Supplementary Figures

Repurposing Cofilin-Targeting Compounds for Ischemic Stroke through Cheminformatics and Network Pharmacology

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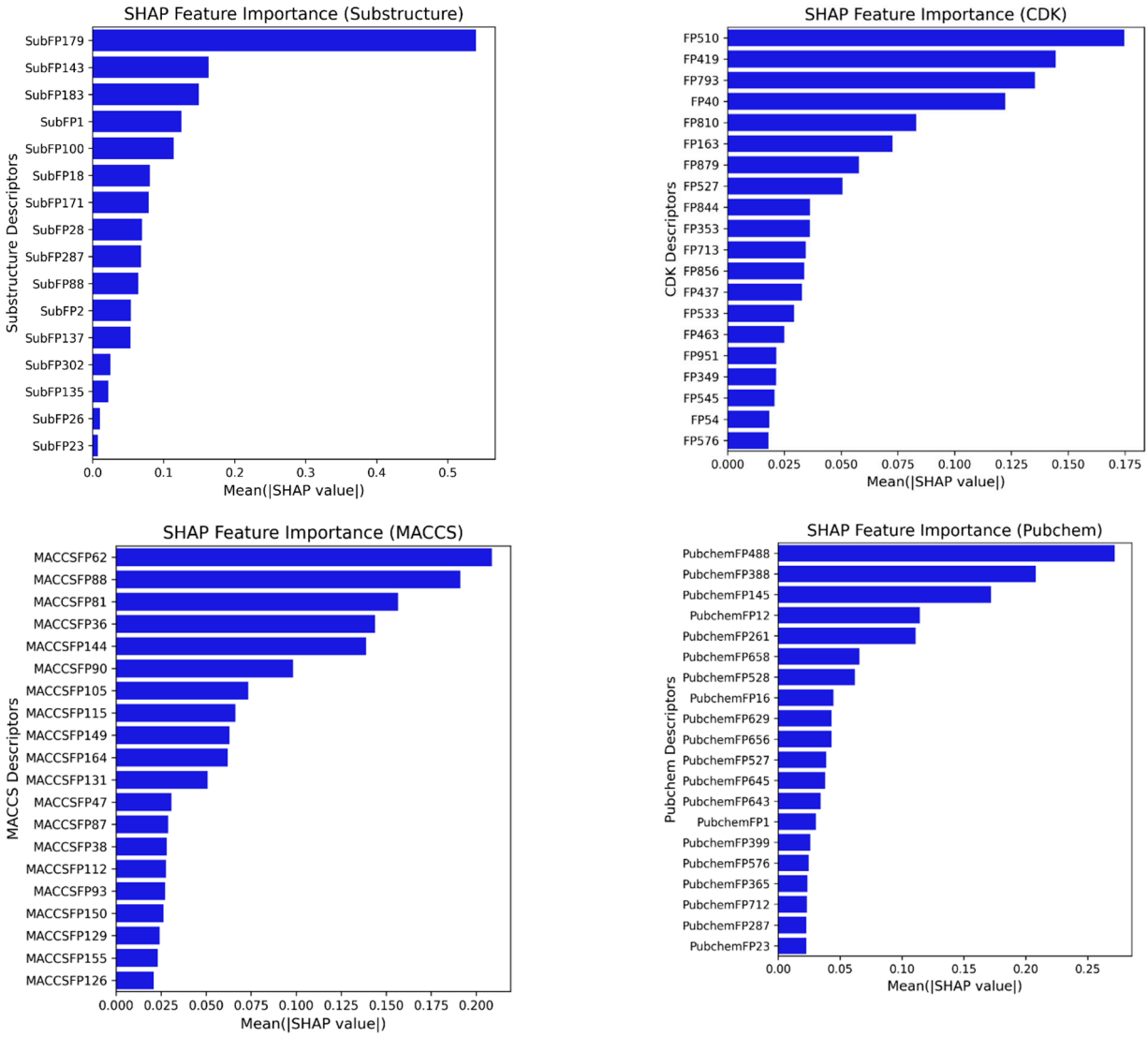

Figure S1: SHAP features importance description of all selective descriptors.

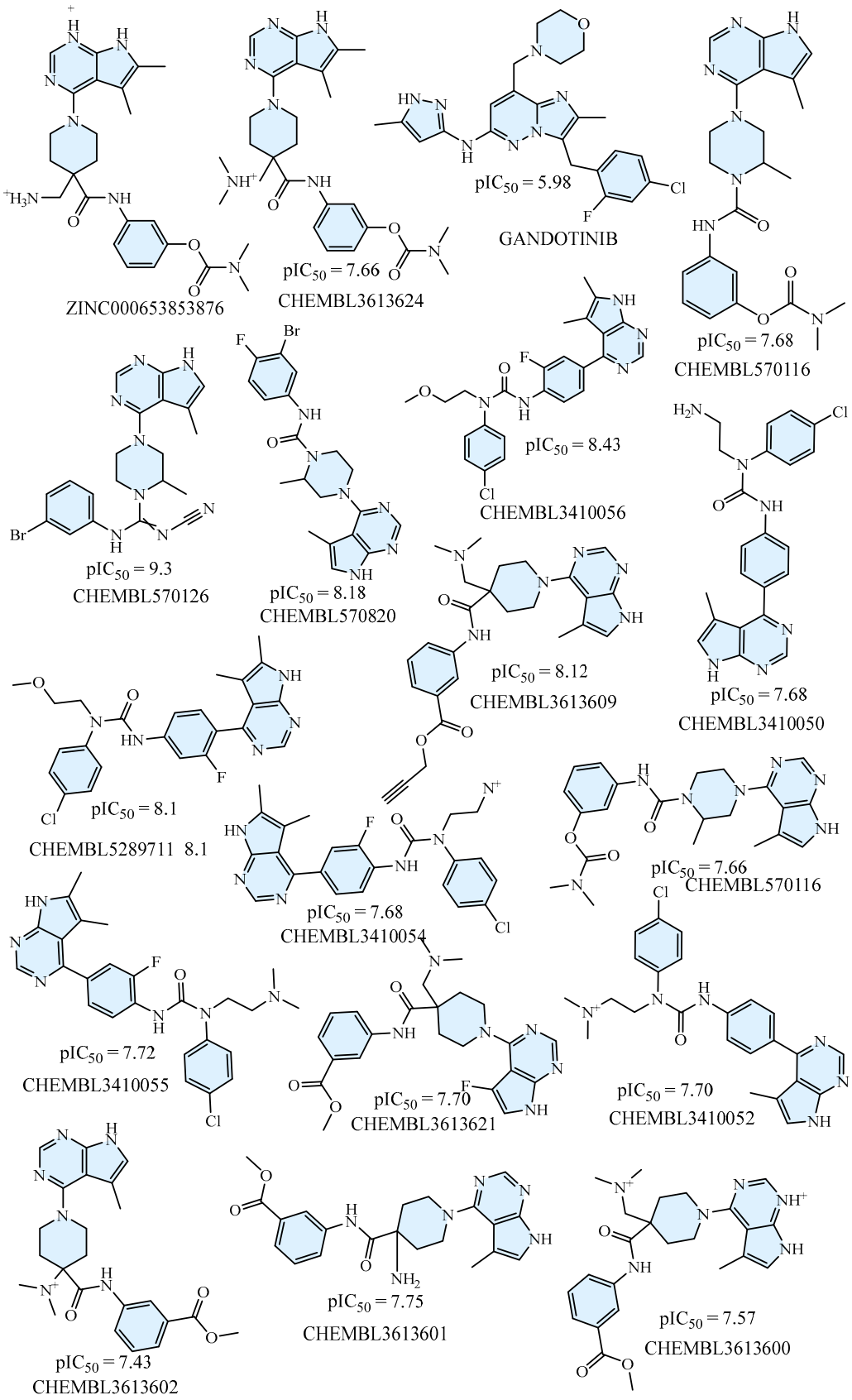

Figure S2: Top hits active compound structures from QSAR.

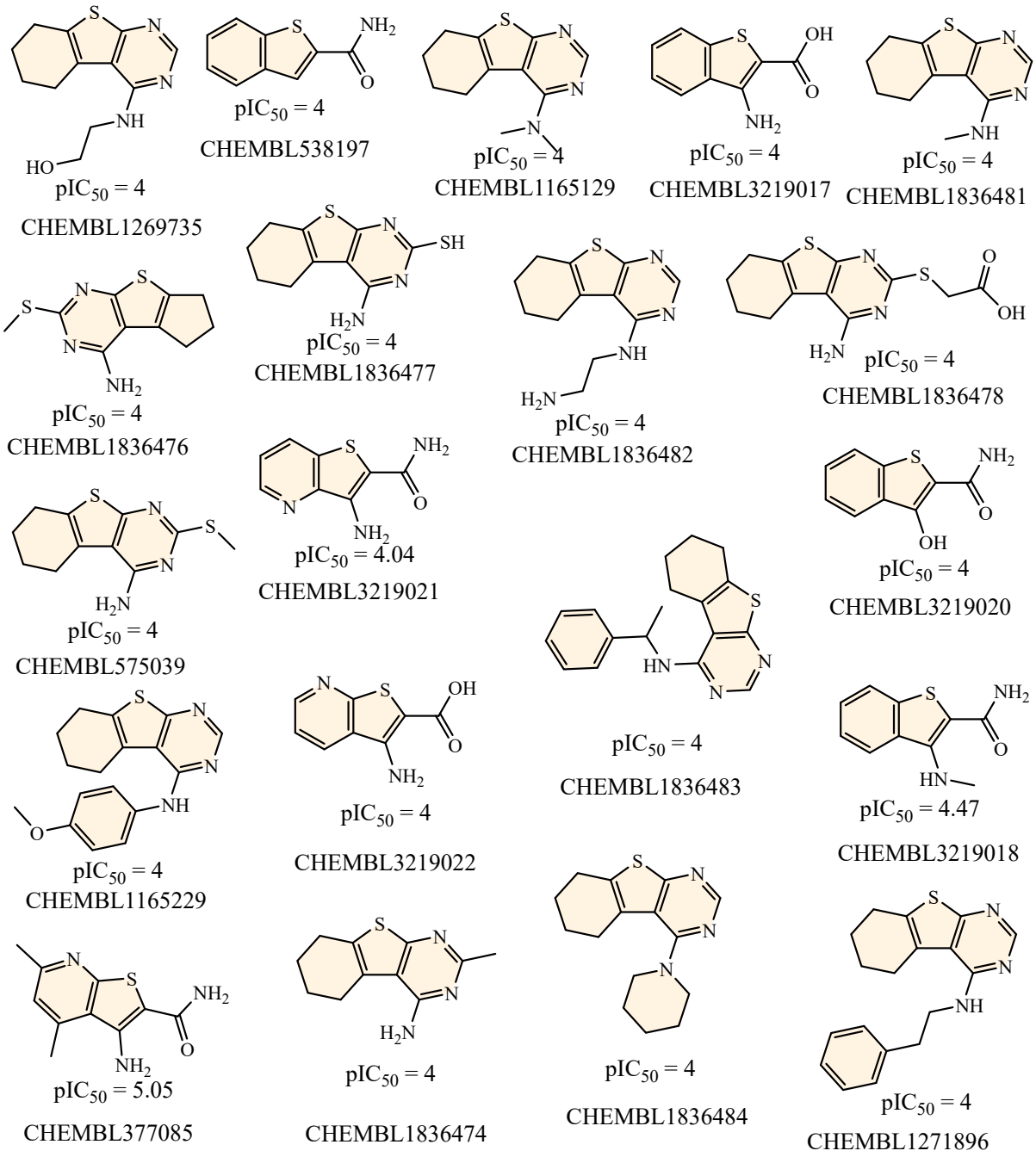

Figure S3: Top hits inactive compound structures from QSAR.

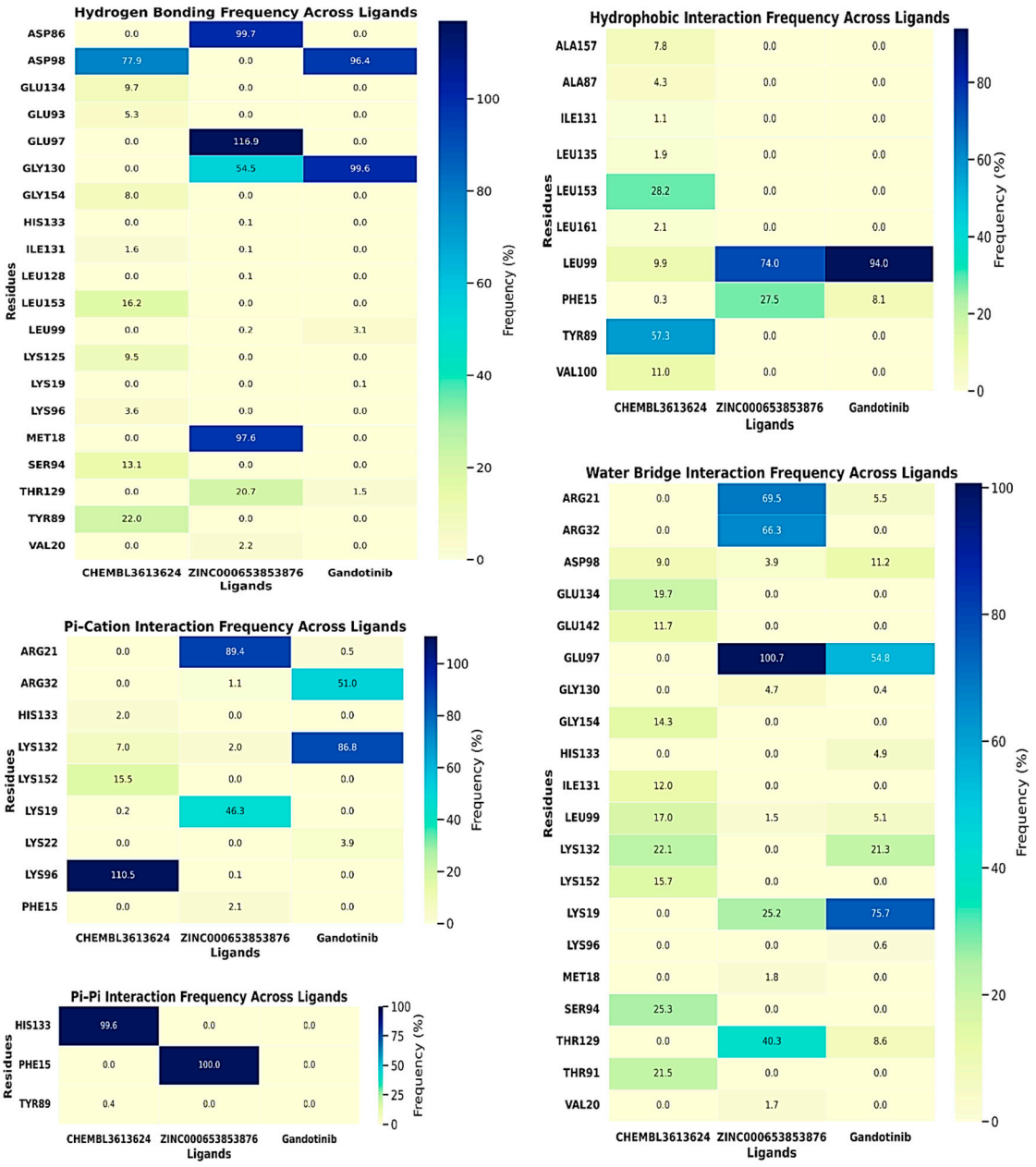

Figure S4. Interaction frequency maps of cofilin with CHEMBL3613624, ZINC000653853876, and Gandotinib during molecular dynamics simulation. Heatmaps show hydrogen bonding, hydrophobic interactions, water bridges, π-cation, and π–π stacking interactions across key residues.

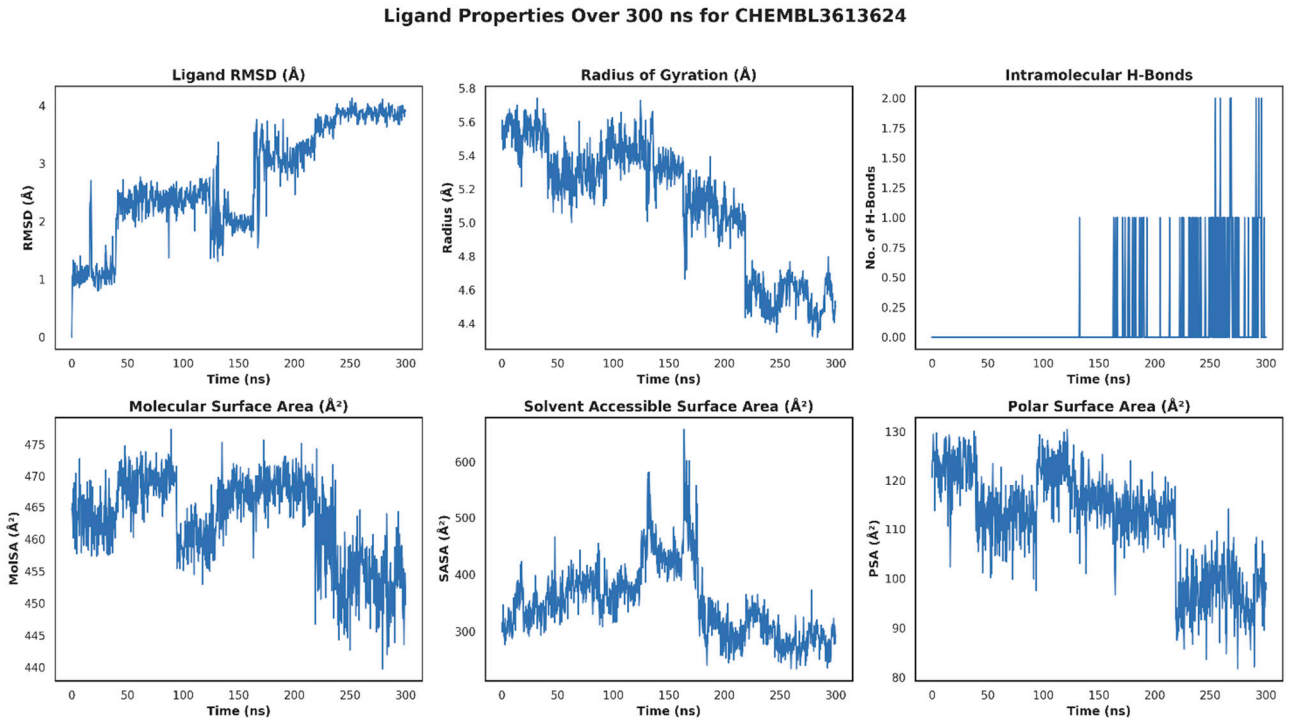

Figure S5: Ligand properties analysis over 300ns for compound CHEMBL3613624.

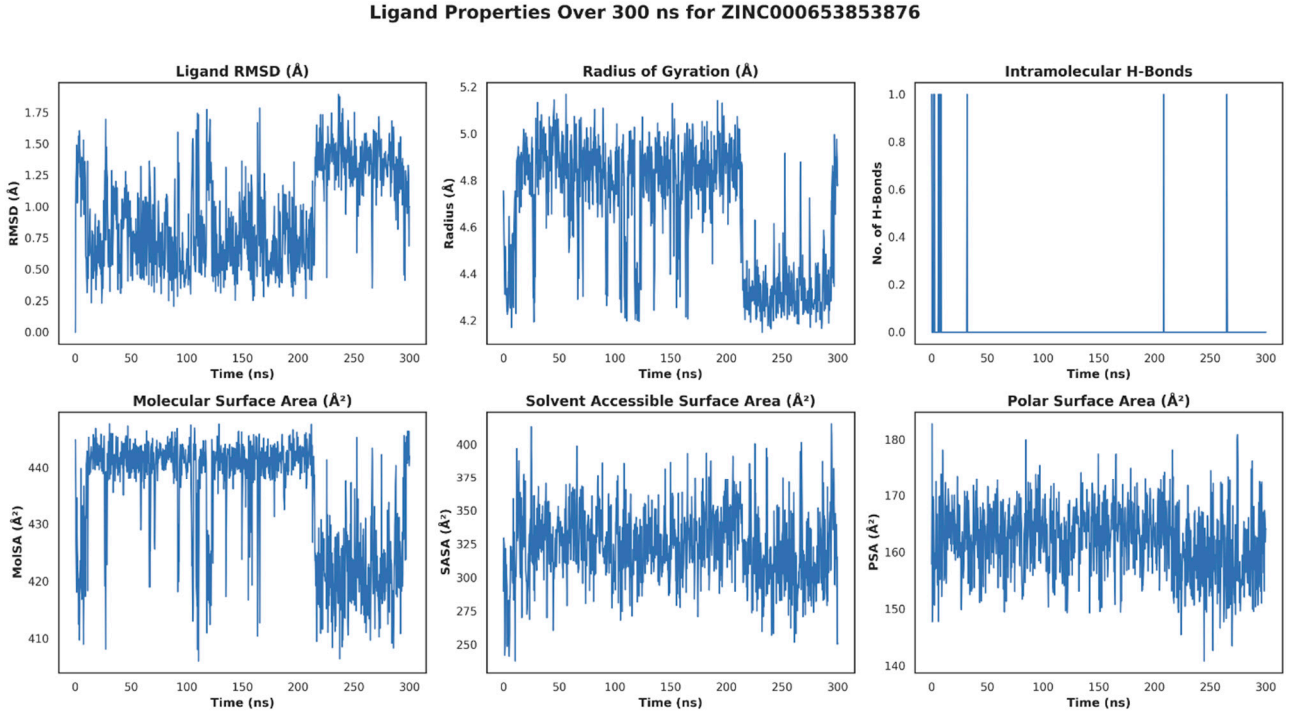

Figure S6: Ligand properties analysis over 300ns for compound ZINC000653853876.

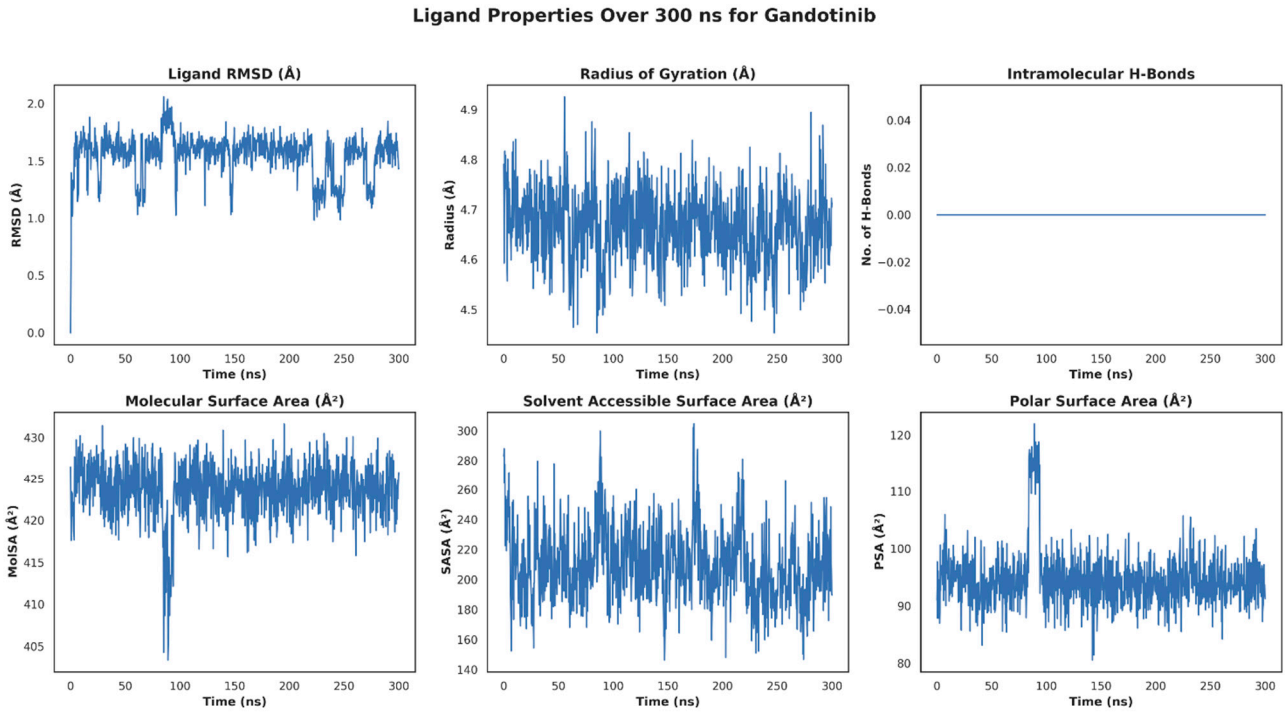

Figure S7: Ligand properties analysis over 300ns for compound Gandotinib.



Figure S8. Gene ontology analysis of different molecular and functional annotations.