

Supplementary file

DATA AVAILABILITY

The data supporting this research are available from the following links:

1. PubChem (<https://pubchem.ncbi.nlm.nih.gov/> accessed on January 10, 2026)
2. ADMETlab3.0 (<https://admetlab3.scbdd.com/> accessed on January 10, 2026)
3. ProTox3.0 (<https://tox.charite.de/> accessed on January 10, 2026)
4. SwissTargetPrediction (<https://swisstargetprediction.ch/> accessed on January 10, 2026)
5. Super Pred (prediction.charite.de/ accessed on January 10, 2026)
6. SEA Search Server (<https://sea.bkslab.org/> accessed on January 10, 2026)
7. ChEMBL (<https://www.ebi.ac.uk/chembl/> accessed on January 10, 2026)
8. GeneCards (<https://www.genecards.org/> accessed on January 11, 2026)
9. OMIM (<https://www.omim.org/> accessed on January 11, 2026)
10. Venny (<https://bioinfogp.cnb.csic.es/tools/venny/> accessed on January 11, 2026)
11. STRING (<https://cn.string-db.org/> accessed on January 11, 2026)
12. DAVID (<https://davidbioinformatics.nih.gov/> accessed on January 11, 2026)
13. The microbiome visualization cloud platform
14. RCSB PDB (<https://www.rcsb.org/pages/about-us/index/> accessed on January 12, 2026)
15. GAWs (<https://gwas.mrcieu.ac.uk/> accessed on January 13, 2026)
16. eQTL (<https://www.eqtlgen.org/> accessed on January 13, 2026)
17. GTEX (<https://gtexportal.org/> accessed on January 13, 2026)

Figure 1. Research workflow of integrative analysis for nicotine-depression molecular mechanism based on network toxicology, molecular docking and Mendelian randomization

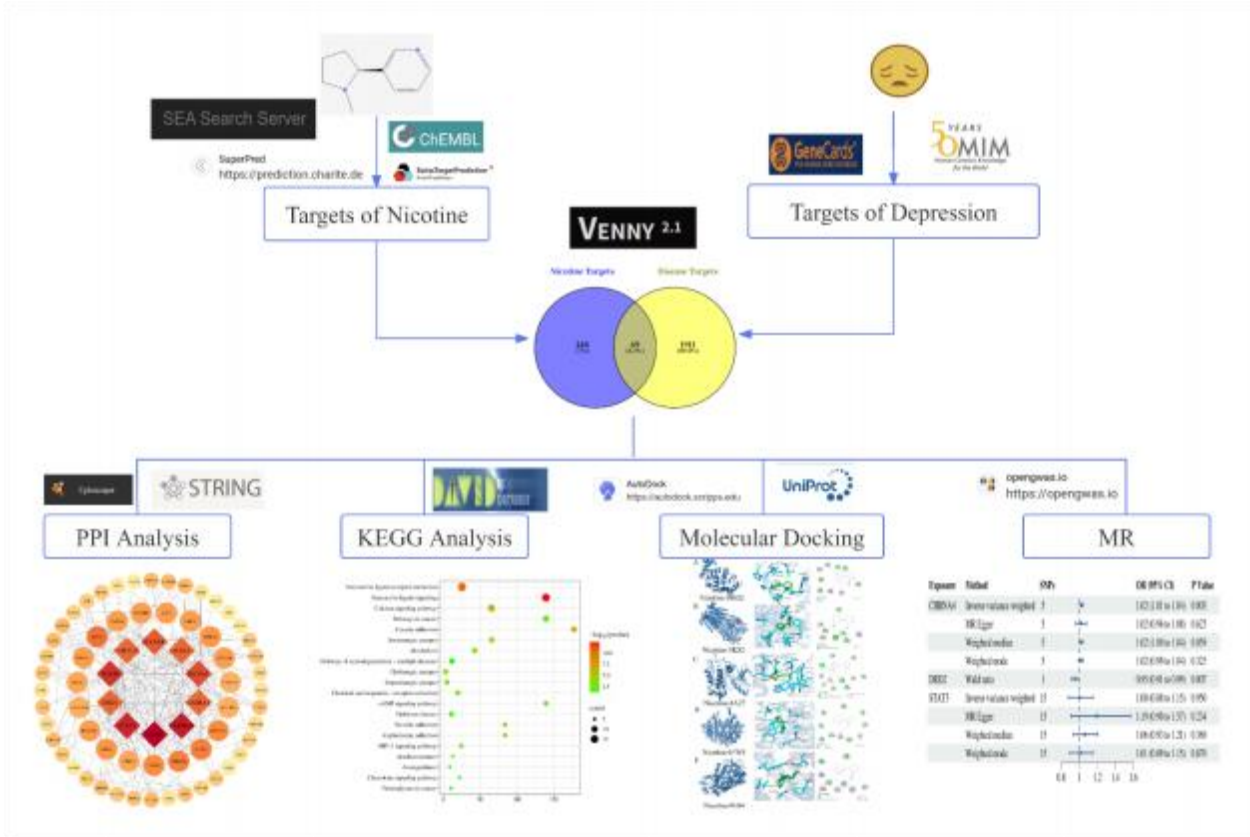


Figure 2. Potential toxic effect distribution of nicotine from in silico analysis based on ADMETlab 3.0 and ProTox3.0 databases

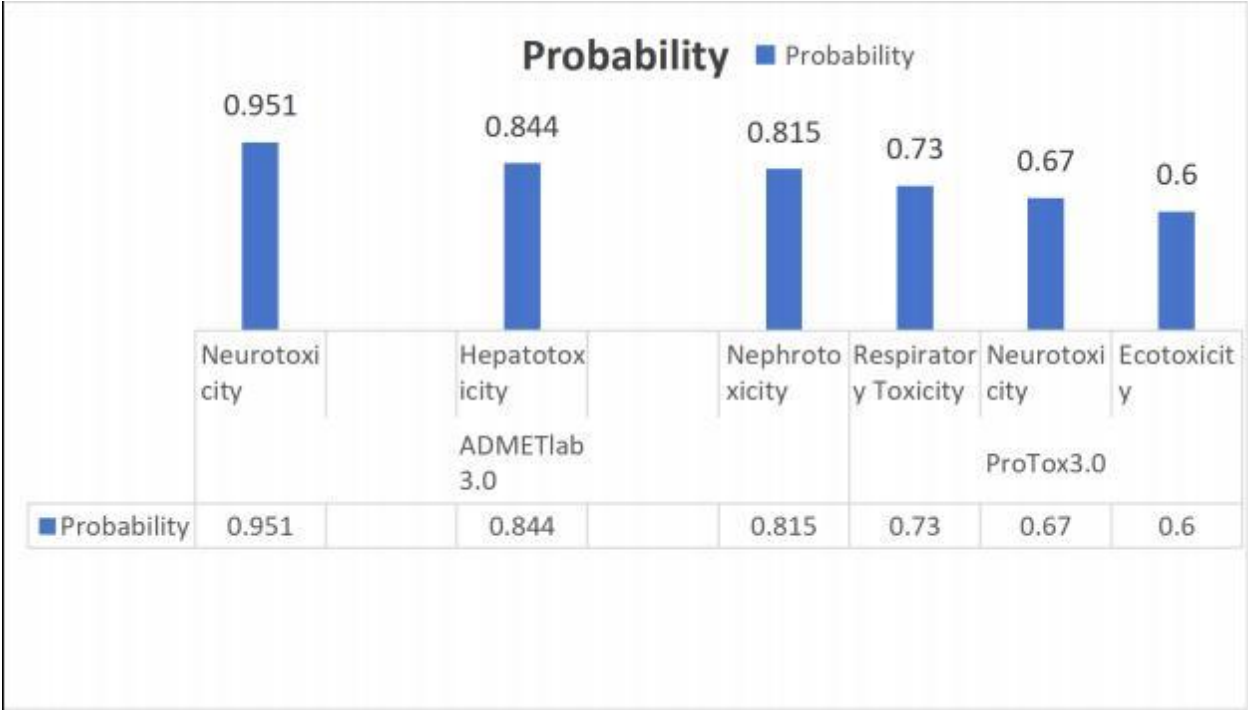
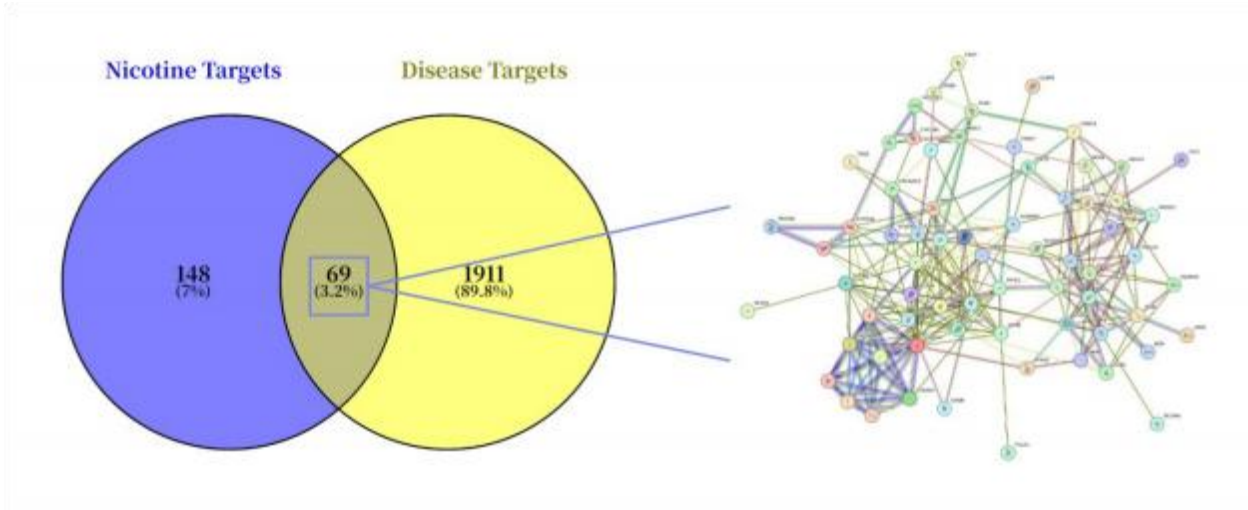


Figure 3. Venn diagram of overlapping targets between nicotine-related genes and depression-related genes



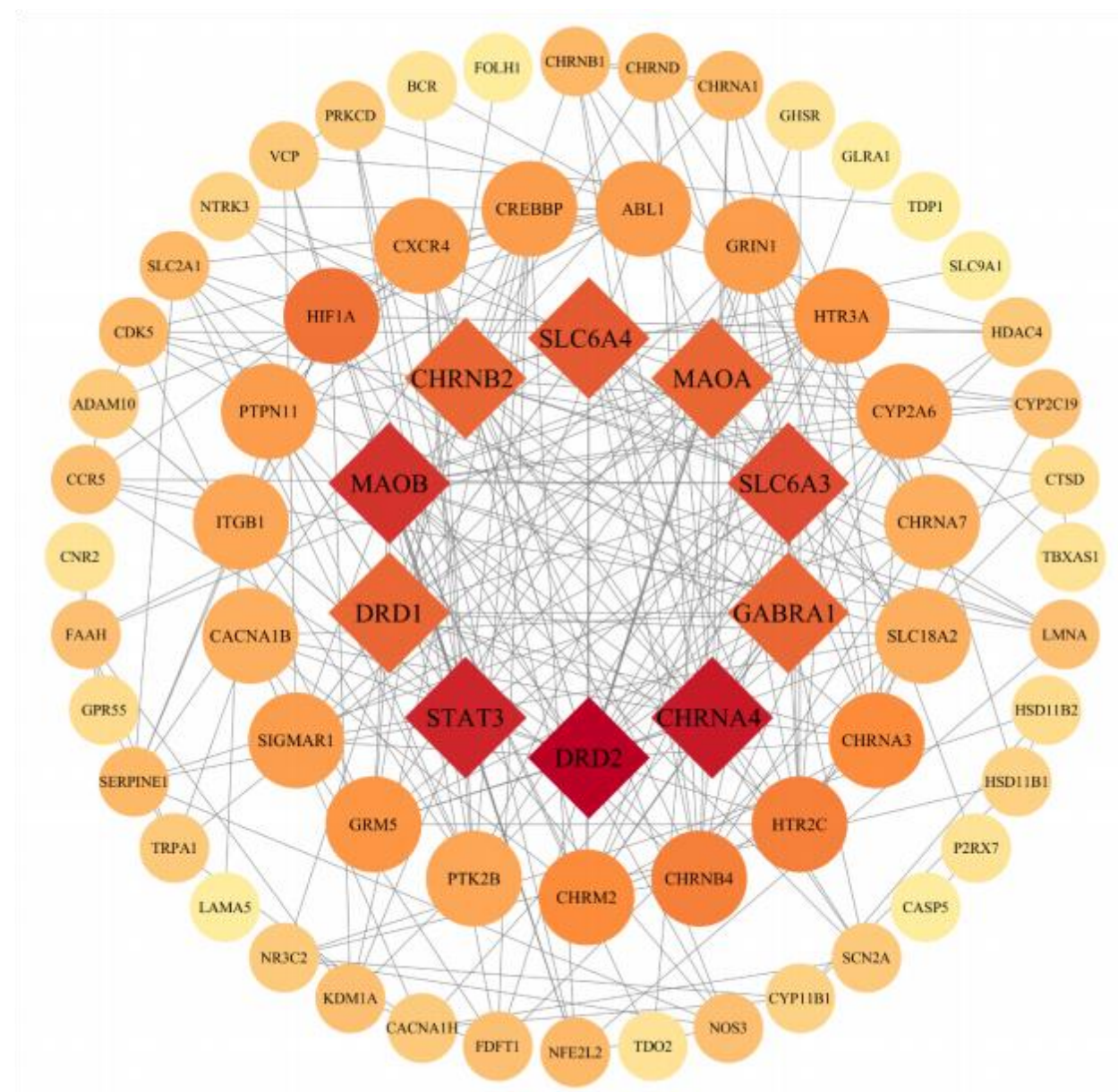


Figure 5. Top 10 core target nodes in nicotine-depression PPI network

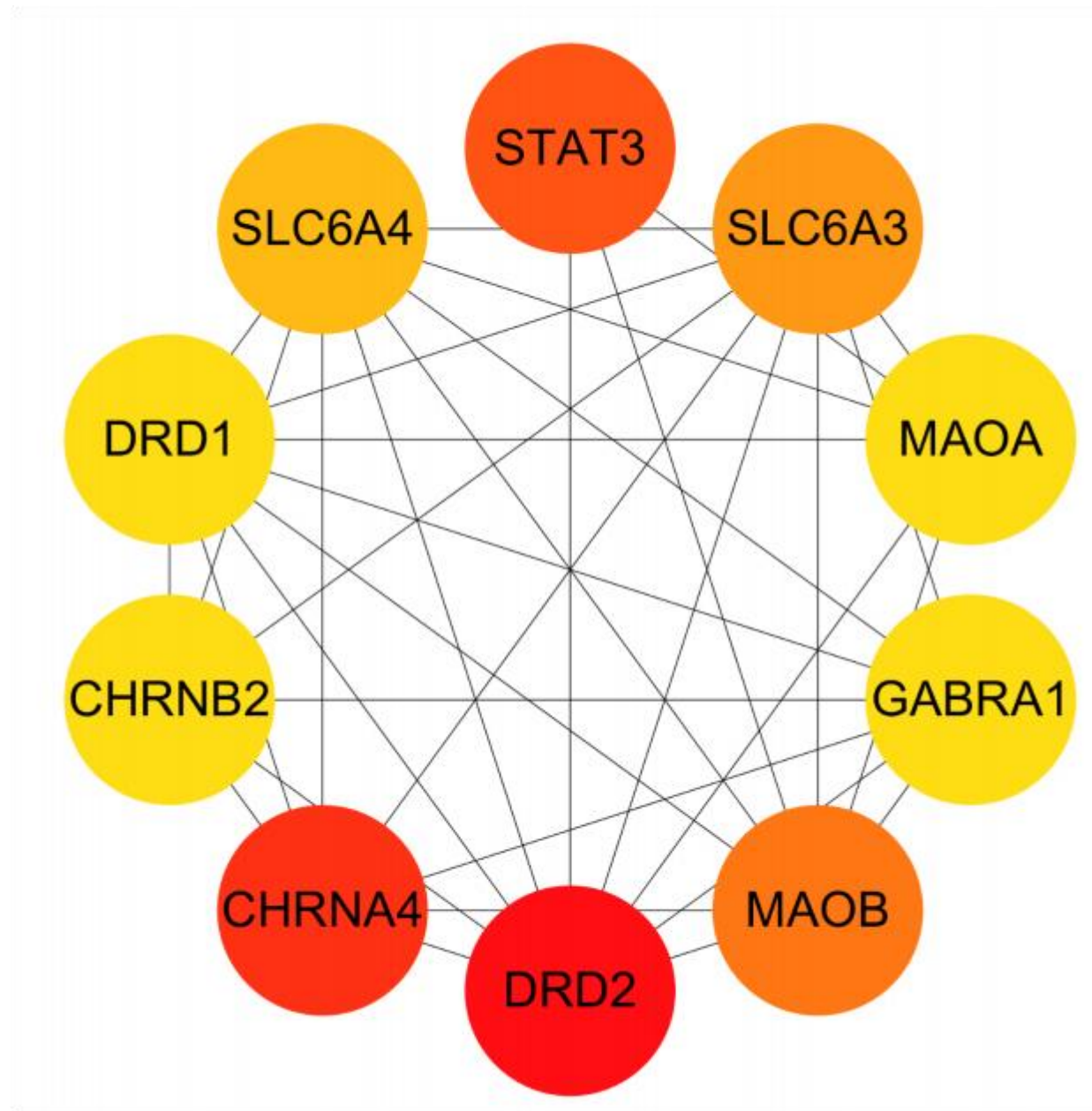


Figure 6. GO functional enrichment and KEGG pathway enrichment analysis results of nicotine-depression overlapping targets

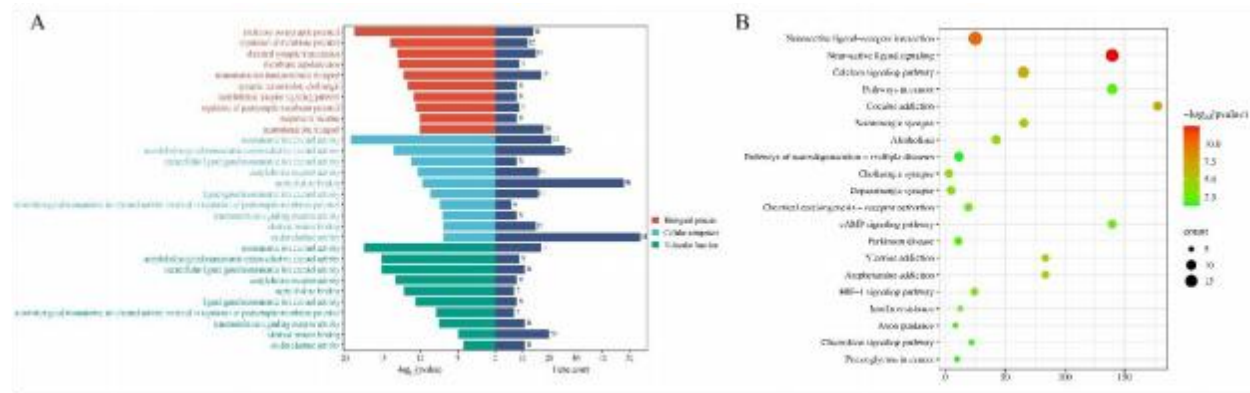


Figure 7. 2D and 3D molecular docking binding maps of nicotine with depression core targets

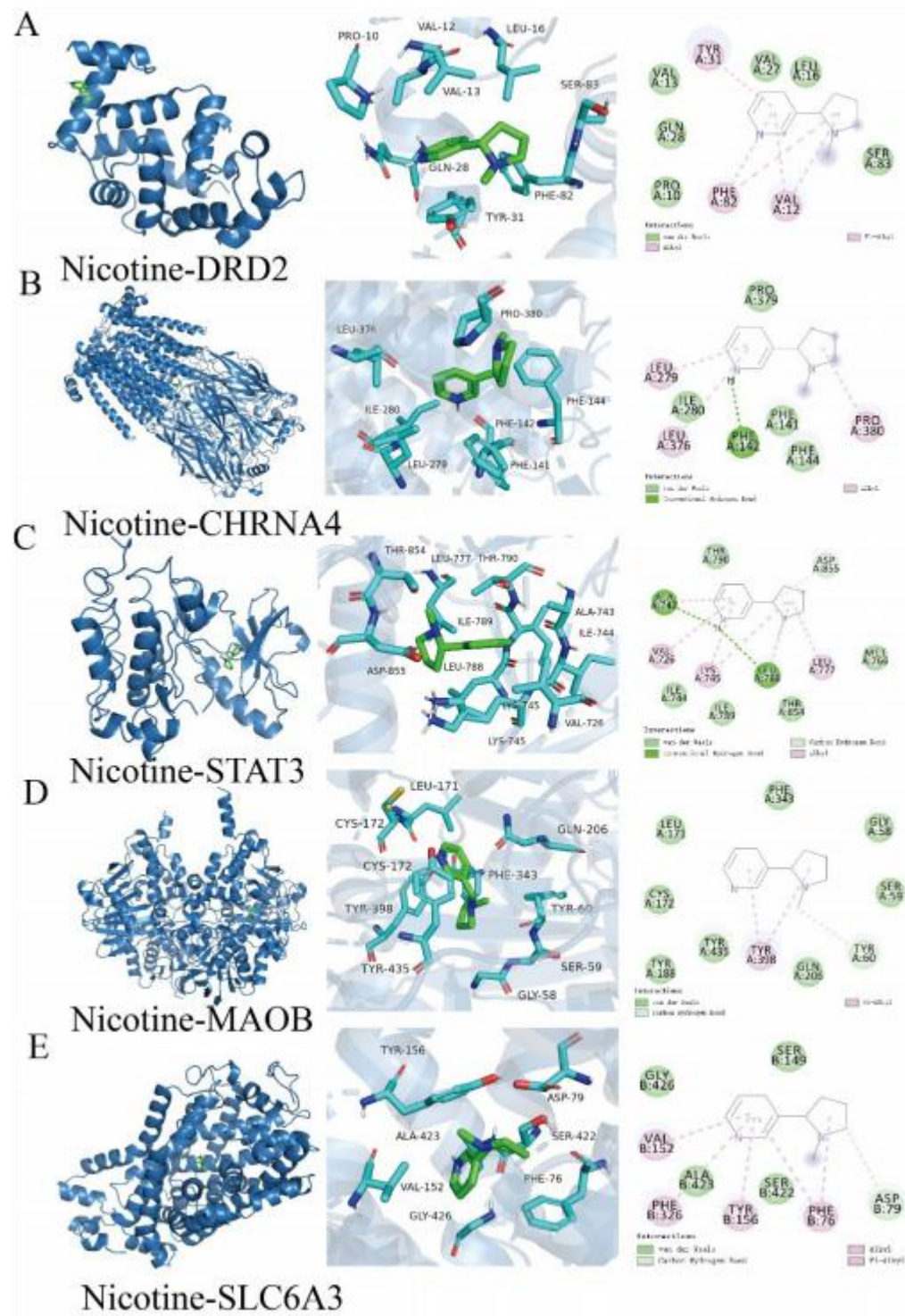
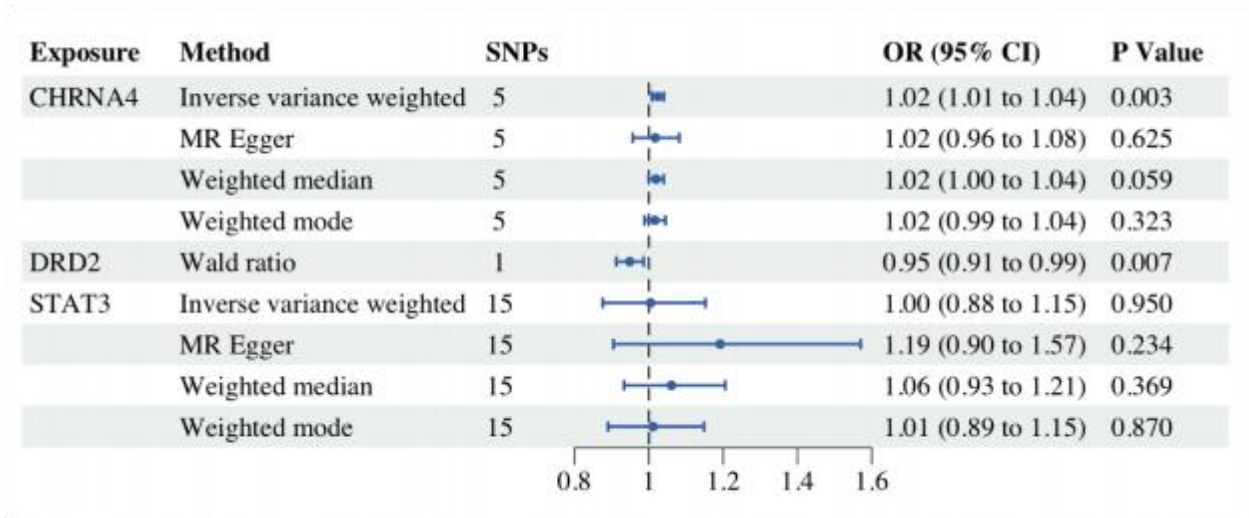


Figure 8. Forest plot of Mendelian randomization analysis for the causal association between 3 core genes and depression risk



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