Reproducible Virtual Screening Pipeline using AutoDock Vina

End-to-end ligand prep, docking, ranking, and binding pose visualization

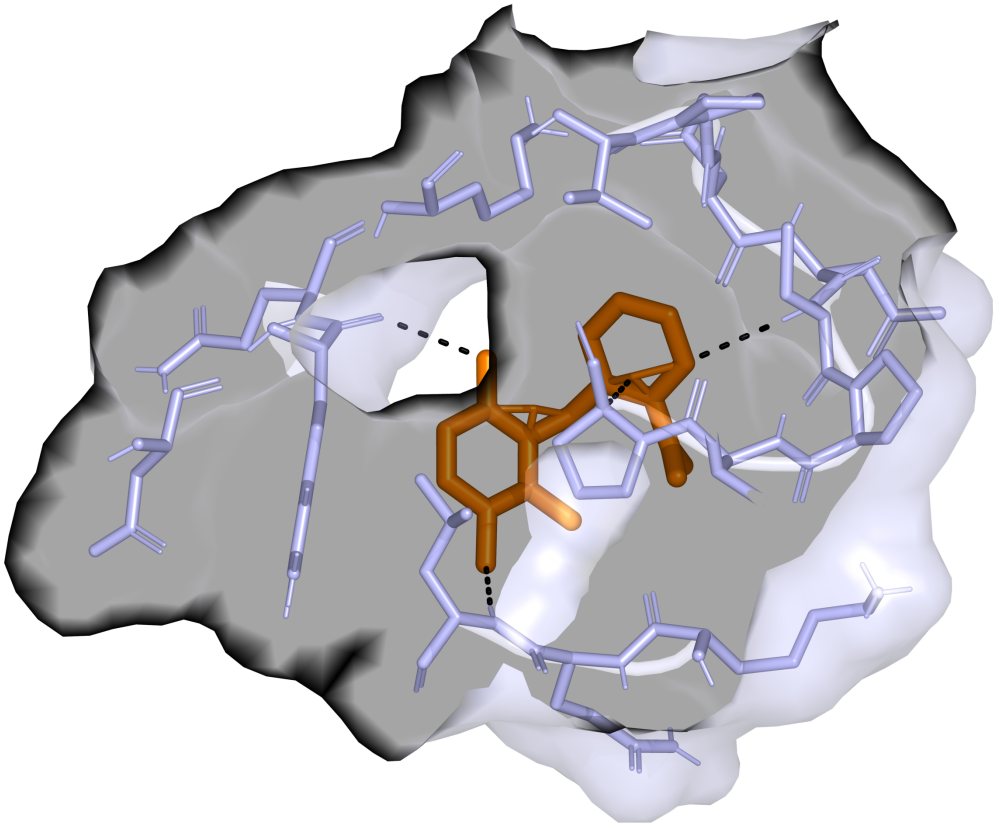
Objective

Build a reproducible pipeline that prepares ligands, converts structures to PDBQT, runs batch docking with AutoDock Vina, ranks candidates, and visualizes top binding poses.

Key Result

Top-ranked ligand: **F_pos006**
Best docking score: **-6.908 kcal/mol (Vina)**

Figure 1. Top docking pose (PyMOL render).



Top Ranked Ligands

Ligand	Affinity (kcal/mol)
03_docking/out/F_pos006_out.pdbqt	-6.908
03_docking/out/F_pos002_out.pdbqt	-6.899
03_docking/out/OH_pos017_out.pdbqt	-6.492

03_docking/out/Cl_pos002_out.pdbqt	-6.49
03_docking/out/Me_pos017_out.pdbqt	-6.456
03_docking/out/F_pos000_out.pdbqt	-6.429
03_docking/out/OH_pos002_out.pdbqt	-6.4
03_docking/out/Me_pos002_out.pdbqt	-6.32
03_docking/out/F_pos001_out.pdbqt	-6.248
03_docking/out/F_pos008_out.pdbqt	-6.231

Reproducibility

All scripts and minimal inputs are provided in this repository. Docking can be reproduced by rerunning the batch docking stage and regenerating results.csv.