70852.88444	68499.03664	67445.69081	55161.45458	59132.50717	56501.81189
8.02	256.0594m/z	256.0593978	8.8195666667	neg	HDBA	44870	Unclassified	Unclassified	Unclassified			36.7	0	M-H2O-H	C14H13NO5	-7.756141852	1.89032775	0.000921753	0.008219751	-0.46143348	0.726264275	33240.79649	45769.56026	32884.05468	33116.24183	33722.09297	43105.6246	47861.66723	46341.38896
4.95	568.1539n	613.1519297	4.94705	neg	6,8-Dimethoxy-2,3-trans-2-(4-hydroxy-2,3-dimethoxyphenyl)-9	51478	Unclassified	Unclassified	Unclassified			36.8	0	M-H, M+FA-H	C29H28O12	-7.348269935	1.887923522	1.65739E-05	0.000756661	-6.600882264	0.010302353	127.3617337	12362.39231	110.0209105	185.0016479	87.06264281	13336.5316	11685.01482	12065.63052
4.36	407.0943m/z	407.0942546	4.3623	pos	5-(3',4'-Dihydroxybenyl)-gamma-valerolactone-4'-O-glucuroni	HMDB0059989	Organic oxygen compounds	Carbohydrates and carbohydrate conjugates	*			43.9	25.5	M+Na	C17H20O10	-1.595636984	1.884386633	7.31441E-05	0.001783532	-2.465189985	0.18109392	2704.683396	14935.25347	2746.882745	2716.381865	2650.786179	13487.45644	15763.02676	15555.27721
7.56	447.1657m/z	447.1656679	7.56	pos	4-Linolenoyl-5-[rhamnosyl-(1->6)-glucoside]	HMDB0030422	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		40	5.16	M+H	C22H32O10	0.996282824	1.881640826	0.004528514	0.023468162	-0.912695104	0.55645076	18256.84906	10559.7175	18487.98485	19704.23226	18962.19411	7178.178	8156.655865	
1.42	324.0728m/z	324.0727564	1.421683333	neg	HHPAA glucuronide	HMDB0240379	Organic oxygen compounds	Organic oxygen compounds	Carbohydrates and carbohydrate conjugates			42.2	16.5	M-H2O-H	C14H17NO9	0.776321604	1.878747398	0.000299332	0.004105014	-3.234549329	0.106243808	1456.979054	13713.54319	1574.526652	1442.715401	1353.695108	15175.89154	11700.34359	14264.39444
8.97	357.2782m/z	357.2781541	8.67276667	neg	THA	LMFA01030222	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids	*	C13802	38.9	0	M-H	C24H36O2	-1.831988911	1.877616632	0.001242305	0.009839537	-1.719666731	0.30361885	5413.880415	17831.17356	5600.894977	5270.230201	5370.516067	14785.43008	19291.72458	19416.36602
5.66	424.1339n	425.141212	5.656316667	pos	Apterin	89790	Phenylpropanoids and polyketides	Coumarins and derivatives	Furanocoumarins			38.8	8.22	M+H, M+Na	C20H20O10	-7.10017491	1.876527223	0.000106097	0.002209089	-0.804271588	0.572651137	16283.47357	28435.24185	15735.33155	16808.77471	16306.31446	28088.65082	27379.41349	29837.66125
8.67	357.2782m/z	357.2781541	8.672766667	pos	Violerolactam	624671	Organic oxygen compounds	Organoheterocyclic compounds	Piperidines	*		49.5	51.5	M+H, M+Na	C19H39NO4	2.742391279	1.874356113	0.000269004	0.001212368	0.611689145	0.823033979	3572.345704	15798.4578	3663.606223	3727.616791	3664.512	15266.29996	31894.43183	30687.82963
5.22	563.1338m/z	563.1337968	5.222166667	neg	Homocysteine-penicillamine disulfide	1733	Unclassified	Unclassified	Unclassified			36.9	0	2M-H	C9H18N2O4S2	-0.930458873	1.868992548	0.000712735	0.006959725	-0.442463201	0.735877127	34064.10369	46290.4776	34477.813	34749.30172	32965.19634	46519.22597	44149.26532	48202.94152
2.72	158.0823m/z	158.082319	2.72215	pos	Epsilon-caprolactam	HMDB0062769	Organoheterocyclic compounds	Lactams	Caprolactams	**	C06593	48.3	42.1	M+H	C6H11NO	0.433688984	1.868706362	0.002221882	0.014495495	-0.373493485	0.77191105	42033.18206	54453.40115	41230.65441	42538.73685	42330.15491	50986.07713	56233.38193	56140.74439
4.68	281.1008m/z	281.1007905	4.660833333	neg	5-Aminomethyldihydropoamide	HMDB0006239	Lipids and lipid-like molecules	Fatty Acyls	Fatty amides			40.2	14.4	M+FA-H	C9H20N2OS2	1.773176999	1.866259604	0.003405701	0.016264037	-0.157502494	0.635611679	18130.5754	31305.67495	18130.57541	28213.8049	32435.02499	18823.83219	20435.30544	19132.67557
0.80	161.0686n	162.0758453	0.796983333	neg	Acetylhomoserine	HMDB0029423	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		39	0	M+NH, M+Na, M+H2O	C6H11NO4	-1.483836107	1.865480414	0.00017689	0.002968146	0.366422873	1.289152443	33666.38466	41629.19983	54578.64822	53589.76376	52830.74199	40243.95774	42764.83841	41878.80333
1.31	179.1176m/z	179.117634	1.30655	pos	Z'-Hydroxynicotine	HMDB0001329	Organoheterocyclic compounds	Pyridines and derivatives	Pyrrolidinylpyridines			44.3	28.9	M+H	C10H14N2O	-1.434761329	1.864515768	2.67284E-06	0.000307608	2.644508404	6.25282614	14172.79155	2266.621721	14730.73448	13957.18494	13830.45522	2514.286258	2174.108867	2111.470038
5.26	320.1828m/z	320.1828402	5.26135	pos	Dinor-10-NO2-CLA	LMFA01120008	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates			49	50.2	M+Na	C16H27NO4	-1.308216051	1.862386548	0.000226401	0.003472549	-0.488366255	0.71283187	29825.45148	41840.79408	30371.21577	29408.03231	29697.11557	40058.4073	42433.61981	43030.35512
5.18	197.0806m/z	197.0802048	5.1777	pos	3,4-Methylene suberic acid	HMDB0059768	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		47.1	38.8	M+H	C10H16O4	0.617393148	1.861638827	0.000143351	0.002618436	0.046832401	1.927624457	24884.56554	12909.44689	23418.87158	25813.49939	25421.32565	12753.09683	13201.45773	13673.81609
5.58	506.2510n	507.2583567	5.581883333	pos	11-Hydroxyprogesterone 11-glucuronide	HMDB0010364	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	*		51.3	61.1	M+H-H2O, M+H	C27H38O9	-1.092129406	1.860689198	0.000595409	0.006222804	0.522183587	1.43612725	39777.75216	27697.93008	39586.7741	37794.10074	41952.38164	27957.70443	27898.91706	27237.16873
0.97	217.0161m/z	217.0161248	0.967616667	neg	4,4'-Biphenyldithiol	70164	Unclassified	Unclassified	Unclassified			36.4	0	M-H	C12H10S2	4.627692407	1.85964405	0.008230211	0.035906255	1.3550436	2.558048469	20996.17274	8207.886987	24135.42973	19048.54896	19804.53953	4352.797494	11557.13414	8713.729324
7.43	298.1887n	299.195934	7.432366667	pos	Diphthamide	HMDB0060473	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues			44.1	24.9	M+H, M+Na	C13H24N5O3+	2.491591527	1.85420522	7.24093E-05	0.001773818	1.308338356	2.476561343	19874.09731	8024.875847	19926.39438	20418.73974	19277.1578	6955.009104	9102.097273	8017.521163
4.41	285.1154n	267.122683	4.41	pos	Sapidolide A 1	HMDB0041582	Organic oxygen compounds	Organic oxygen compounds	Lactones	*		38.3	0	M+H, M+Na	C14H18O5	-0.064135664	1.853557332	0.001312368	0.011689145	0.673483926	0.644617862	21944.5492	34042.7259	23241.85561	21125.49673	21286.29996	31894.43183	36567.82963	33665.74091
6.68	547.1462m/z	547.1461782	6.680966667	neg	3,4,5-trihydroxy-6-[3-[(E)-2-(4-hydroxyphenyl)ethenyl]-5-[[3,4,5	HMDB0128508	Phenylpropanoids and polyketides	Stilbenes	Stilbene glycosides	*		46.9	37.8	M-H2O-H	C26H30O14	0.818984842	1.849075796	0.043854388	0.121803629	0.379787305	1.301150014	61390.34585	47181.60489	64386.73894	63819.85447	65964.44412	39053.0013	51175.8505	51315.96286
3.89	383.0986m/z	383.0986316	3.8906	neg	3-O-p-Coumaroylquinic acid	HMDB0029681	Organic oxygen compounds	Organic oxygen compounds	Alcohols and polyols			42.1	14.4	M+FA-H	C16H18O8	0.772541947	1.848704285	3.82642E-07	0.000126917	-2.476994761	0.179618174	2560.816848	14257.00299	2691.297872	2521.21865	2469.934021	14007.8502	14590.72925	14172.4295
0.78	245.0437m/z	245.0432924	0.778533333	neg	Phosphatidyl glycerol	186	Unclassified	Unclassified	Unclassified			39.5	0	M-H	C6H15O8P	0.466578417	1.845639419	0.004430844	0.023121207	-0.590844382	0.663954194	24338.14655	36656.36392	23610.36139	25861.52417	23542.55409	32681.24927	38656.27099	38629.5715
1.29	141.1152n	159.1488628	1.285033333	neg	Cuphylinine	HMDB0033364	Organoheterocyclic compounds	Piperidines	Unclassified	*		39.7	2.12	M+H, M+NH4	C8H15NO	-1.365675351	1.844211216	9.48858E-05	0.002028599	-2.605865	0.164289279	2304.559882	14029.1593	2289.131654	2408.539482	2216.00821	12580.84853	15035.01285	14001.6168
4.41	447.0788m/z	447.0787822	4.41115	neg	N-Adenylylanthranilate	65950	Unclassified	Unclassified	Unclassified			37.8	0	M-H2O-H	C17H19N6O8P	-7.669740607	1.844126574	0.000242022	0.00359488	-1.3673644	0.38759869	7452.197869	19226.58167	7769.73895	7678.76893	6908.085726	18696.15082	20996.2574	17987.33679
6.88	411.1276m/z	411.1276112	6.8759	neg	7-beta-D-Glucuronosyloxybutylidenephthalide	90178	Organic oxygen compounds	Carbohydrates and carbohydrate conjugates	*			38.1	0	M-H	C18H22O8	-5.624672717	1.840713066	0.042233274	0.118345186	0.171246612	1.1260451	125732.7372	11658.7046	122917.5126	132816.5831	121464.1159	110801.8049	117551.7163	106622.5926
6.23	318.1587m/z	318.1586389	6.230633333	neg	4-[4-(3-Hydroxypropyl)-2-methoxyphenoxy]-1,3-propanediol 1-	HMDB0041552	Organic oxygen compounds	Organic oxygen compounds	Carbohydrates and carbohydrate conjugates			39.8	5.75	M-H	C16H24O7	0.855037724	1.838527138	0.000846892	0.004778549	-0.775323182	0.548012889	28923.57187	17134.89267	31111.27	30816.84526	29640.03353	16741.34107	20843.19247	20844.31192
6.63	613.1178m/z	613.117844	6.63275	neg	Neobignonoside	HMDB0033006	Phenylpropanoids

4.48	377.0947m/z	377.0946988	4.477166667	neg	Butamifos	68779	Unclassified	Unclassified	Unclassified		37.7		0	M+FA-H	C13H21N2O4PS	1.599344837	1.488233288	0.000980454	0.00849969	0.790380264	1.72953027	18422.4063	10651.68192	20125.09385	17867.62417	17274.50088	11107.39434	10442.58563	10405.06578
6.86	479.1151m/z	479.1151357	6.86375	neg	3'-O-Methyl-(-)-epicatechin 7-O-glucuronide	96020	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	*	36.3		0	M+H	C22H24O12	-9.089326735	1.48685571	0.010997109	0.044307739	0.20325278	1.151291196	63181.59896	54878.90397	63215.58195	65437.78532	60891.42962	53884.4856	57473.26358	53278.96272
6.62	331.1401m/z	331.140113	6.61635	neg	Tryptophyl-Glutamine	HMDB0029081	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	39.5	6.73	0	M+H	C16H20N4O4	-3.208470741	1.483974763	0.049605537	0.133491443	0.207207372	1.154451346	69312.08556	60038.98373	71201.3527	67727.26097	69007.643	53696.64328	63363.23195	63057.07597
12.95	814.6309m/z	814.6308737	12.94628333	pos	PC(16:0/22:2(13Z,16Z))	LMGP01014173	Lipids and lipid-like molecules	Glycerophosphocholines	*	37.1		0	M+H	C46H88NO8P	-1.423441943	1.483644219	0.010954633	0.041889878	-1.300759356	0.405912492	5628.728386	13866.85185	6093.434846	6414.630395	4378.119918	16923.30948	13724.31235	10952.93372
6.34	505.2662m/z	505.266192	6.339663333	pos	SLF	64652	Unclassified	Unclassified	Unclassified		36		0	M+H2O-H	C30H36N2O6	-8.781230196	1.482077378	0.003539381	0.019770294	0.442643451	0.735785193	22007.3943	29910.08043	21733.65122	23180.12738	21108.40428	28364.09045	29259.40465	32106.74617
8.09	481.1826m/z	481.1826002	8.085633333	pos	Noroxymorphone-3-glucuronide	1423	Unclassified	Unclassified	Unclassified		39		0	M+NH4	C22H25NO10	2.00510246	1.481265876	8.805215e-05	0.001969787	-0.691820907	0.619071991	12295.21268	19860.71549	12791.85687	12246.68759	11847.09357	19144.43072	19980.97696	20456.73881
4.79	427.1224m/z	427.1224164	4.792316667	neg	Lucuminic acid	HMDB0035007	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		38.9	8.79	0	M+FA-H	C19H26O12	-4.861092646	1.481021881	0.004939757	0.024979468	-0.327400519	0.796971192	31211.64871	30534.48568	32944.37445	30156.08599	37118.29424	40953.33192	39416.86916
6.01	607.2378m/z	607.2378083	6.007266667	neg	Eriocarpin	67232	Unclassified	Unclassified	Unclassified		37.7		0	M+FA-H	C29H38O11	-3.213260495	1.478756646	0.000325279	0.004304125	0.259276952	1.196878704	46168.07183	38573.72655	46610.58657	45496.75381	46396.87512	38958.49529	39300.84914	37461.83521
1.92	165.0418m/z	165.0418092	1.926916667	pos	7-Methylxanthine	58075	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	**	C16353	45.5	34.3	M+H	C6H6N4O2	0.061197588	1.478200154	0.042421107	0.118745322	0.253914954	1.192438576	56195.61996	47126.63702	50733.5833	51753.20557	50733.58353	40100.071	46940.04725	49406.74866	45033.11515
8.10	437.2140m/z	437.2139629	8.104816667	pos	(4R,5S,7R,11x)-11,12-Dihydroxy-1(10)-spiroveriten-2-one 12-	HMDB0030895	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*	46.5	38.2	N/a	C21H34O8	-1.510779704	1.475661999	0.000749877	0.00717297	-0.635133694	0.643881144	13768.57398	21383.71982	13949.3447	13719.97096	13636.40628	19997.19601	22819.85969	21334.10376
3.98	190.0497m/z	190.0496848	3.979183333	pos	4-(2-Aminophenyl)-2,4-dioxobutanoic acid	HMDB0000978	Organic oxygen compounds	Organooxygen compounds	Carbonyl compounds	**	C01252	52.9	67.4	M+H+H2O	C10H9NO4	-0.892152762	1.474525199	0.021470743	0.071882685	0.211306799	1.157736392	62206.63559	53731.26045	64854.8819	60064.6366	61700.38827	51256.45889	57316.86823	52620.45423
0.82	207.0474m/z	207.0146728	0.819566667	neg	Hydroxypyruvic acid	HMDB0001352	Organic acids and derivatives	Hydroxy acids and derivatives	Beta hydroxy acids and derivatives	**	C00168	45	26.2	2M-H	C3H4O4	0.151454515	1.471507867	0.000109759	0.00351909	0.771439701	1.71039519	18550.79129	10553.57932	17388.45254	18819.06651	17944.85483	9780.13444	10850.48512	11030.11839
5.79	589.3036m/z	589.303645	5.785316667	neg	Urobilin	HMDB0004160	Organic oxygen compounds	Tetrapyrroles and derivatives	Bilirubins	**	C05794	38.5	0	M-H	C33H42N4O6	0.82380264	1.469885594	0.01148354	0.01106399	-0.686559433	0.621333854	12508.31552	20131.39224	11739.62451	13004.84993	12780.47212	21257.56565	20786.125	18350.48608
1.29	231.0837m/z	231.0836745	1.285033333	pos	Ethyl beta-D-glucopyranoside	HMDB0029968	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		39.1		0	M+Na	C8H16O6	-1.126290171	1.466799808	7.82644E-05	0.001854977	-0.851298073	0.55428579	9214.819237	16624.67161	9314.102486	9221.270859	9109.084367	16043.20136	17496.80725	16334.00623
5.97	368.2200n	413.2183145	5.965483333	neg	5(6)-Epoxy Prostadlandin E1	LMFA03020068	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids	*	C04741	38.5	0	M+H2O-H, M+FA-H	C20H32O6	0.311822759	1.466501799	0.000137733	0.002553197	-1.094797419	0.468201863	6537.442738	13962.87211	5861.873122	7233.38629	6517.068802	13378.26708	13975.05404	14535.29521
0.70	175.1438m/z	175.1437963	0.698133333	neg	Tranexamic Acid	HMDB0014447	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C12535	48.9	55.8	M+NH4	C8H15NO2	-1.960103825	1.46499412	0.005894172	0.02822503	0.146978459	1.107248052	81035.12118	73186.05896	78452.36483	83333.97938	81319.01935	72678.42085	72938.32417	73941.43186
6.09	427.1973m/z	427.197284	6.087383333	neg	Cincassaid A	HMDB0035164	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*	38.4	0	M+FA-H	C20H30O7	-0.19565902	1.463857523	0.000211885	0.003315336	-1.155834449	0.448806523	6041.077223	13460.3151	5768.536375	5795.340571	6559.354723	12454.10225	13763.0657	14163.77735
4.23	467.1194m/z	467.1194225	4.234483333	neg	Plicatic acid	HMDB0256643	Unclassified	Unclassified	Unclassified		39.3		2.59	M+FA-H	C20H22O10	-0.182984786	1.463256988	4.34208E-05	0.001317744	-2.615509804	0.163174802	1435.564546	8797.709732	1576.604529	1222.089701	1507.999407	8249.446967	9496.789	8646.89323
4.54	431.0968m/z	431.0968435	4.542216667	pos	naringenin-7-O-glucuronide	HMDB0029209	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	*	47	40	M+H+H2O	C21H20O11	-0.958951506	1.462664426	1.24974E-05	0.000633643	5.523448684	45.99638848	7501.372628	163.0861221	7986.659777	7489.126822	7028.331285	173.3611395	90.92782974	224.9693971
5.79	413.1779m/z	413.177899	5.790833333	pos	(-)-11-hydroxy-9,10-dihydrojasmonic acid 11-beta-D-glucoside	LMFA02020206	Lipids and lipid-like molecules	Fatty Acyls	Octadecanoids	*	45	31.1	N/a	C18H30O9	-0.854277677	1.459700049	0.002083157	0.013935281	1.855883154	1.811055807	15897.15163	9329.986615	18731.16251	15944.51652	16023.77585	8229.113429	9903.919803	9856.926912
1.16	173.1394m/z	173.1394387	1.157483333	pos	Acetylagmatine	65718	Unclassified	Unclassified	Unclassified		40.8		14.8	M+H	C7H16N4O	-1.445967555	1.457461032	3.4823E-05	0.001143585	-2.792024587	0.144383262	1231.661753	8530.502309	1210.413729	1152.166767	1332.404763	8071.908328	9230.911253	8288.687345
4.79	176.0704m/z	176.0704131	4.7912	pos	Betamipron	HMDB0034250	Benzenoids	Benzene and substituted derivatives	Unclassified		49.1		48.5	M+H-H2O	C10H11NO3	-0.993950439	1.455926285	0.00059179	0.006206833	0.837569241	1.787036672	16793.68052	9397.501899	18065.6987	16268.15399	16047.18889	8649.382138	9971.567987	9571.555572
3.73	305.0339m/z	305.0338969	3.730516667	neg	4-Hydroxy-5-(3',5'-dihydroxyphenyl)-valeric acid sulfate	HMDB0240457	Unclassified	Unclassified	Unclassified		41.5		23	M-H	C11H14O8S	0.775376136	1.45317493	0.000703656	0.006925341	-1.216197154	0.430415771	5580.537252	12965.45719	6643.196041	5901.664903	4196.750812	13276.91049	13192.13116	13327.32992
5.24	409.1460m/z	409.1459803	5.238833333	neg	NNAL-N-glucuronide	HMDB0060498	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	49.2	52.1	N/a	C16H24N2O8+	1.087217857	1.451880418	7.95631E-05	0.001868759	0.359197167	1.315122481	30321.06048	25958.75154	29894.6137	30087.46019	22880.39605	23777.96018	22508.75947	
4.88	383.1347m/z	383.1347473	4.880083333	neg	15-Acetyl-4-deoxynivalenol	HMDB0033444	Nucleosides, nucleotides, and analogues	Purine nucleosides	Purine 2'-deoxyribonucleosides	*	41.6	11.7	N/a	C17H22O7	-0.025493613	1.451762492	0.000164048	0.002833823	0.24399856	1.18427043	46832.57463	39545.50704	46618.89888	47172.52547	46706.29955	40548.88307	39107.71616	38979.92189
4.41	146.0692n	145.061842	4.41115	neg	Alanylglycine	HMDB0029049	Organic acids and derivatives	Amino acids, peptides, and analogues		*	44.9	31.3	N/a	C5H10N2O3	0.130433996	1.451404689	0.002032169	0.013698466	-0.714640649	0.609356893	11669.57212	19150.6361	12013.92538	11352.92801	11641.86291	17139.27506	20539.58891	19773.04432
4.57	839.5498m/z	839.549846	4.5698	neg	Citrusin C	HMDB0038708	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		41.3	10.7	M+FA-H	C41H74O17	0.854497977	1.450699295	0.000345031	0.001987319	0.445977655	0.881135949	13665.38923	6629.96812	13555.00803	12867.08348	14559.90286			
5.27	342.1924m/z	342.192425	5.271716667	neg	N-(3-oxododecanoyl) homoserine lactone	LMFA08030001	Lipids and lipid-like molecules	Fatty Acyls	Fatty amides		42.8	18.3	M+FA-H	C16H27NO4	0.719247263	1.450404345	0.024046799	0.078331287	-0.464902828	0.724519875	21815.61433	30110.44289	23851.52035	20424.79761	21170.52503	31932.08091	25921.01788	32478.22988
7.14	391.1354m/z	391.1354116	7.13965	pos	b-D-Glucopyranosiduronic acid, 6-(3-oxobutyl)-2-naphthalenyl	1377	Unclassified	Unclassified	Unclassified		40.8	20	M+H	C20H22O8	-8.542003539	1.44665049	5.7513E-05	0.001563228	0.543172163	1.457172994	22963.67883	15759.06115	23437.84549	22689.75812	22763.43287	15337.00555	16398.52561	15541.6534
6.17	407.0962m/z	407.096284	6.171316667	no	Khellol glucoside	67349	Unclassified	Unclassified	Unclassified		37.4	0	M+H	C19H20O10	-5.19966482	1.446439055	0.001610017	0.011713862	-0.969281212	0.510760474	7726.832139	15128.09338	7152.872552	7607.936639	8419.687259	13420.33838	15484.32901	16479.61274
5.22	371.1995m/z	371.1994832	5.21759	pos	4-hydroxy-3,5-bis(1-methylethyl)phenyl glucuronide	LMFA02020206	Lipids and lipid-like molecules	Fatty Acyls	Fatty amides		46.3	37	M+H	C18H29NO8	-0.854277677	1.445700049	0.002083157	0.013935281	1.855883154	1.811055807	15897.15163	9329.986615	18731.16251	15944.51652	16023.77585	8229.113429	9903.919803	9856.926912
11.72	762.5985m/z	762.5985109	11.71891667	pos	PA(24:1(15Z)/15:0)	HMDB0115457	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphates		36.3	0	M+NH4	C42H81O8P	-2.98264401	1.442400935	0.032102627	0.096854327	-1.344271127	0.393852919	5438.74432	13809.07456	6525.155477	5624.408842	4166.668642	18422.00467	13182.79581	9822.423187
0.88	156.0533n	174.0870845	0.8802	pos	5-Hydroxymethyl-4-methyluracil	HMDB0000544	Organoheterocyclic compounds	Diazines	Pyrimidines and pyrimidine derivatives	*	42.5	19.8	M+H+H2O, M+NH4, M+Na	C6H8N2O3	-1.32933998	1.441186327	0.036183925	0.106089761	0.253158989	1.191813909	52504.81328	44054.5398	57305.03953	51878.38645	48331.01385	43073.12969	45606.52249	43483.96721
0.82	138.9707m/z	138.9706736	0.819566667	neg	Sulfoacetic acid	HMDB0258590	Unclassified	Unclassified	Unclassified		38.5	0	M-H	C2H4O5S	0.041484713	1.441107592	8.41495E-05	0.00192919	0.48265388	1.3973117	25174.91198	18016.67586	24945.42701	25857.64681	24721.66231	18240.68914	17476.64552	18332.69293
6.71	415.1978m/z	415.1978424	6.7005	neg	(8S,7E,9S)-9-Hydroxy-4,7-megastigmadien-3-one 9-glucoside	HMDB0036822	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid glycosides	*	42.3	17.1	M+FA-H	C19H30O7	1.313396772	1.441855352	0.000394132	0.001586825	0.327147358	0.568991324	16924.168	60277.54472	51639.36981	61414.22127	57836.70841	46817.2714	55555.00803	12867.08348	14559.90286
2.33	651.3870m/z	651.3870187	6.230633333	neg	D-Phosphatidylglycerol	4194	Unclassified	Unclassified	Unclassified		38.5	0	M-H2O-H	C32H63O12P	-1.27427709	1.438660906	3.32653E-05	0.001113701	-1.608467366	0.327946557	3470.81205	10583.46848	3734.664406	3671.954221	3005.817523	10075.9414	10899.2702	10775.19384
3.96	303.0182m/z	303.0182002	3.957583333	neg	5-(3',4',5'-Trihydroxyphenyl)-gamma-valerolactone-4'-O-sulpha	HMDB0059987	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*	45.3	34.9	M-H	C11H12O8S	0.619401344	1.438154596	0.000113992	0.002304294	-1.799996356	0.287972638	2885.899697	10021.43717	2775.530418	3033.204637	2878.964035	9086.552858	10573.09289	10404.66576
6.67	548.5158n	571.14139	6.670416667	no	Mirificin	HMDB0254749	Lipids and lipid-like molecules	Polyketides	Flavonoids		46.3	37.5	M+NH4, M+Na	C28H28O13	-2.115758677	1.437913379	0.03118548	0.094818604	0.354028554	1.275020863	38475.06903	30176.03095	39738.53622	34539.72642	41146.94444	29111.59624	33262.24681	28154.24998
5.38	274.1312n	243.122801	5.382166667	no	Polyethylene, oxidized	HMDB0032472	Organic acids and derivatives	Keto acids and derivatives	Unclassified	*	51.9	63.2	M+FA-H2O-H, M-H	C12H20O5	0.580159857	1.437444106	0.263101604	0.530055839	1.857066145	1.870447807	47491.96475	47749.66641	45980.87861	35762.11807	41818.56292	40038.93541		
11.97	799.5443m/z	799.5442699	11.97468333	pos	PG(18:0/18:1(9Z))[U]	40860	Unclassified	Unclassified	Unclassified		37.4	0	M+NH4	C42H81O10P	-2.171367572	1.43656409	0.019302349	0.066676245	-0.548706998	0.683632553	17265.3426	25255.29617	19065.05268	17758.55633	14972.4188	28690.13995	23178.9696	23896.77896
8.66	395.1713m/z	395.1713226	8.6638	neg	Calonectrin	HMDB0034915	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	*	39.2	0	M+FA-H	C19H26O6	0.517256907	1.436362149	0.000373294	0.004669795	0.962800375	1.949089549	14718.68672	7551.570285	15848.61405	14092.06991	14215.37621	8134.486574	7439.198464	7081.025851
0.82	244.0778m/z	244.078118	0.818166667	neg	N-Acetyl-D-glucosamine	HMDB0000215	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C00140	46.1	34.5	M+Na	C8H15NO6	-1.537183418	1.435665768	0.00047197	0.002173842	0.024173847	1.170425835	51357.16519	43879.04268	52816.72332	50243.73306	51011.04014	44984.86227	44915.02567	
0.72	206.0898n	245.0529628	0.717716667	neg	Seryithreonine	HMDB0029049	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	38.6	0	M+Na, M+K	C7H14N2O5	-2.171167724	1.435326775	0.001282794	0.01003959	0.32972476	1.256773582	35584.03332	28313.798	34047.24118	36807.8239	35897.03489	27604.03817	28952.2338	28385.12201
7.30	413.2184m/z	413.2183696	7.29525	neg	Δ17-6-keto PGF1α	36198	Unclassified	Unclassified	Unclassified		36.6	0	M+H	C20H32O6	0.755000103	1.435156498	0.000872489	0.007921882	-0.727942668	0.603764289	11002.48236	18223.14198	11441.67558	10648.2774	10917.49409	16677.03695	19092.54962	18899.83938
4.84	373.1143m/z	373.1142725	4.836566667	neg	Ethylvanillin glucoside	HMDB0037682	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		43.4	21.4	M+FA-H	C15H20O8	0.76797363	1.434914082	0.008276775	0.036019819	-0.266219337	0.831495674	37568.80193	45182.19768	38029.36112	37127.53479	37549.59887	42136.63605	47152.97892	46256.97807
5.59	197.1957m/z	197.1957175	5.592833333	neg	Palmatisolide C	Unclassified	Unclassified	Unclassified	Unclassified		37.6	0	M+FA-H	C12H30O2	0.115864592	1.434859382	0.000384503	0.001477577	-1.694845676	0.398962312	3597.197766	11050.53854	3922.362193	3127.410652	9199.862356	11338.55106	10512.20205	
1.84	422.0120m/z	422.011964	1.841666667	neg	5-Amino-4-hydroxy-3-(phenylazo)-2,7-naphthalenedisulfonic ac	HMDB0033381	Benzenoids	Naphthalenes	Naphthalene sulfonic acids and derivatives		36.6	0	M-H	C16H13N3O7S2	-0.594173251	1.4348426	0.004240812	0.022407053	-0.608287598	0.655974847	14204.62691	21654.24296	14579.60933	14053.97144	13980.29997	24013.50111	19718.32892	21230.84485
3.65	519.1359m/z	519.1358643	3.64965	neg	trans-Caffeic acid [apiosyl-(1->6)-glucosyl] ester	89479	Phenylpropanoids and polyketides	Isoflavonoids	Furanoisoflavonoids		39.1	34.9	M-H	C11H12O8S	0.619401344	1.438154596	0.000113992	0.002304294	-1.799996356	0.287972638	2885.899697	10021.43717	2775.530418	3033.204637	2878.964035	9086.552858	10573.09289	10404.66576
6.52	453.1384m/z	453.1384449	6.123483333	neg	Nodakenin	67571	Unclassified	Unclassified	Unclassified		37.2	0	M+FA-H	C20H24O9	-4.386417571	1.432614171	0.000849299	0.007778319	0.456683484	1.372383308	26521.57946	19325.19822	25682.34564	27360.02363	26522.36912	18114.31936	19582.4917	20278.7836
5.38	593.1651m/z	593.1664827	5.312566667	neg	1,2,10-Trihydroxydihydro-trans-linalyl oxide 7-O-beta-D-gluco	HMDB0033237	Lipids and lipid-like molecules	Prenol lipids	Monoterpenoids	*	41.8	15	M+FA-H	C16H30O10	1.064178853	1.431564987	0.000159612	0.00142363	0.311705373	1.144556245	32645.82103	33526.82102	33960.6607	46383.88624	37335.14178	33265.32562		
5.20	383.1714m/z	383.1713924	5.20005	neg	Pinolidoxin	HMDB0030836	Unclassified	Unclassified	Unclassified		40.2	7.18	M+FA-H	C18H26O6	0.742076388	1.431834107	0.000289284	0.004030098	-0.716700526	0.608487475	11057.4265	18171.98703	10460.8125	11017.22394	11694.24307	18967.57964	17301.90056	18246.48089	
6.38	527.1881m/z	527.1881357	6.3814	pos	Physalin F	89711	Lipids and lipid-like molecules	Steroids and steroid derivatives	Physalins and derivatives		37.6	0	M+H	C28H30O10	-5.77334224	1.43059115	0.00039828	0.004855797	-1.175678438	0.442675539	5652.624447	12769.227	5986.723427	5690.028894	5281.12102	11532.64335	13384.10796	13390.92969
3.22	405.0416m/z	405.041586	3.22245	neg	2,4',6,6'-tetranitro-2',4-azoxytoluene	71193	Unclassified	Unclassified	Unclassified		36.8	0	M-H	C14H16N6O9	-5.081742473	1.428559512	2.58218E-06	0.000420441	-1.983631765	0.067749885	507.8485962	7495.932958	759.0771444	395.4029276	369.0657511	7235.332809	7747.881549	7438.583638
4.95	473.1987m/z	473.1986761	4.948983333	neg	Cymorosin diglucoside	93962	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	36.8	0	M+H+H2O	C22H34O12	-6.246712748	1.427815918	0.003944785	0.021317809	-0.525502333	0.694717174	16746.60939	24105.65051	18261.53703	15148.2503	16830.04085	22486.5594	25312.51205	24517.88009
4.95	396.1680m/z	396.1679887	4.948983333	pos	Meperidinic acid glucuronide	1135	Unclassified	Unclassified	Unclassified		39.7	13.6	M+H	C19H25NO8	6.816398584	1.424555089	0.000921863	0.008219751	0.767272345	1.702048733	17244.97649	10131.89349	18696.3983	16294.52831	16744.00284	9483.199061	10328.96145	10583.51997
4.41	665.1846m/z	665.1846185	4.41115	neg	Ethalfluralin	72592	Unclassified	Unclassified	Unclassified		36	0	2M-H	C13H14F3N3O4	6.925613181	1.423060818	3.40031E-05	0.001131219	-2.813259873	0.142273624	1153.84778	8110.061102	905.9202541	1692.17074	863.4523468	8042.233818	8500.484363	7787.465124
4.43	116.0661m/z	116.0661714	4.425	neg	2-Acetyl-4-methylpyridine	HMDB0037071	Organic oxygen compounds	Carbonyl compounds	Unclassified		45.4	36.4	M+H+H2O	C8H9NO	0.33848024	1.421629305	0.000639212	0.006537778	-0.515190403	0.568332041	9294.108848	16353.30789	10065.97197	8813.093146	9003.151424	15253.3602	17387.65188	16418.9116
5.18	509.1942m/z	509.1942301	5.1777	neg	Karwinskione	68031	Unclassified	Unclassified	Unclassified		37.2	0	M-H2O-H	C32H32O7	-5.172350698	1.419179469	0.000372803	0.004669339	-0.52081279	0.696979056	16106.0217	23108.32952	16353.05347	16230.87724	15734.1344	24299.01892	22371.72895	22654.24069
1.96	629.1916m/z	629.1915506	1.95955	neg	Flusilazole	HMDB0039815	Benzenoids	Benzene and substituted derivatives	Halobenzenes		C18733	37.7	0	2M-H	C16H15F2N3Si	-2.91010767	1.418700859	4.5478E-05	0.001356751	-22.23359759	2.02778E-07	0.001403199	0.001403199	0.001403199	7036.119019	7485.49411	6238.053933	
8.02	158.0689n	141.0656284	0.8181166667	pos	1-(Hydroxymethyl)-5,5-dimethyl-2,4-imidazolidinedione	HMDB0031670	Organoheterocyclic compounds	Azolidines	Imidazolidines		43.8	24.1	M+H+H2O, M+NH4	C6H10N2O3	-1.426719313	1.415500521	0.003188763	0.018462091	0.212834212	1.158962761	52457.11722	45262.12488	52094.78131	52605.57774	52670.99261	43156.18375	46986.3723	45643.81858
4.29	468.1253n	468.1150839	4.29	neg	Catechin-4-ol 3-O-beta-D-galactopyranoside	47415	Unclassified	Unclassified	Unclassified		38.4	0	M+H, M+Na	C21H24O12	-1.001258313	1.414542235	6.82697E-05	0.002042041	-1.175986185	0.554.2404	743.4966383	1009.921264	810.3615144	7327.962057	7790.760505	6946.465041		
5.81	453.0994m/z	453.0993729	5.806016667	neg	Hydroxynicorandil	1522	Unclassified	Unclassified	Unclassified		38.5	0	2M-H	C8H9N3O5	-3.944940558	1.414168468	0.011526393	0.04578431	0.642391753	1.560914757	20854.92811	13360.70917	23858.62292	18970.22046	19735.94093	14840.9285	12347.32806	12893.87094
6.74	356.2426m/z	356.2425859	6.738266667	pos	Idebenone	HMDB0253376	Unclassified	Unclassified	Unclassified		38.9	0.292	M+H4	C19H30O5	-1.666689784	1.412388158	0.002937443	0.017503604	0.481716197	1.396403809	25186.55505	18036.72755	23919.60777	25795.506	25844.55139	16244.57327	19153.02342	18712.58597
5.13	265.1195m/z	265.1194961	5.132616667	pos	Phenylalanylthreonine	HMDB0029005	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	39.1	2.54	M+H	C13H18N2O4	0.453816494	1.411743984	0.008465669	0.038612241	-0.753101991	0.593326452	10786.97911	18180.51271	11066.11297	10414.58663	10880.23773	17033.1581	16316.68044	21189.70389
3.72	193.0971m/z	193.0970231	3.716333333	pos	1-(2a-Hydroxypachyrrhizone	HMDB0030774	Phenylpropanoids and polyketides	Isoflavonoids	Pterocarpans	*	46.5	0	M+H	C20H14O6	0.255330722	1.410988089	0.010019332	0.002246791	0.052910198	1.383.109683	7241.758299	1379.156619	1384.633185	513.9010944	6401.094832	7916.765016	7404.384438	
6.41	545.1309m/z	545.1308602	6.408833333	neg	Apiin	HMDB0030843	Phenylpropanoids and polyketides	Flavonoids	Flavonoid glycosides	***	C04858	38.3	0	M-H2O-H	C26H28O14	1.410450367	1.406857795	4.29106E-05	0.001306062	1.422711655	2.680889313	10857.44094	4049.940028	11287.88016	10966.09369	10318.34897	4389.141002	4092.45281	3668.226272
1.27	195.0334m/z	195.0334001	1.26875	neg	(±)-2-Hydroxy-4-(methylthio)butanoic acid	HMDB0031161	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*	45	28	M-H	C5H10O3S	0.880139236	1.403698382	0.000245778	0.003637115	-1.380807523	4197.498403	11022.62469	4617.667533	4124.05001	3850.777664	10227.92649	11957.69497	10882.25261	
5.60	330.2934m/z	5.602	neg	Methlvid	Unclassified	66681	Unclassified	Unclassified	Unclassified		36.3	0	M+FA-H	C21H29NO2S2	-4.628810127	1.403211486	5.74591E-05	0.001563228	0.184187787	2.241070116	12245.99644	5452753	12432.61949	12132.80992	12532.37231	5840.042267	5751.982174	5840.042267		
7.44	369.1739m/z	369.1739049	7.440866667	pos	Androstenediol 3-sulfate	HMDB0248416	Lipids and lipid-like molecules	Steroids and steroid derivatives	Sulfated steroids		47.9	47.6	M-H	C19H30O5S	-0.577276141	1.400994227	0.000726416	0.007050308	0.282558365	1.216349955	38631.94453	31760.55079	39095.84252	38528.00023	38271.99086	31250.39333	33131.31906	30899.93999
8.00	411.0588m/z	411.0588855	8.000366667	neg	1-(5'-Phosphoribosyl)-5-formamido-4-imidazolecarboxamide	3506	Nucleosides, nucleotides, and analogues	Imidazole ribonucleosides and ribonucleotides	1-(5'-phosphoribosyl)-5-formamido-4-imidazolecarboxamides	**	C04734

2.30	298.9536m/z	298.9535784	2.303733333	neg	catechol disulfonate	1832	Unclassified	Unclassified	Unclassified			36.5	0	M+FA-H	C6H6O7S2	-0.468698349	1.34543695	3.36356E-09	1.63904E-05	-2.867471125	0.137026694	983.3268494	7176.169993	1017.991335	986.5895247	945.3996885	7155.848702	7153.326975	7219.334302
5.84	398.1933n	399.2007945	5.843716667	pos	Ptaquiloside	73198	Unclassified	Unclassified	Unclassified			41.7	16.1	M+H+H2O, M+H	C20H30O8	-1.966134752	1.345364879	0.003444108	0.019423295	-0.344558825	0.787548772	24119.76367	30626.37457	23677.03926	24155.51045	24526.7413	28712.78155	30968.81305	32197.52914
7.55	485.2350m/z	485.2350218	7.553266667	pos	Neryl rhamnosyl-glucoside	HMDB0029349	Lipids and lipid-like molecules	Prenol lipids	Terpene glycosides	*		40	6.27	M+Na	C22H38O10	-1.506242913	1.344484761	0.000622383	0.00641608	-0.316351148	0.803098501	25745.47723	32057.68308	24930.36811	26382.47606	25923.58752	32862.08467	31182.37048	32128.59409
0.68	161.1281m/z	161.1281323	0.6788	pos	Isoputreanine	HMDB0006009	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		51.7	63.4	M+H	C7H16N2O2	-2.010438013	1.343657854	3.02893E-05	0.001057718	0.298593302	1.229944573	33167.28139	26966.48461	33529.04574	32619.61093	33353.18748	26815.39451	26935.65813	27148.40117
7.99	372.2659n	355.2625876	7.987716667	pos	3-oxo(hd-4-en-24-oic acid	LMST04010233	Unclassified	Unclassified	Unclassified			44.1	26.7	M+H+H2O, M+H	C24H36O3	-1.528865971	1.341698394	2.41234E-05	0.000920092	-1.501261193	0.353244272	3375.410882	9555.45823	3437.871811	3701.380294	2986.980541	9364.524284	9921.908173	9379.942233
4.19	242.9969m/z	242.996913	4.189783333	neg	(2E)-3-[3-(sulfooxy)phenyl]prop-2-enoic acid	HMDB0124975	Phenylpropanoids and polyketides	Cinnamic acids and derivatives	Hydroxycinnamic acids and derivatives	*		47.6	42.5	M-H	C9H8O6S	0.124726626	1.341527569	0.002822144	0.017006536	-1.178256497	0.441885196	5098.656455	11538.41881	4738.561005	4649.880975	5907.527384	13328.89992	10743.97514	10542.38138
4.28	308.0778m/z	308.0777995	4.278183333	neg	Indoxyl glucuronide	HMDB0010319	Lipids and lipid-like molecules	Steroids and steroid derivatives	Steroidal glycosides	*		42.4	16.8	M-H	C14H15NO7	0.725150798	1.341439307	9.65491E-06	0.000564774	-4.216636296	0.053785597	350.7053734	6520.432841	341.8934958	311.5014482	398.7211762	6729.597247	6748.572245	6083.12903
1.16	340.0674m/z	340.0674386	1.160166667	neg	Triglochinin	66921	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			37.6	0	M+H2O-H	C14H17NO10	0.094644633	1.340731605	8.92076E-05	0.001974362	-4.679982899	0.039010792	251.5722013	6448.784759	0.001403199	754.7137974	0.001403199	6828.653145	5869.039837	6648.661294
7.27	439.1933m/z	439.1932512	7.274666667	neg	8-Prenylneoisoeriodictyol	93233	Organic oxygen compounds	Isoquinolines and derivatives	Benzylisoquinolines	*		36.9	0	M+H	C25H30O9	-6.86420514	1.339756151	0.005831615	0.028503478	0.643913015	1.562561545	18187.42288	11639.49218	19940.2352	17049.8874	17572.14603	9970.594268	12571.3483	12376.53396
5.80	589.3012m/z	589.3012292	5.799966667	neg	D-Urobilin	58223	Unclassified	Unclassified	Unclassified			37.7	0	M+H	C33H40N4O6	-1.414621816	1.33885912	0.000368501	0.004631961	2.548769128	5.851348427	7516.192398	1284.52313	6730.460655	7281.528465	8536.588076	1026.409825	1588.667747	1238.491819
0.88	172.0845n	173.0918252	0.8802	pos	Prolylglycine	HMDB0011178	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.8	0	M+H, M+Na, M+H-H2O	C7H12N2O3	-1.414754282	1.338664201	2.9015E-06	0.000313766	0.574132564	1.488782048	18702.91583	12562.56136	18717.52922	18740.15349	18651.06478	12474.94533	12872.71342	12340.02533
8.07	745.2025m/z	745.2024789	8.074016667	pos	Deferasirox	85530	Organoheterocyclic compounds	Azoles	Triazoles	*		39.6	0	2M-H	C21H15N5O4	-3.69408824	1.337354684	0.000716993	0.009555188	-2.547127389	0.171066208	1590.206304	7542.145908	1904.939437	1885.750658	778.9288177	6626.707719	8688.863381	7109.866623
7.26	483.2214m/z	483.2214904	7.262266667	neg	Eriodictyol 8 -A	HMDB0038028	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		44.2	33.9	M-H2O-H	C24H38O11	-4.142563923	1.335930906	0.005505531	0.026954451	0.301746434	0.810457133	27777.69312	34287.2794	27838.40712	27185.42901	28309.24323	32355.441	34175.23915	36331.15806
5.56	949.1902m/z	949.1901695	5.56185	neg	Chondroitin 6-sulfate	5570	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*	C00635	36.6	0	2M-H	C15H25NO14S	-1.794366153	1.335177114	0.003055336	0.01791223	0.76124917	1.694957583	15614.14175	9212.113569	14405.98593	17152.51705	15283.92227	8670.090808	10383.64901	8582.600886
7.95	415.1978m/z	415.197822	7.949583333	neg	5-Hexagistimen-7-yne-3,9-diol 9-glucoside	HMDB0032841	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		37.5	0	M+FA-H	C19H30O7	1.258357299	1.334238677	0.000719498	0.006999835	0.965746698	1.953072762	12763.80818	6535.244577	13032.84569	12022.93497	13235.64387	6026.190941	7630.206018	5949.336774
5.84	490.2642m/z	490.2641864	5.843716667	pos	BAY-u9773	63071	Unclassified	Unclassified	Unclassified			37.1	0	M+NH4	C27H39NO5S	2.263833975	1.333805914	0.000857221	0.007830455	0.689169138	1.61235468	16419.85334	10183.77255	15496.90415	16823.98068	16938.67519	9388.363114	10002.25283	11160.70172
0.86	151.0071m/z	151.0070612	0.86335	neg	2-Mercaptopropanoic acid	HMDB0031520	Organic acids and derivatives	Carboxylic acids and derivatives	Carboxylic acids	*		46	33.1	M+FA-H	C3H6O2S	0.074648182	1.333791484	0.000162012	0.002813412	-0.543679411	0.686019072	13437.36624	19587.45288	13921.06915	12772.46511	13618.56445	19459.5656	20134.40689	19168.38614
7.65	487.2553m/z	487.2553253	7.6458	neg	4-Hexagistimene-6a,9R-diol 9-[apiosyl-(1->6)-glucoside]	HMDB0041580	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*		40.8	10.4	M-H2O-H	C24H42O11	0.897277327	1.331964732	0.010276488	0.042111237	0.241961192	1.182599189	42874.19175	36254.20359	42970.55279	40652.56623	44999.46622	34846.45312	37247.01265	36669.14501
3.24	322.1232m/z	322.1232472	3.238016667	pos	Saxitoxin	HMDB0029368	Phenylpropanoids and polyketides	Saxitoxins, gonyautoxins, and derivatives	Unclassified	Unclassified	C13757	44.9	28	M+Na	C10H17N7O4	-0.586736211	1.331681711	0.000114082	0.002304294	0.441112283	1.357560639	23232.79304	17112.49741	23058.89025	23697.09679	22942.39209	17751.78239	16632.75228	16952.95755
7.26	235.0953m/z	235.0953029	7.259166667	neg	DIHYDRO-8-TUBAIC ACID	44213	Unclassified	Unclassified	Unclassified			37.8	4.04	M-H	C13H16O4	-9.655230148	1.329154004	0.001491527	0.011099124	4.945820253	1.410122266	21441.74261	15205.59118	21890.52051	20526.04854	21908.65878	13960.27884	15442.21056	16214.28415
4.26	340.9951m/z	340.995139	4.2568	neg	L-Homocysteine sulfonic acid	6566	Organic acids and derivatives	Organic sulfonic acids and derivatives	Organosulfonic acids and derivatives	*		36.4	0	2M-H	C3H9NO3S2	-6.885353901	1.326536716	0.000117827	0.00233832	-0.632743229	0.644948903	11035.90067	17111.27907	11766.29062	10589.02768	10752.38373	16800.35263	17403.73503	17129.74956
5.52	358.1491m/z	358.1490886	5.5209	pos	Simmondsin	HMDB0030394	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		40	6.28	M+H+H2O	C16H25NO9	-1.478031839	1.325901766	1.93515E-05	0.000806645	-1.457533462	0.364115116	3457.6894	9496.143535	3600.547097	3133.622394	3638.89871	9798.932048	9121.722612	9567.775944
1.81	129.0425n	130.0497632	1.807733333	pos	(R)-(+)-2-Pyrrolidone-5-carboxylic acid	63632	Unclassified	Unclassified	Unclassified			42.2	14.8	M+H, M+Na	C5H7NO3	-0.82726625	1.32562311	0.000285601	0.003999929	-0.826878873	0.563747535	7872.595723	13964.75413	8135.257118	8001.588434	7480.941617	13216.0562	14835.40497	13842.80121
2.14	166.0488n	167.0561139	2.135	pos	9-Methylxanthine	96280	Organoheterocyclic compounds	Imidazopyrimidines	Purines and purine derivatives	*		40	8.14	M+H, M+Na	C6H6N4O2	-1.43206875	1.321653052	0.033489784	0.099353625	0.127156098	1.092138708	83824.56242	76752.69801	86559.25928	84129.38623	81685.13176	74290.69533	80485.56628	75481.83242
4.48	445.0822m/z	445.0822389	4.477166667	neg	(4aS,5aS,12aS)-7-chloro-4-(dimethylamino)-3,6,10,12,12a-per	HMDB0144089	Phenylpropanoids and polyketides	Tetracyclines	Unclassified	*		38.2	28.3	M-H2O-H	C21H21ClN2O8	3.095726755	1.314720624	0.000545974	0.005905479	0.914478786	1.884887981	12832.10704	6807.888409	13932.03175	11940.76401	12623.52535	6792.127216	7035.958624	6595.579388
2.03	214.0158m/z	214.015784	2.026633333	pos	Benzeneacetamide-4-O-sulphate	HMDB0059994	Organic acids and derivatives	Benzenoids	Arylsulfates	*		38.9	14.2	M+H-H2O	C8H9NO5S	-4.636430548	1.313716044	7.77468E-06	0.000510852	-3.411983614	0.093429139	609.7084562	6525.891831	674.7919323	613.7591449	540.5742916	6176.064763	6854.698597	6546.912133
7.12	254.0396m/z	254.0395679	7.123666667	pos	Stepsisicaloneoside A/B/D	HMDB0033602	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*		38.4	4.14	M+H+H2O	C12H19NO5	4.869132005	1.311302964	0.000450918	0.005304172	0.040460848	0.533514572	6841.869378	12824.14715	6903.86818	6478.420634	7202.429555	13617.84841	13014.70466	12482.25398
1.50	233.1128m/z	233.1128448	1.500483333	pos	N6-Acetyl-L-L-2,6-diaminoheptanedioate	63453	Unclassified	Unclassified	Unclassified			51.1	60.3	M+H	C9H16N2O5	-1.522000584	1.312219255	0.000361999	0.004583005	0.672081318	1.593370001	16062.18856	10080.6395	16990.27236	15492.06716	15704.22616	9650.122373	10539.99214	10051.80397
7.10	571.1026m/z	571.1026063	7.097333333	neg	5'-Phosphoribosylglycinamide (GAR)	3411	Unclassified	Unclassified	Unclassified			37.1	0	2M-H	C7H15N2O8P	-5.805477516	1.308620164	0.000381478	0.004730241	0.639869363	1.558188058	16632.72555	10674.40189	15652.85741	17491.98888	16753.33037	10529.23412	10754.81159	10739.15996
6.43	473.1815m/z	473.1815367	6.433933333	neg	1-Isomanganostin hydrate	HMDB0029984	Organoheterocyclic compounds	Benzopyrans	1-benzopyrans	*		38.5	0	M+FA-H	C24H28O7	-0.395524654	1.308361413	8.31582E-05	0.001921109	-0.995815458	0.501452673	5937.097994	11839.79727	5802.832451	5852.193976	6156.267554	12301.18733	11164.4416	12053.76288
7.59	216.9153m/z	216.9153604	7.589166667	neg	LysoPI(0:0/18:0)	HMDB0061704	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoinositols	*		38.6	0	M+NH4	C27H55O12P	-1.547364811	1.308228353	0.000269178	0.002616317	0.153161392	2.926516117	1023.342414	851.8286449	1023.342414	851.8286449	7015.046787	7836.225104	7931.071992	7447.605148
8.13	577.2636m/z	577.2635722	8.12973333	neg	Calotropin	3590	Unclassified	Unclassified	Unclassified			37.7	0	M+FA-H	C29H40O9	-3.501044372	1.306560306	0.000301479	0.004121061	0.5390162	1.452981365	19008.74651	13082.58108	19295.87848	18975.96073	18754.40033	12237.41939	13898.91397	13111.40988
5.22	274.2009m/z	274.2009072	5.21595	pos	Heptanoylcarnitine	LMFA07070068	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*		42.1	16.3	M+H	C14H27NO4	-1.381921133	1.306112595	0.000166872	0.002856862	0.538990981	1.452955967	18915.48513	13018.62242	19631.29913	18971.30429	18143.85197	12941.63694	13048.67892	13065.55141
4.68	327.0723m/z	327.0723214	4.682483333	neg	6-(3-carboxymethyl)phenoxy]-3,4,5-trihydroxyoxane-2-carboxy	HMDB0125161	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		43.6	20.9	M-H	C14H16O9	0.505341911	1.305442269	0.000387375	0.004772494	-0.969426384	0.510709081	6184.868498	12110.35545	6536.691317	5375.021964	6642.892212	12259.28337	12634.4477	11437.33527
4.45	399.1991m/z	399.1990196	4.454861667	neg	Propofol glucuronide	HMDB0060933	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		39.3	3.99	M+FA-H	C16H24O8	0.744103535	1.304311942	0.000732468	0.016387575	-0.594535651	0.662257757	11919.79196	7996.99673	12629.03997	12187.13642	10943.73948	8466.181771	9601.584534	8966.2898
7.18	519.0583m/z	519.0582948	7.178516667	neg	Norswertianin	68122	Unclassified	Unclassified	Unclassified			38	0	2M-H	C13H8O6	2.682932406	1.303024181	0.013747414	0.051927016	0.352390182	1.276674003	29762.05013	23312.17684	29278.8241	31694.31176	28313.01453	21340.57176	25366.57887	23229.37989
4.41	134.0612m/z	134.0611855	4.41115	neg	5-(2-Furanyl)-3,4-dihydro-2H-pyrrole	41	Organic oxygen compounds	Heteroaromatic compounds	Unclassified			6.74	6.74	M-H	C8H9NO	0.355184571	1.302460159	0.000726691	0.007050308	-0.977307629	0.507926754	6123.171878	12055.22614	6475.32978	6318.930529	5775.255326	10933.93081	12793.80809	12437.39523
6.52	624.3394m/z	624.339454	6.526166667	neg	(3a,5b,7b)-24-(f(carboxymethyl)amino)-7-hydroxy-24-oxocholan	6724	Unclassified	Unclassified	Unclassified			37.7	0	M-H	C32H51NO11	0.797957658	1.300819803	0.00055299	0.005821764	-1.599201263	0.330599662	2906.105022	8804.787092	2891.192454	3128.963525	2598.159447	7714.884452	9191.338928	9035.137624
7.29	176.0770n	177.0842892	7.285333333	pos	Biotin sulfone	HMDB0004818	Organoheterocyclic compounds	Thienoimidazolidines	Unclassified	*		38	0	M+H, M+Na	C10H16N2O3S	-1.247334505	1.300747211	0.000879502	0.007971837	0.458170676	0.316838152	2749.327104	6872.265461	2886.114033	2846.102224	2635.765149	7453.44056	7931.071992	7447.605213
4.95	462.2325m/z	462.232521	4.948983333	pos	Cynaroside A	HMDB0040532	Lipids and lipid-like molecules	Prenol lipids	Terpene lactones	*		38.6	0.707	M+NH4	C21H32O10	-1.91751233	1.300330828	0.001660116	0.011926149	0.590863741	1.506148208	17814.86622	11828.09642	18778.82851	18262.03799	16403.73218	11345.09152	12466.90081	11672.29694
9.74	479.1901m/z	479.1901429	9.7401	neg	Myristicanol A	95723	Unclassified	Unclassified	Unclassified			37.6	0	M+FA-H	C23H30O8	-4.900842141	1.299766936	0.000542582	0.005886902	0.561699291	1.476006721	18274.6275	12381.12756	17726.17841	17796.42915	19301.26595	12208.5378	12924.78649	12010.05841
3.91	215.1157n	238.1046876	3.911666667	pos	1-Hydroxyphenazine 4-enoylglycine	HMDB0094755	Organic acids and derivatives	Amino acids, peptides, and analogues				40.9	8.24	M+H+H2O, M+H, M+Na	C10H10N4O	-0.446026809	1.299642351	0.004769233	0.024344779	0.024344779	0.657633299	14074.45888	20199.78157	15196.82002	13516.82002	18554.10086	21743.19256	20561.61309	19437.08247
1.62	188.9865m/z	188.9864721	1.615883333	neg	4-Sulfocatechol	66486	Unclassified	Unclassified	Unclassified			38.4	0	M-H	C6H6O5S	0.811732391	1.294447088	2.82823E-06	0.000309083	0.840248055	0.558547525	7264.100207	13005.33953	7440.071053	7112.850502	7239.379065	13221.86872	12821.86398	12972.28589
6.99	331.1448m	354.1340497	6.988366667	pos	AMBELLINE	43630	Unclassified	Unclassified	Unclassified			37.2	0	M+H, M+Na	C18H21NO5	8.662956927	1.293645125	0.002892078	0.017285267	0.702425608	1.627238376	15537.02137	9548.091789	16244.88968	16325.18845	14040.98599	8690.050131	9415.513073	10538.71126
1.16	364.0628m/z	364.0628438	1.157483333	pos	N-Glycolylneuraminic acid	HMDB0000833	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C03410	37.9	0	M+K	C11H19NO10	-3.722289982	1.293503992	4.28027E-06	0.000310852	-4.319983614	0.093429139	609.7084562	6525.891831	674.7919323	613.7591449	540.5742916	6176.064763	6854.698597	6546.912133
7.72	314.1911m/z	314.1911207	7.705833333	pos	13-oxo-10,11-dihydro-20-COOH-LTB4	HMDB0012549	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38.7	0	M+FA-H	C20H30O6	0.761623114	1.290491705	0.000327818	0.003332661	-1.622502568	0.664339119	1504.633919	13271.72291	2112.915324	6793.568431	12853.99413	13914.70496	13617.94844	13017.25398
3.13	259.0129m/z	259.0129319	0.778533333	neg	(E)-C-HDMAPP	64798	Unclassified	Unclassified	Unclassified			39.3	7.72	M-H	C16H14O7P2	-4.875341535	1.290392613	0.004934717	0.024971941	0.417585134	1.335689928	24072.99403	18022.89104	22621.89744	25119.47047	24477.61417	16689.69391	18008.30089	19370.67831
7.55	647.2668m/z	647.2668003	7.547766667	neg	Glabranin	52653	Unclassified	Unclassified	Fatty Acyls	*	C09752	38.1	0	2M-H	C20H20O4	2.712620008	1.290194741	0.000754356	0.007199491	0.470613822	1.385698914	20951.10433	15119.52136	20674.19451	21227.02929	20952.0892	14195.37535	16268.10159	14895.08713
0.78	129.0657m/z	129.0657079	0.776666667	pos	2-amino-4-cyano-butanoic acid	35948	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates	*	C05717	52	64.2	M+H	C5H9N2O2	-1.140209781	1.290164321	0.008140187	0.035672724	0.195602446	1.145202278	48475.74132	42329.41397	50220.11847	48117.5693	47089.53619	40790.62739	42443.10511	43754.50941
4.12	289.0389m/z	289.0388535	4.181333333	neg	4-Hydroxy-5-(2-hydroxyphenyl)-valeric acid-4'-O-sulphate	HMDB0059976	Lipids and lipid-like molecules	Fatty Acyls	Fatty acids and conjugates	*		38	0	M-H	C11H14O7S	0.365867844	1.289987141	0.004453449	0.021703127	-5.309797	0.153352187	1449.750369	9139.936515	1433.965867	1384.321161	1290.296961	8104.844702	8067.995925	8346.205464
1.03	332.3728m/z	332.3727604	1.032333333	neg	1-O-(2R-hydroxy-nonadecyl)-sn-glycerol	LMGL01020065	Lipids and lipid-like molecules	Glycerolipids	Monoradylglycerols	*		38.8	0	M+NH4	C22H46O4	-1.803519204	1.289348633	0.002446772	0.015446665	0.244428393	1.841508189	32120.99978	38051.28543	31126.03928	31998.92343	33238.03663	39148.95359	36998.96283	38005.93986
5.63	549.1614m/z	549.1614471	5.628083333	neg	6-Hydroxy-5-methyl-3',4',5'-trimethoxyaurone-4-O-alpha-L-rhar	LMPK12130045	Unclassified	Unclassified	Unclassified			38.1	0	M+FA-H	C25H28O11	0.163713045	1.286973668	0.000220784	0.003417281	-1.603973008	0.328969786	2814.565484	8555.696006	2969.583068	2418.765915	3055.347469	8915.855254	7746.675546	9004.557217
4.34	194.0597m/z	194.0597414	4.3405	neg	Vanillin acetate	HMDB0029663	Benzenoids	Phenol esters		*		48.4	45.7	M+H+H2O, M+H	C10H10O4	-1.150508326	1.28677444	0.000396933	0.004423809	-0.344102555	0.523416934	3073.980498	9036.683098	3259.880006	3074.742961	3127.202842	7894.286567	9665.126567	9035.132632
8.50	446.2916m/z	446.2916218	8.503666667	neg	Myxalamid B	69330	Unclassified	Unclassified	Unclassified			38.7	0	M-H	C25H39NO3	1.058620684	1.286536268	0.000134715	0.002525704	-3.15282758	0.112435726	724.1831456	6440.863359	770.6315663	478.5215863	923.3962843	5692.331685	6788.951177	6841.307222
6.61	353.1015m/z	353.1014887	6.613233333	pos	Lunatone	HMDB0303339	Lipids and lipid-like molecules	Polyketides	Flavonoids			46.3	45.7	M+H+H2O	C20H18O7	-1.286080611	1.286175973	0.000601131	0.006245844	1.323507887	2.502739071	9612.576584	3840.822519	10726.10557	8981.315171	9130.309012	3532.208972	4161.958086	3828.300499
3.73	230.9970m/z	230.9969863	3.730516667	neg	2-[3-(sulfooxy)phenyl]acetic acid	HMDB0125163	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*		45.8	35.8	M-H	C8H8O6S	0.447414103	1.285600517	0.000301988	0.004123745	0.719468859	1.646576863	14611.70059	8873.986336	14551.17894	15005.91416	14278.00866	7992.768038	9314.650403	9314.540566
0.80	208.0324m/z	208.0303238	0.800366667	neg	D-Glucarate	3343	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	**	C00818	51.5	65	M-H	C6H10O8	0.157090788	1.282992831	0.000143723	0.002620058	0.183174418	2.904267798	26450637	8060.047412	8537.142454	9423.167381	2948.009426	2949.37664	3061.998644	
4.88	263.0514m/z	263.0514478	4.880083333	neg	bis(4-fluorophenyl)-Methanone	2735	Unclassified	Unclassified	Unclassified			38	0	M+FA-H	C13H8F2O	-4.936411042	1.279054057	7.80984E-05	0.001854977	0.396688061	1.316482242	23458.94485	17819.41609	22882.05325	23807.50721	23687.27411	18162.50135	17731.07027	17564.67666
4.19	401.0550m/z	401.0550234	4.189783333	neg	Shoyuflavone B	90052	Phenylpropanoids and polyketides	Isoflavonoids	Isoflav-2-enes	*		36.6	0	M-H	C19H14O10	8.969197928	1.276818606	0.001099159	0.009073763	-2.144979392	0.226098074	1675.73357	7411.534027	1513.906065	1557.946177	1955.348467	8696.903817	6451.826143	7085.872121
5.45	234.0773m/z	234.0773196	5.451166667	neg	Phensuximide	HMDB0014970	Organoheterocyclic compounds	Pyrrolidines	Phenylpyrrolidines		C07437	51.9	61.6	M+FA-H	C11H11NO2	0.730419645	1.276518023	0.002173991	0.014308847	-1.168402416	0.444913748	4648.486201	10448.0615	4756.75228	4451.621802	4737.084522	12079.96618	9478.218372	9785.999962
4.37	424.0983m/z	424.0804424	4.367166667	neg	4,5,7,3',4',5'-pentahydroxyflavanone	88586	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	*		36.5	0	M+FA-H, M-H	C15H12O7	-5.413688815	1.275103817	0.000181184	0.002609073	-5.613742328	0.326749667	2735.671955	8372.378703	3346.551067	2930.67648	8102.844702	8067.995925	8346.205464	
0.86	375.0527m/z	375.0527327	0.859583333	neg	4-(4-Deoxy-α-D-gluc-4-enuronosyl)-D-galacturonate	63148	Unclassified	Unclassified	Unclassified			38.3	0	M-H	C12H16O12	-1.885840125	1.275656845	0.000113285	0.002301931	1.281739543	2.431319589	9540.701161	3924.083533	9952.415573	9373.374441	9296.313471	4192.323189	4274.404849	3305.522561
8.99	471.2429m/z	471.2428607	8.9919	neg	Ursodeoxycholic acid 3-sulfate	LMST05020033	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	*		36.5	0	M-H	C24H40O7S	1.402782718	1.27496401	5.80912E-05	0.001570867	-1.290974715	0.408674827	3870.270026	9470.292206	4182.857705	3493.497512	3934.454861	9586.34119	9007.533502	9817.001924
7.06	146.0692n	145.0619439	0.757316667	pos	D-Glutamine	63630	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	**	C00819	53.3	72.9	M+H2O-H, M-H	C5H10N2O3	0.365818111	1.273328173	0.044442249	0.122999072	-0.349253799	0.784990011	24577.46595	31309.27222	21194.14233	24995.80934	27542.44618	28474.96522	32851.70613	32601.1453
5.32	259.0910m/z	259.0910099	5.3203133	neg	4-Hydroxy-5-methyl-3(2H)-thiophenone	88358	Organic acids and derivatives	Vinylogous thioesters	Vinylogous thioesters	*		38.3	0	2M-H	C5H6O2S	-1.248043897	1.273287381	0.014627167	0.054383506	2.580649121	1.149374638	43784.98059	47256.3576	44917.41371	48715.42329	47762.1213	40512.71609	40505.35193	40505.35193
4.86	507.1874m/z	507.1873764	4.858383333	neg	13-Hydroxy-5'-O-methylmelledonal	HMDB0035864	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids	**		40.6	9.88	M+FA-H	C24H30O9	0.413302039	1.271228296	1.45811E-05	0.00068802	-0.913567204	0.066358855	394.0234271	5937.767146	496.3915187	331.8233637	353.8553989	5775.864628	6360.53757	5676.89924
5.13	335.1352m/z	335.135191	5.132616667	neg	Trimethoprim	HMDB0014583	Benzenoids	Phenol ethers	Anisoles		C01965	39.4	5.83	M+FA-H	C14H18N4O3	-3.109926297	1.271019419	0.046170363	0.126482405	0.350287521	1.274814666	31191.18614	24467.23197	32577.62287	29635.47561	31360.45994	22063.65042	22487.2231	28850.82239
6.00	290.1780m/z	290.1780765	5.995733333	pos	Ibopamine	9617	Unclassified	Benzenoids	Phenol esters			36.6	0	M+H+H2O	C17H25NO4	0.978749927	1.271325844	4.53072E-05	0.001355489	-0.955365828	0.936389971	1513.19222	5163.107	1591.155869	1535.558063	5724.503231	5974.060769	5657.155499	6209.52783
3.42	303.0723m/z	303.0723312	3.417666667	pos	Lepidimoic acid	HMDB0041096	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates			45.1	28.8	M+H2O-H	C12H18O10	0.545075619	1.269679644	0.00039371	0.004827985	-0.234458491	0.850

5.87	795.1270m/z	795.1270139	5.866533333	neg	Sulfasalazine	2551	Organoheterocyclic compounds	Azobenzenes	Unclassified	C07316	37.3	0	2M-H	C18H14N4O5S	-3.379807415	1.217874187	0.003022641	0.017813228	-0.729152446	0.603258212	8095.574565	13419.7503	9057.436889	7579.36771	7649.919095	14008.29007	12073.24531	14177.71551
5.06	285.1346m/z	285.1345887	5.05975	neg	Imiquimod	HMDB0014862	Organoheterocyclic compounds	Quinolines and derivatives	Imidazoquinolines		42.7	22.6	M+FA-H	C14H16N4	-4.625256142	1.217710308	0.002576446	0.015968969	0.362896135	1.286004896	23778.09563	18489.8951	23441.85278	22973.04622	24919.38788	17746.646	18213.00309	19510.03622
5.73	229.0177m/z	229.017694	5.727283333	neg	Polystyrene sulfonate	HMDB0015435	Benzenoids	Benzene and substituted derivatives	Benzenesulfonic acids and derivatives		43.1	22	M+FA-H	C8H8O3S	0.412920682	1.217391409	0.00141653	0.010727516	-1.022556231	0.492243401	5069.740902	10299.25621	4965.2844	5422.727831	4821.210475	9029.767832	10788.94487	11079.05594
4.84	287.1503m/z	287.1502569	4.836566667	neg	Botrydiolpidin	HMDB0036594	Organoheterocyclic compounds	Tetrahydrofurans			45.1	30.3	2M-H	C7H12O3	0.849590032	1.216821568	0.001294489	0.010099655	0.531118888	1.445049475	16963.18316	11738.82518	17269.45194	16986.90653	16633.19101	19227.78465	12710.16655	10578.52434
2.38	234.9644m/z	234.9643764	2.382833333	neg	(6-(but-3-en-1-ynn-1-yl)-1,2-dithiin-3-yl)methanol	LMFA12000373	Lipids and lipid-like molecules	Fatty Acyls	Oxygenated hydrocarbons		38.6	9.64	4H-K	C9H8OS2	-2.237761004	1.216306468	9.23956E-05	0.002030008	0.326541678	0.003115023	15.93055879	5114.107054	0.001403199	30.58143876	17.2088344	4646.531935	5729.774411	4966.014814
2.03	433.1231m/z	433.123095	2.025516667	neg	Sulfinpyrazone sulfide	HMDB0060943	Organosulfur compounds	Thioethers	Aryl thioethers	*	43.4	29.9	M+FA-H	C23H20N2O2S	0.884269391	1.215633981	0.015376114	0.056490679	0.411571391	1.330133814	22741.38953	17097.06895	23903.75904	22302.21334	22018.1962	16270.80402	19573.90045	15446.50236
7.79	505.1493m/z	505.1492695	7.793283333	neg	Oxytetracycline	1690	Phenylpropanoids and polyketides	Tetracyclines	Unclassified	** C06624	36.8	0	M+FA-H	C22H24N2O9	6.272538687	1.212538149	0.03614155	0.10600717	0.291812057	1.224176906	32652.67621	26673.16795	35158.5846	31388.50158	31410.94245	23770.47811	28465.58397	27783.44178
7.67	464.3020m/z	464.3020225	7.66825	neg	Myxalamid S	69328	Unclassified	Unclassified	Unclassified		38.9	0	M+FA-H	C25H41NO4	0.622173203	1.212130405	0.000465933	0.005343919	-0.872977148	0.546018922	6153.336755	11269.45699	5943.513866	6099.477072	6417.019327	10346.72922	11604.05925	11857.5825
6.10	269.1011m/z	269.1011381	6.101666667	neg	Aspidinol	68482	Unclassified	Unclassified	Unclassified		37	0	M+FA-H	C12H16O4	-8.584401189	1.211132042	0.00094447	0.005338534	-0.579374477	0.669253889	10418.12791	15566.77979	10771.11884	10717.49673	10763.76803	14721.12146	15559.594	16419.62391
2.68	356.0963m/z	357.1035517	2.677116667	pos	2-O-beta-D-Glucopyranuronosyl-D-mannose	HMDB0039722	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		50.4	59	M+H, M+Na	C12H20O12	2.244245991	1.209819175	0.003077202	0.018011094	0.418499241	1.336536504	20816.5167	15574.97056	21207.66929	20457.13572	20784.7181	14237.68493	15512.06463	16975.16247
11.10	762.5992m/z	762.5992092	11.09875	pos	PA(15:0/24:1(15Z))	HMDB0114832	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphates		37	0	M+NH4	C42H81O8P	-2.044788002	1.20960278	0.041242973	0.11643646	-1.931270658	0.262198137	2144.987651	8180.789048	2681.324923	1648.360745	2105.277286	11988.76615	7402.381136	5151.219858
5.65	349.1506m/z	349.1506209	5.650916667	neg	(2S)-2-Butanol-O-(b-D-Apiofuranosyl-(1->6)-b-D-glucopyranos	HMDB0041255	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		40.1	5.7	M+H2O+H	C15H26O10	0.583663595	1.208445201	0.002356421	0.013194723	0.657583976	1.573437753	14325.92191	9081.766863	15264.1902	13833.40303	13880.1825	10089.76107	7704.842071	9450.697443
7.71	413.1776m/z	413.1775831	7.709666667	neg	2,2-Dimethyl-3,4-bis(4-methoxyphenyl)-2H-1-benzopyran-7-ol	70521	Unclassified	Unclassified	Unclassified		36.1	0	M+H+H2O	C27H26O5	6.619177786	1.208253081	0.011319374	0.0451576	0.548481916	1.462545816	17322.43536	11844.02921	18971.26285	16963.71669	16032.32654	10355.97704	13392.63622	11783.47438
0.80	132.0766m/z	132.0766282	0.796983333	pos	Creatine	7	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	** C00300	49.5	50.2	4H-H	C4H9N3O2	-0.951640491	1.208113	0.00094431	0.008338534	0.42799512	1.345362658	19957.83627	14834.54008	19837.2739	19554.77633	20481.45859	13864.75299	15635.49196	15003.37529
3.26	117.0557m/z	117.0557621	2.36465	neg	5-hydroxy valeric acid	LMFA01050010	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates		42.5	14.4	M-H	C5H10O3	0.375457352	1.208040317	0.005917794	0.028309846	0.257811238	1.195663346	32597.77458	27263.33854	33137.30578	33150.52009	31505.49787	25613.33167	28322.65648	27854.02745
7.12	448.3073m/z	448.3072583	7.719166667	neg	N-Palmitoyl phenylalanine	HMDB0062339	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues		38.5	0	M+FA-H	C25H41NO3	1.012291964	1.207779171	0.000103561	0.002179944	-1.169434902	0.261277736	1779.955294	6812.502757	1810.272033	1643.238309	1886.35554	6191.968788	6996.972017	7248.567466
6.79	1017.3157m/z	1017.31573	6.7874	neg	Alpha-cyclodextrin	85154	Unclassified	Unclassified	Unclassified		37.4	0	M+FA-H	C36H60O30	0.603520953	1.204349741	0.001222933	0.009750357	-2.288391139	0.204703668	1314.955151	6423.700962	1503.053586	556.1360861	1885.675781	5524.538	7187.360109	6559.204779
3.91	298.0966m/z	298.0965629	3.911966667	pos	5'-Deoxy-5'-<WBR>(methylthio)adenosine	3425	Unclassified	Unclassified	Unclassified	*	55.8	85.4	4H+H	C11H15N5O3S	-0.921931563	1.203999756	6.86813E-05	0.001720966	0.504474685	1.418606718	16922.45053	11928.92315	17129.18297	16897.58646	16740.58216	11420.00624	12336.72299	12030.04024
0.88	203.0370m/z	203.0369904	0.884633333	neg	1,4-Dihydroxy-2-naphthoic acid	64746	Unclassified	Unclassified	Unclassified		38.1	10.8	M-H	C11H8O4	9.841692217	1.203966058	0.04232896	0.118518839	1.070493574	2.100151747	11428.21602	5441.614416	13420.18121	7934.351427	12930.11544	3630.452589	7214.030357	5480.360303
6.57	213.1134m/z	213.113397	6.570233333	neg	2,2'-(3-methylcyclohexane-1,1-diyl)diacetic acid	96295	Unclassified	Unclassified	Unclassified		53.9	72.9	M-H	C11H18O4	0.767727971	1.203905282	0.002023828	0.013664078	0.397403966	1.317135679	21404.91472	16251.10842	21589.77248	21428.56889	21196.40279	15225.63365	17618.62179	15909.09897
11.64	836.5411m/z	836.5410674	11.63681667	pos	PS(18:2(9Z,12Z)/20:1(11Z))	LMGP03010357	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoserines	*	36.9	0	M+Na	C44H80NO10P	-0.169210232	1.202969412	0.031550007	0.095569832	-0.592226764	0.663318301	11471.02975	17293.40158	11145.59927	11199.18366	12068.30633	20768.78114	14975.85377	16135.56982
0.86	310.1504m/z	349.1099533	0.859583333	pos	Demethylcitalopram	1782	Unclassified	Unclassified	Unclassified		36.5	0	M+Na, M+K	C19H19FN2O	7.157139146	1.200961046	0.03802133	0.109945968	-0.183555835	0.880530062	43437.56243	49331.1521	43590.32981	43398.1317	43324.22579	45525.04377	51796.8391	50671.57343
8.95	406.2720n	405.2647708	8.953233333	neg	3,7-Dihydroxy-12-oxocholanoic acid	5389	Lipids and lipid-like molecules	Steroids and steroid derivatives	Bile acids, alcohols and derivatives	*	38.5	0	M-H, M+FA-H	C24H38O5	0.302543695	1.200679965	0.000947181	0.003348491	-1.976778411	0.254056554	1723.957582	6785.7237	1547.461816	1840.643985	1783.766944	6007.737745	6446.905543	7902.527812
1.52	182.0671m/z	182.0670978	1.52285	pos	S-2-Propyl-L-cysteine	HMDB0037541	Organic acids and derivatives	Thiosulfinic acid esters	Thiosulfinic acid esters		39.3	11.3	M+H	C6H13O2S2	1.801170665	1.200535984	0.00200575	0.013585512	0.310074697	1.239772121	28464.30418	21346.10264	27180.84866	26206.53308	26005.53301	20205.59229	22314.99545	21517.72317
4.41	376.1375n	377.1447796	4.4062	pos	(1x,2x)-Guaiacylglycerol 2-glucoside	89157	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates		38.5	0	M+H, M+Na	C16H24O10	1.478803959	1.199108076	0.017570459	0.062326963	0.385134224	1.305981286	23580.12416	18055.48396	25417.2772	22076.20222	23246.89305	16124.61769	19617.50579	18424.32842
3.00	279.0987m/z	279.0987252	3.004583333	neg	S-4-Hydroxymephenytoin	HMDB0013894	Organoheterocyclic compounds	Azolidines	Imidazolidines	*	40.7	6.52	M+FA-H	C12H14N2O3	0.341912658	1.198742882	0.000335479	0.004526766	0.313492057	1.242712059	25587.87328	20590.34762	25586.97184	26098.37942	25078.26859	20395.04877	21236.99526	20138.99882
0.84	182.0809m/z	182.0809224	0.859583333	pos	Propetamphos	36	Organoheterocyclic compounds	Benzofurans	Unclassified		41.4	14.3	M+H, M+Na	C10H15O3P	1.198712355	1.198712355	0.000738439	0.007188822	0.36532258	1.288186626	22465.57744	17439.92172	23467.23389	22071.98434	21882.45411	17054.15173	18473.56373	17588.06027
8.33	413.2183m/z	413.2182569	8.3263	neg	6,15-Diketo,13,14-dihydro-PGF1a	HMDB0001979	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids	*	38.7	0	M+FA-H	C20H32O6	0.448977352	1.197764079	0.000658674	0.006640461	-0.791849483	0.577603151	6857.329777	11872.04358	7493.718814	6397.515763	6680.754754	11063.10248	12342.73916	12210.28911
5.41	609.0885m/z	609.0885189	5.406433333	neg	EPIGALLOCATECHIN 3,5-DIGALLATE	43930	Unclassified	Unclassified	Unclassified		36.8	0	M-H	C29H22O15	-0.122388192	1.197584944	0.006133625	0.029019836	0.439455414	1.356092336	20004.32683	14751.44893	20061.4945	21260.3982	18691.0878	15738.16081	15017.32826	13498.85772
7.04	271.1553m/z	271.1552843	7.044716667	neg	Riesling acetal	HMDB0037562	Organoheterocyclic compounds	Tetrahydrofurans	Unclassified		52.2	64.6	M+FA-H	C13H22O3	0.826385665	1.197435269	0.000536209	0.005844137	0.82186019	1.767617587	11519.78617	6517.125793	12025.88408	11795.99898	10737.47544	6477.273938	7046.356413	6027.747028
5.12	699.1087m/z	699.1087127	5.122166667	neg	Tricetin 7,3'-diglucuronide	49271	Lipids and lipid-like molecules	Polyketides	Flavonoids		36.3	0	M+FA-H	C27H26O19	5.627850371	1.194215781	0.013555748	0.046289729	0.725257534	1.531015813	15724.39152	16039.9602	15389.5806	13002.1666	19603.07406	18202.66209	21339.23884	25671
3.96	319.1037m/z	319.1037371	3.957583333	neg	Dikegulac	72590	Unclassified	Unclassified	Unclassified		38.3	0	M-H	C12H18O7	1.026300009	1.194210122	0.000607882	0.006300462	0.59370746	1.509119929	14749.26101	9773.418748	15242.32337	13958.63264	15046.82701	9146.635813	10064.40244	10109.21799
4.59	302.1959m/z	302.1958736	4.58805	pos	3-hydroxy-cis-5-octenoylcarnitine	LMFA07070038	Lipids and lipid-like molecules	Fatty Acyls	Fatty esters		48.1	45.8	M+H	C15H27NO5	-1.081648226	1.193037441	0.000421416	0.00501538	0.38754527	1.308165679	21023.1509	16070.70972	21203.18609	21520.38022	20345.8864	15585.37258	16015.88582	16610.87077
5.38	455.1542m/z	455.1542348	5.384216667	neg	XANTHYLETIN	43779	Unclassified	Unclassified	Unclassified		37.3	0	2M-H	C14H12O3	9.257316685	1.192487454	0.004031647	0.021637529	0.468822164	1.401412981	17936.80571	12799.08632	16930.64057	19492.71217	17387.06438	13361.10975	12142.83386	12893.31535
4.07	302.1959m/z	302.195893	4.069166667	neg	TEGASEROD	44186	Unclassified	Unclassified	Unclassified		37.8	1.44	4H+H	C16H23N5O	-5.457882695	1.190828205	0.000226939	0.002437549	0.567473295	1.484564554	15100.96565	12190.05627	15304.16654	14676.44255	15236.34154	9568.861481	10654.77136	10867.06023
5.60	401.0808m/z	401.0807569	5.602	neg	4-Phospho-N-pantothenoylcysteine	6014	Unclassified	Unclassified	Unclassified		36.9	0	4H-K	C12H23N2O9PS	4.58948913	1.19071219	5.22855E-05	0.001493097	1.274753974	2.419575528	8316.727101	3437.266994	8607.128389	8179.006848	8164.046066	3657.091201	3664.102896	2990.606885
3.87	304.1749m/z	304.1749189	3.866916667	pos	Pimelylcarnitine	HMDB0013328	Lipids and lipid-like molecules	Fatty Acyls	Fatty acid esters	*	46.8	42.8	M+H	C14H25NO6	-1.798022332	1.190372494	0.001873767	0.012978922	0.55512261	1.469233499	15744.76384	10715.87389	16111.68299	16439.63819	14682.97033	9861.369701	11207.87064	11078.38132
8.52	531.1828m/z	531.1827831	8.5245	neg	METHOXYVONE	43575	Unclassified	Unclassified	Unclassified		38.7	0	2M-H	C17H14O3	2.763807278	1.190213197	0.003119972	0.018184063	-0.848731185	0.55527287	6341.526484	11420.55884	6583.29755	5679.334359	6761.947544	10023.81127	12449.03713	11788.82811
2.86	254.1400m/z	254.1399531	3.4	neg	3,4-DMMA	96606	Unclassified	Unclassified	Unclassified		38.9	0	M+FA-H	C12H19NO2	0.819571722	1.190060564	0.000104234	0.001167722	-0.759861106	0.590553183	9744.933797	13937.66104	9837.480243	9680.310919	9222.574857	11484.83882	11949.56571	11693.25671
0.78	262.1045m/z	262.1045042	0.778533333	neg	Glutaminylalanine	HMDB0028790	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	42.6	13.4	M+FA-H	C8H15N3O4	0.2087009	1.188406313	0.028749659	0.089330213	-0.224530102	0.855873746	33357.45353	38974.73628	33332.68748	34316.4667	32423.20641	36073.10287	41547.19616	39303.90981
6.93	419.1927m/z	419.1926995	6.926366667	neg	2,6-Dihydroxypseudooxynicotine	63863	Unclassified	Unclassified	Unclassified		38.7	0	2M-H	C10H14N2O3	-2.162552461	1.187443757	0.001262547	0.009932667	0.950065018	1.931959724	10297.28539	5329.968973	11052.38308	10254.41658	9585.056499	4445.3498	5732.687774	5811.869346
5.98	369.1519m/z	369.151077	5.9826	neg	Phenylacetyl-L-Gln-glucoside	HMDB0031956	Lipids and lipid-like molecules	Fatty Acyls	Fatty acyl glycosides	*	45.4	32.7	M-H2O-H	C19H26N2O10	0.957430843	1.185711663	0.005485578	0.026888843	0.391570723	1.518220853	21575.50083	16446.9722	21853.19883	22761.50323	19273.16547	15457.39847	17209.09782	16774.94921
6.22	311.1503m/z	311.150333	6.215	neg	Humulinic acid A	86723	Organic acids and derivatives	Carboxylic acids and derivatives	Vinylogous acids	*	38.9	0	M+FA-H	C15H22O4	1.194630627	1.184811653	4.24322E-05	0.001297999	0.721560998	1.648965252	12259.39736	7434.600178	12596.23474	11927.63169	12254.32566	7267.937898	7283.906305	7751.956332
7.74	341.1972m/z	341.197192	7.738233333	neg	(1(10)E,4a,5E)-1(10),5-Germacradiene-12-acetoxy-4,11-diol	HMDB0038798	Lipids and lipid-like molecules	Prenol lipids	Sesquiterpenoids		38.5	0	M+FA-H	C17H28O4	0.775629711	1.184406509	5.52888E-05	0.001532394	1.491960736	2.812709849	7492.65843	2663.857572	7732.665726	7752.401477	6992.908087	2473.899821	2765.257829	2752.415067
6.63	387.1280m/z	387.1279551	6.63275	neg	Sphalleroside A	88694	Organic oxygen compounds	Carbohydrates and carbohydrate conjugates			37.4	0	M+FA-H	C16H22O8	-5.0140377	1.18406553	0.000425879	0.005049268	-1.564059318	0.338198152	2492.761483	7370.712904	2598.696943	2637.881618	2241.705887	6508.828838	7683.540085	7919.769789
4.45	497.1835m/z	497.1835056	4.451833333	neg	4'-Hydroxyverdilid	HMDB0013947	Organoheterocyclic compounds	Indoles and derivatives	Carbazoles		43.6	29.5	M+FA-H	C28H26N2O5	2.855778185	1.184213829	0.015405158	0.056570354	0.465527592	1.722406187	14284.42458	11978.7111	14615.59289	14584.92453	13902.05322	11819.38336	17586.06023	16485.56877
1.44	216.0337m/z	216.0336879	1.43735	neg	o-Toluenesulfamide	3056	Unclassified	Unclassified	Unclassified		39.1	0	M+FA-H	C7H9NO2S	0.500031566	1.181725267	0.000210586	0.003304822	1.469577219	2.769407244	7560.366604	2729.958413	8245.800842	7052.671777	7382.627193	2903.206578	2498.621036	2788.047626
4.30	245.0126m/z	245.0126071	4.300033333	neg	3-(4-(sulfooxy)phenyl)propanoic acid	HMDB0013048	Organic acids and derivatives	Organic sulfuric acids and derivatives	Arylsulfates	*	43.1	21.3	M-H	C9H10O6S	0.302987616	1.181178341	0.000199631	0.003201993	-1.844421525	0.278467039	1862.386368	6687.99574	1973.361287	2136.973261	1876.824555	6154.28584	7235.97294	6673.728439
0.72	781.3539m/z	781.3539179	0.717716667	pos	PA-PI	LMGP20050013	Lipids and lipid-like molecules	Glycerophospholipids	Oxidized glycerophospholipids		36.1	0	M+K	C34H63O15P	0.406565531	1.180758949	0.001370072	0.010474386	-1.094480979	0.468304862	4329.623771	9245.310319	3276.752417	4320.400015	5391.71888	9205.60057	9448.967699	9081.362688
5.78	455.2246m/z	455.2245885	5.795833333	neg	Lischenone a14	52796	Lipids and lipid-like molecules	Polyketides	Flavonoids		36.1	0	M+H+H2O	C30H32O7	1.196845805	1.179947888	0.004450337	0.017394788	0.424632686	1.326068159	3507.582054	8688.003519	3505.024435	3717.341262	3926.643373	8936.853359	8956.437036	8777.027902
8.07	463.2235m/z	463.2234806	8.056183333	neg	1-(4Z,7Z,10Z,13Z,16Z,19Z-docosahexaenoyl)-glycero-3-phosp	HMDB0062307	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphates	*	36.1	0	M-H2O-H	C25H39O7P	-4.185735282	1.180103783	0.000545139	0.005899478	-2.479559727	0.179299115	1060.732449	5959.153775	1131.007758	1147.333441	903.8561474	4971.415413	6480.320187	6296.245726
6.22	307.1624m/z	307.1623976	6.216316667	neg	Citalopram	1781	Unclassified	Benzenoids	Benzene and substituted derivatives	Phenylbutylamines	** C07572	36.6	0	M+H-H2O	C20H21FN2O	5.843827026	1.179393279	0.00070996	0.006949515	0.660263618	1.580371372	13250.47782	8384.407648	13149.21453	12986.41197	13615.80695	7475.380437	9113.20359	8564.639016
7.71	433.2086m/z	433.2083725	7.703333333	neg	zwthl 10,12,13,15-bisezidoxy-16-hydroperoxy-8E-octadecen-1	LMFA01040052	Lipids and lipid-like molecules	Fatty Acyls	Fatty Acids and Conjugates		38.4	0	M+FA-H	C19H32O8	1.163535886	1.178901247	0.000793276	0.004164276	0.397157387	1.210950857	8894.216113	6426.427687	8763.010596	9836.126207	9263.451768	3984.837133	3782.647477	3566.842081
4.43	329.0879m/z	329.0878723	4.432683333	neg	2-O-Benzoyl-D-glucose	HMDB0034618	Organic acids and derivatives	Carboxylic acids and derivatives	Organooxygen compounds		38.6	0	M+FA-H	C13H16O7	0.234310818	1.178668875	0.000747911	0.0071705	-2.271552696	0.207106868	1269.15843	6128.036408	1342.890537	1334.826466	1129.758287	5145.667985	6907.067279	6331.373961
6.74	343.2128m/z	343.2127844	6.739933333	neg	(4R,6S)-4-Hydroxy-1,7-dioxaspiro[5.5]undecane	102846	Unclassified	Unclassified	Unclassified		38.9	0	2M-H	C9H16O3	0.499908333	1.177291201	0.000382149	0.004735774	0.885550058	1.847468874	10507.12859	5687.31021	11033.10175	10565.06564	9923.218372	5224.024221	6235.031968	5602.87444
12.98	771.5133m/z	771.513332	12.98333333	pos	PG(16:0/18:1(9Z))	LMGP04010987	Lipids and lipid-like molecules	Glycerophospholipids	Glycerophosphoglycerols	*	37.7	0	M+Na	C40H77O10P	-1.784803762	1.176106651	0.009594221	0.040127125	-3.275604896	0.103262984	592.4064831	5736.871607	683.1523112	606.9553631	487.1117751	7474.07942	6044.717299	3691.818101
3.79	246.1291m/z	247.1284581	3.781333333	neg	L-beta-aspartyl-L-leucine	62015	Organic acids and derivatives	Peptidomimetics	Peptidomimetics	*	54.1	75.8	M+H, M+Na	C10H18N2O5	-1.584539662	1.175665935	0.002965962	0.017636895	0.544153162	1.351117891	19046.32261	14076.71409	19972.52946	18541.08408	18625.3543	12981.33145	15054.35956	14201.44327
4.54	270.1097m/z	293.0902045	4.542216667	pos	Idebenone Metabolite (Benzenebutanoic acid, 2,5-dihydroxy-3	773	Unclassified	Unclassified	Unclassified		43	20.1	M+H, M+Na, M+H-H2O	C13H18O6	-2.298435489	1.173375344	0.003328099	0.018997634	-0.63383341	0.644461728	8956.813385	13898.13079	9655.492601	8758.035654	8456.9119	12796.96979	15205.65334	13691.76925
5.01	484.0621n	483.0547804	5.014716667	neg	alpha,beta-Dihydroxyethyl-TPP	69564	Unclassified	Unclassified	Unclassified		36.3	0	M-H, M+FA-H	C14H22N4O9P2S	7.817872346	1.172252086	0.001136509	0.009258881	2.089227988	4.254318331	6327.410177	1487.291191	5271.253033	6989.456345	6721.521154	1798.401701	1625.774199	1037.697673
7.92	511.2268m/z	511.2267769	7.915266667	neg	Prednicarbate	43380	Lipids and lipid-like molecules	Steroids and steroid derivatives	Prenone steroids		37.1	0	M+Na	C27H36O8	-7.090631562	1.171822216	0.018918475	0.06570533	0.288376124	1.221264866	29274.64513	23970.75847	30899.30023	27474.51216	29450.123	22767.59941	25902.24368	23242.43232
4.90	323.1327m/z	323.1327131	4.902316667	neg	L-phenylalanyl-L-hydroxyproline	62023	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	37.8	0	M+FA-H	C14H18N2O4	-7.771904806	1.170495423	3.38497E-05	0.001127896	0.638532743	1.558745105	13165.65143	8457.165781	13326.84283	13019.43031	8053.016992	8544.470382	8777.977902
5.81	422.1799m/z	422.1799495	5.806016667	neg	Deaminohydroxyblasticidin S	66067	Unclassified	Unclassified	Unclassified		38.4	0	M-H	C17H25N7O6	1.404523469	1.170478775	0.002774838	0.016803584	0.702583352	1.627416307	12703.03851	7805.647799	13843.11414	12882.40845	11383.59295	8211.167614	7682.677764	7523.098019
5.31	385.1464m/z	385.1464085	5.30655	neg	Ritodrine sulfate 2	2360	Unclassified	Unclassified	Unclassified		36	0	M+NH4	C17H21NO6S	9.873387146	1.168935964	0.014818003	0.054937829	0.164394146	1.120695348	48378.34145	43168.14695	48807.76914	49305.00864	47022.24658	41456.56823	45119.21609	42928.65653
5.91	325.1066m/z	325.1066288	5.9112	pos	2,3-Dehydro-UWM6	72459	Unclassified	Unclassified	Unclassified		51.6	63.5	M+H	C19H16O5	-1.299881117	1.168471367	2.80706E-06	0.000390983	1.83982622	3.576673091	6490.529695	1814.683581	6660.826379	6422.533765	6388.229659	1695.045494	1764.112154	1984.893173
6.55	525.1570m/z	525.1569805	6.548566667	neg	Bleistirene S	68197	Unclassified	Unclassified	Unclassified		36.9	0	M+Na	C30H26O6	3.101336176	1.168212389	0.001520107	0.011241455	0.58600853	1.501087973	14469.21339	9115.150836	15177.87729	13862.07001	9128.250775	14367.69288	18629.94525	16925.5917
6.39	571.1800m/z	571.1799639	6.386066667	neg	Physalin A	HMDB0033773	Lipids and lipid-like molecules	Prenol lipids	Triterpenoids	*	37.1	0	M+FA-H	C28H30O10	-4.059580302	1.16782023	5.80704E-05	0.001570867	-1.622954924	0.324669795	2256.355047	6949.691919	2013.929089	2578.358625	2176.777429	7355.216724	6745.262244	6748.59679
1.20	365.1735m/z	365.1735368	1.199716667	pos	2,3-dinor-11b-PGF2alpha	LMFA03010011	Lipids and lipid-like molecules	Fatty Acyls	Eicosanoids		39.5	7.54	M+K	C18H30O5	3.233090774	1.166304886	0.035680564	0.104990855	0.553841373	1.467989219	17344.20741	11814.94195	19167.95502	15356.76095	17507.96625	9614.247619	14386.84115	11443.73708
5.22	687.1669m/z	687.0350416	5.197033333	neg	Vanillic acid	HMDB0000484	Benzenoids	Benzene and substituted derivatives	Benzoic acids and derivatives	** C06672	58.7	96.5	M-H	C8H8O4	0.352840148	1.166124566	0.000351103	0.001305103	0.155468629	0.231671671	5864.467866	5249.742076	568.7683145	5061.884982	512.8364555	686.763145	5061.884982	5477.13965
5.19	203.0493m/z	203.0493028	5.193566667	neg	AMCC	69065	Organic acids and derivatives	Carboxylic acids and derivatives	Amino acids, peptides, and analogues	*	C11490	37.8	0	M+H+H2O	C7H12N2O4S	3.695209117	1.16432448	2.39935E-06	0.000293302	21.65806916	3309241.516	4643.525208	0.001403199	4457.608491	4613.729071	4859.238062	0.001403199	0.001403199	0.001403199
3.58	332.0736m/z	332.0736384	3.582033333	pos	N-Acetylmuramic acid	3421	Organic oxygen compounds	Organooxygen compounds	Carbohydrates and carbohydrate conjugates	** C02713	39	0	M+H	C11H19NO8	-2.000182332	1.164261155	0.000101412

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