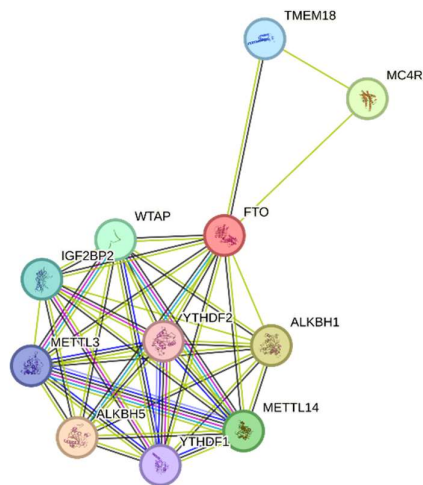
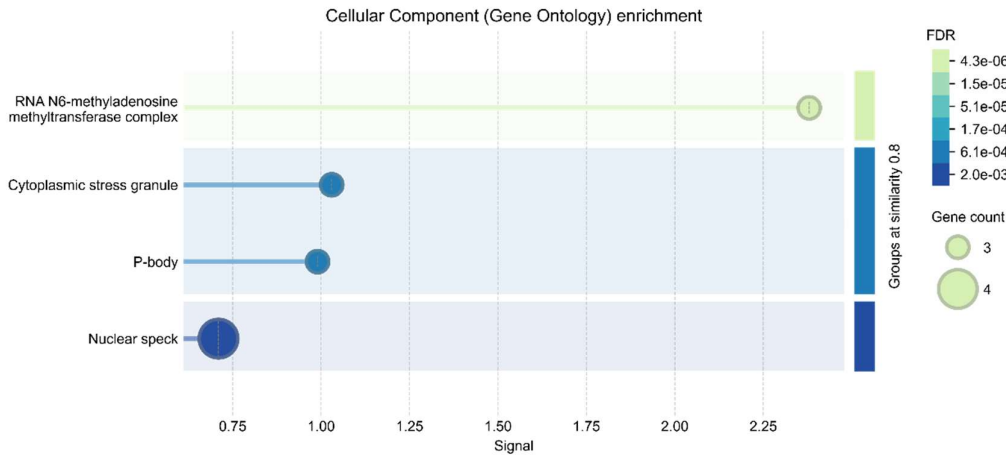


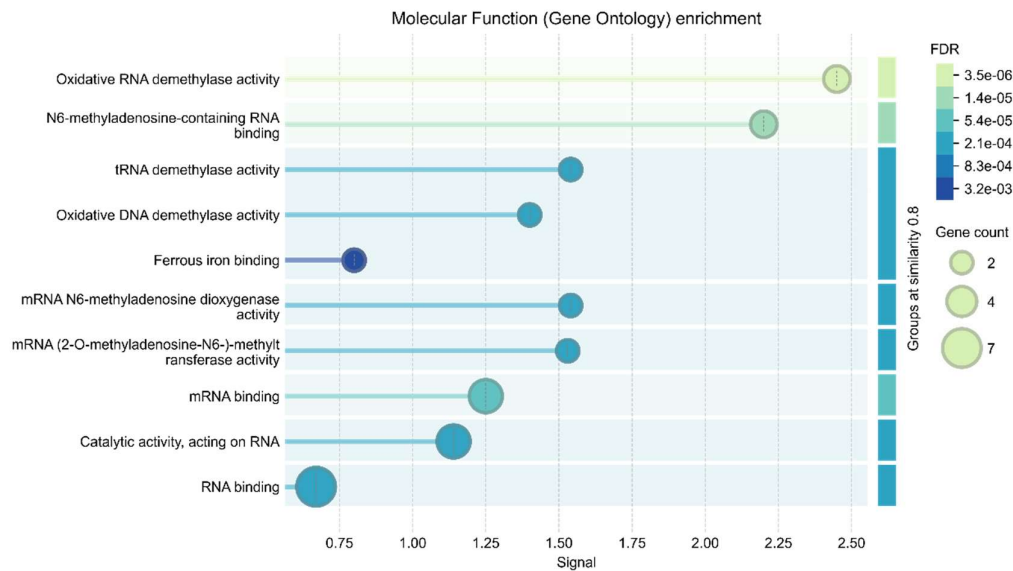
Large-Scale Chemical Space Exploration Identifies DE19725241 as a Novel FTO Inhibitor for Pancreatic Cancer



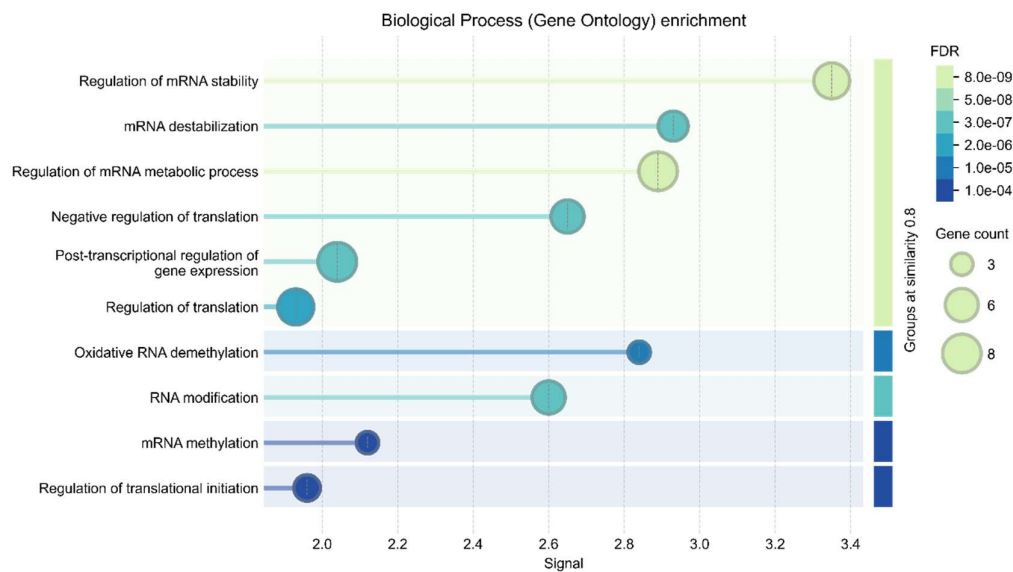
Supplementary Figure S1. Protein–protein interaction (PPI) network involving FTO.



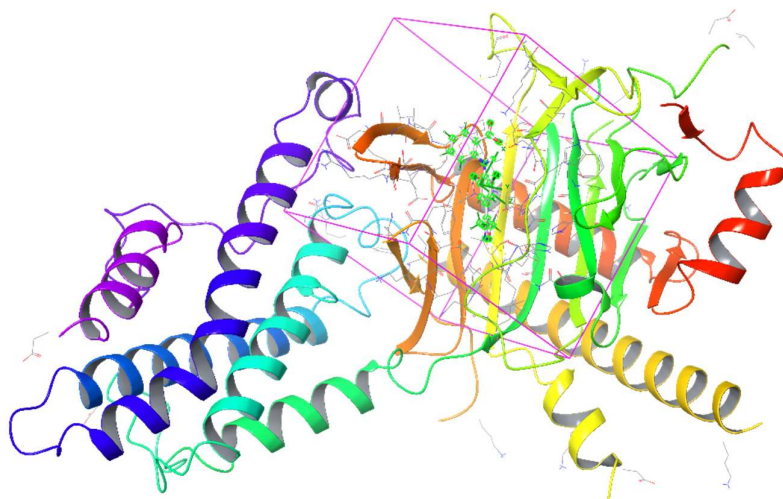
Supplementary Figure S2. Gene Ontology cellular component (GO-CC) enrichment analysis of the FTO-associated PPI network.



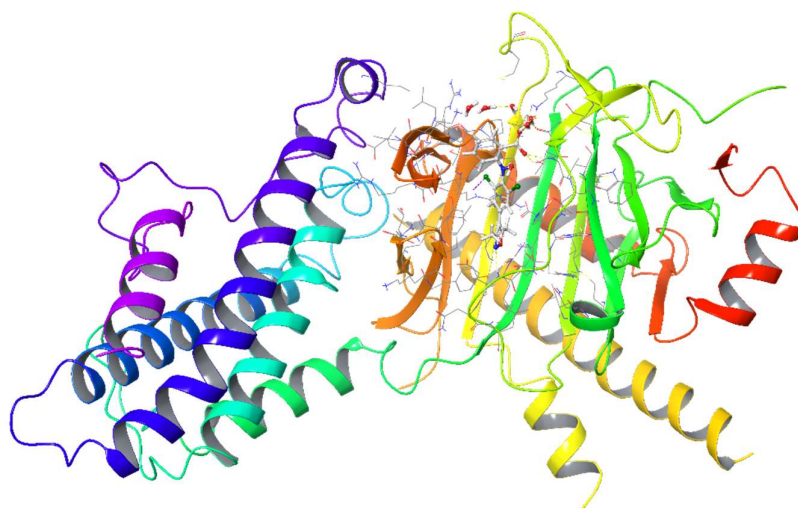
Supplementary Figure S3. Gene Ontology molecular function (GO-MF) enrichment analysis of the FTO-associated PPI network.



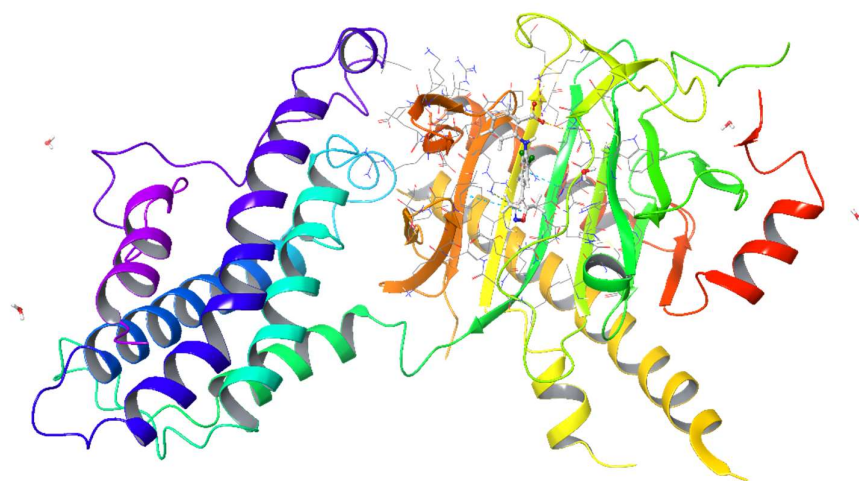
Supplementary Figure S4. Gene Ontology biological process (GO-BP) enrichment analysis of the FTO-associated PPI network.



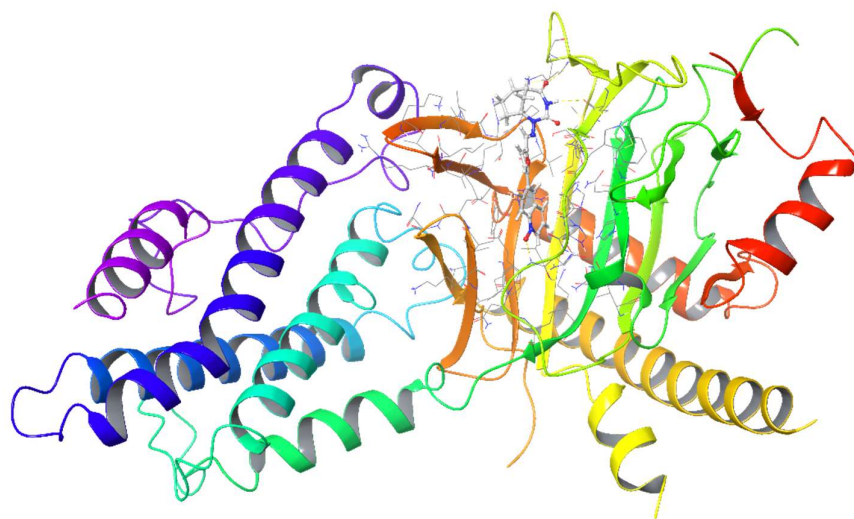
Supplementary Figure S5. Visualization of the FTO ligand-binding pocket used for molecular docking.



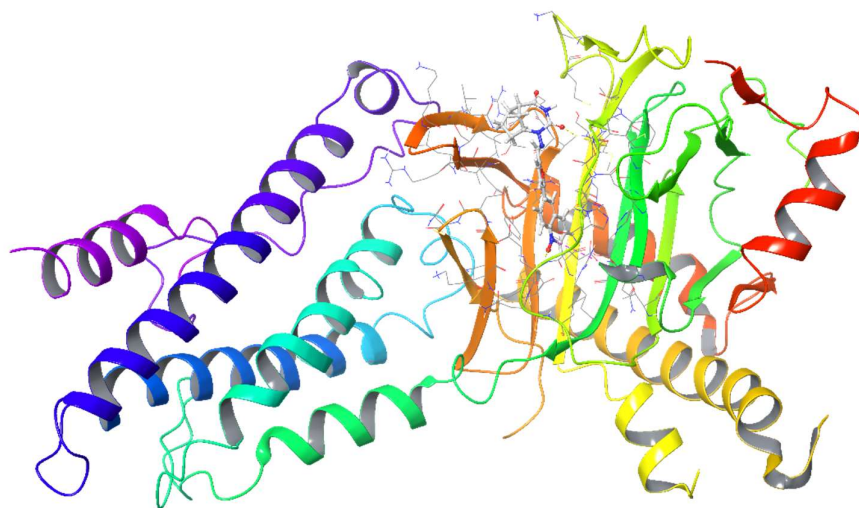
Supplementary Figure S6. Pre-simulation conformation of the FTO-FB23 complex.



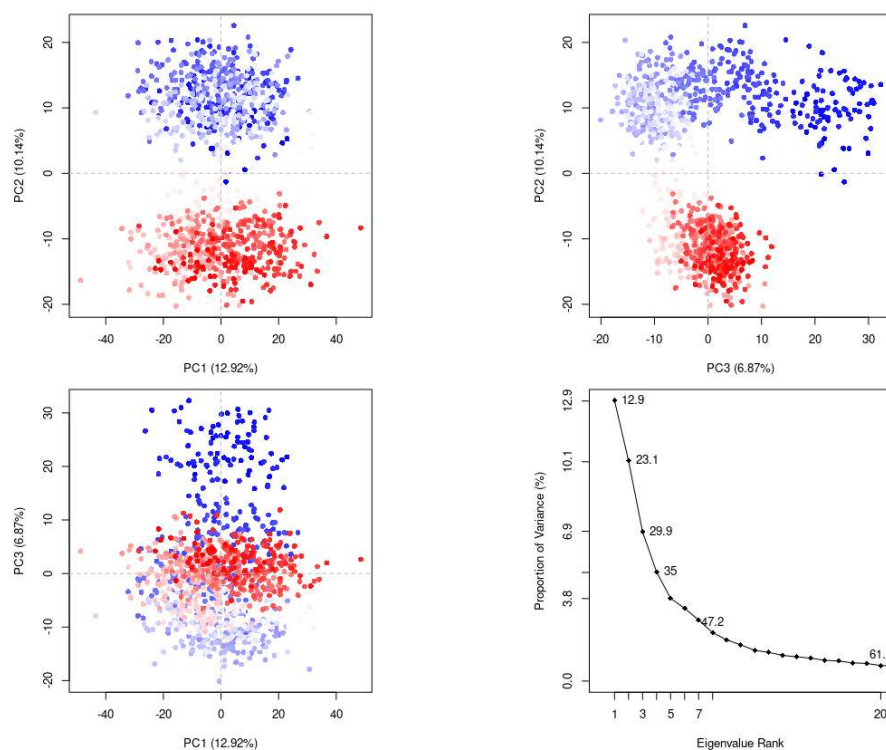
Supplementary Figure S7. Post-simulation conformation of the FTO-FB23 complex.



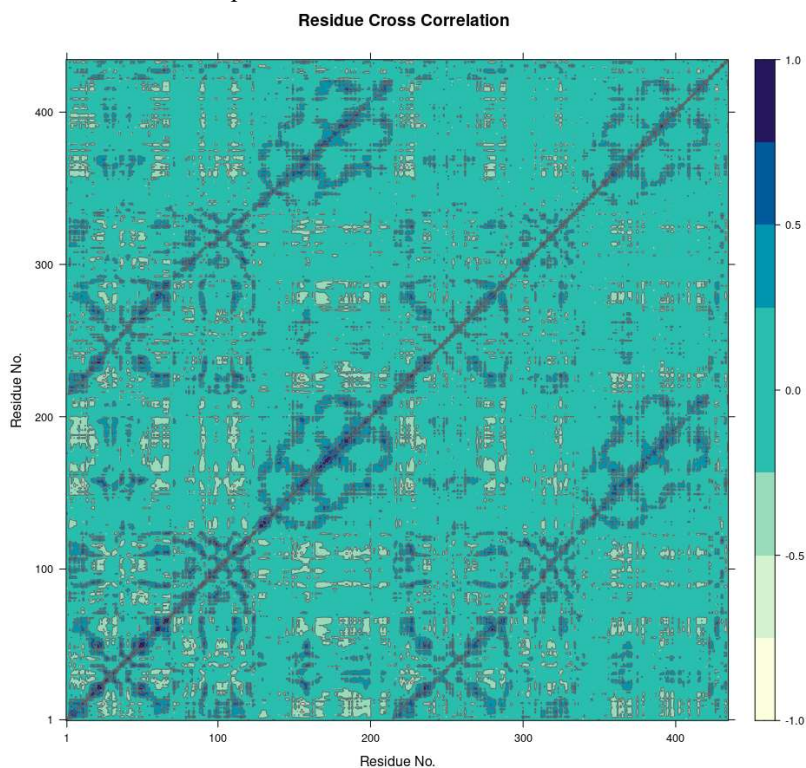
Supplementary Figure S8. Pre-simulation conformation of the FTO-DE19725241 complex.



Supplementary Figure S9. Post-simulation conformation of the FTO–DE19725241 complex.

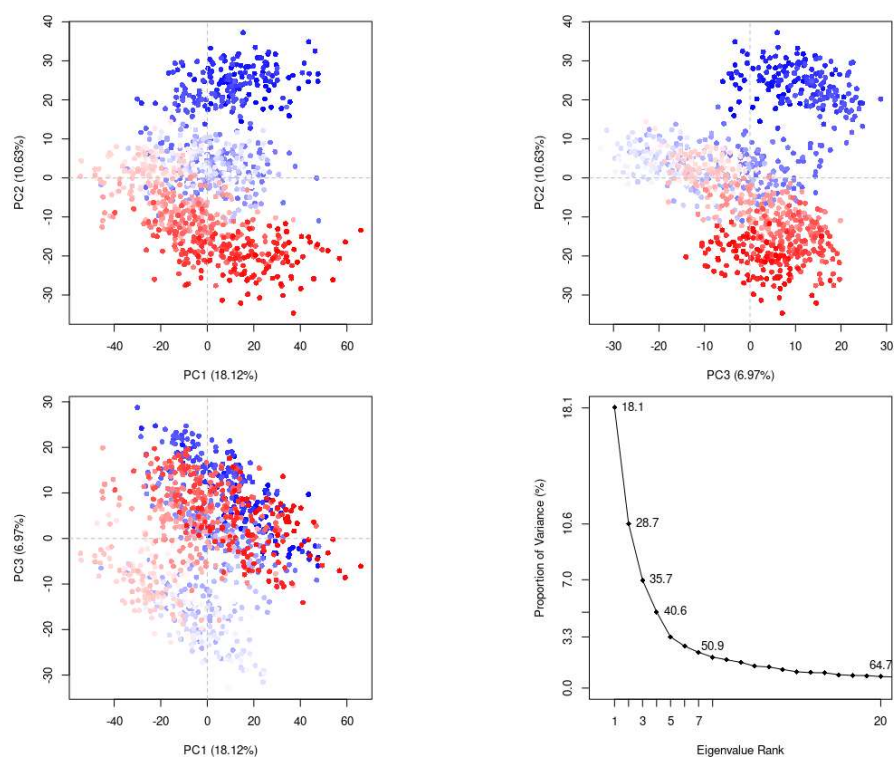


Supplementary Figure S10. Principal component analysis (PCA) of the molecular dynamics (MD) trajectory of the FTO–FB23 complex.

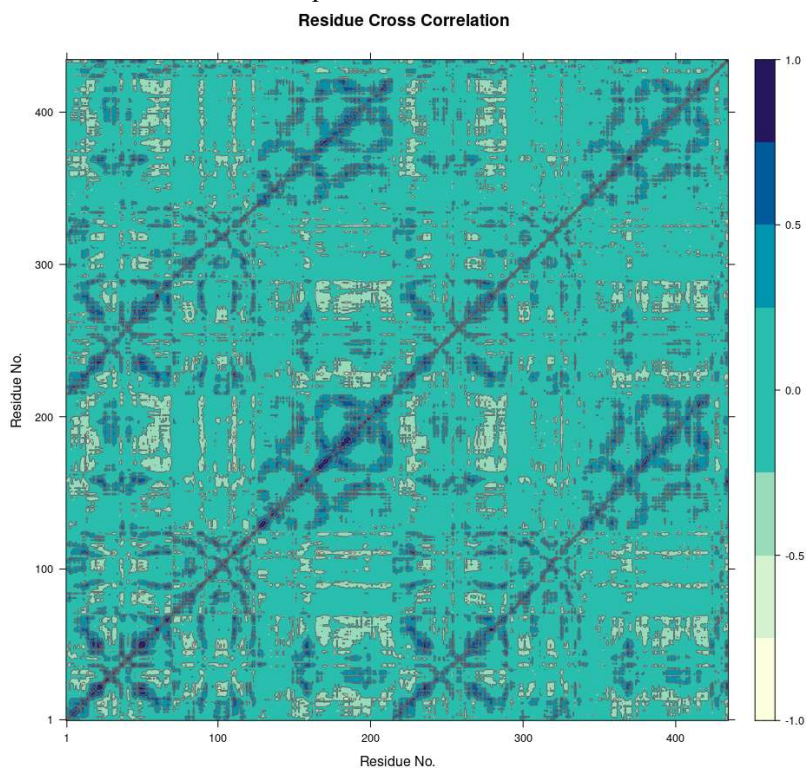


Supplementary Figure S11. Principal component analysis (PCA) of the molecular dynamics (MD)

trajectory of the FTO–FB23 complex.

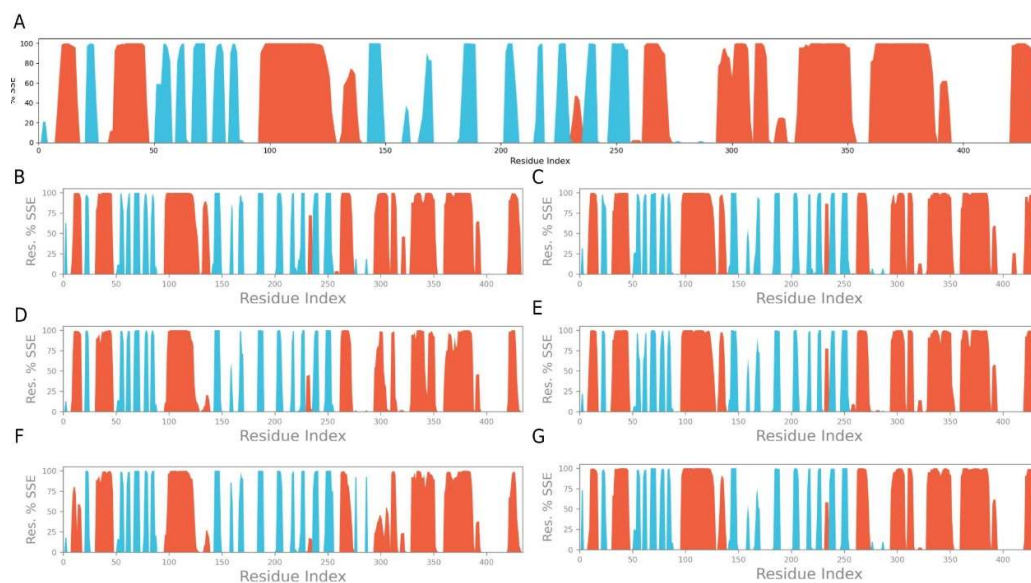


Supplementary Figure S12. Principal component analysis (PCA) of the molecular dynamics (MD) trajectory of the FTO–DE19725241 complex.



Supplementary Figure S13. Principal component analysis (PCA) of the molecular dynamics (MD)

trajectory of the FTO–DE19725241 complex.



Supplementary Figure S14. Comparative secondary-structure profiles derived from molecular dynamics trajectories of wild-type and mutant FTO. Panels A–G depict the time-resolved secondary-structure distributions for WT, R96G, Y108G, A227G, S229G, E234G, and R322G, respectively.