

# Reproducible Virtual Screening Pipeline using AutoDock Vina

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

## Objective

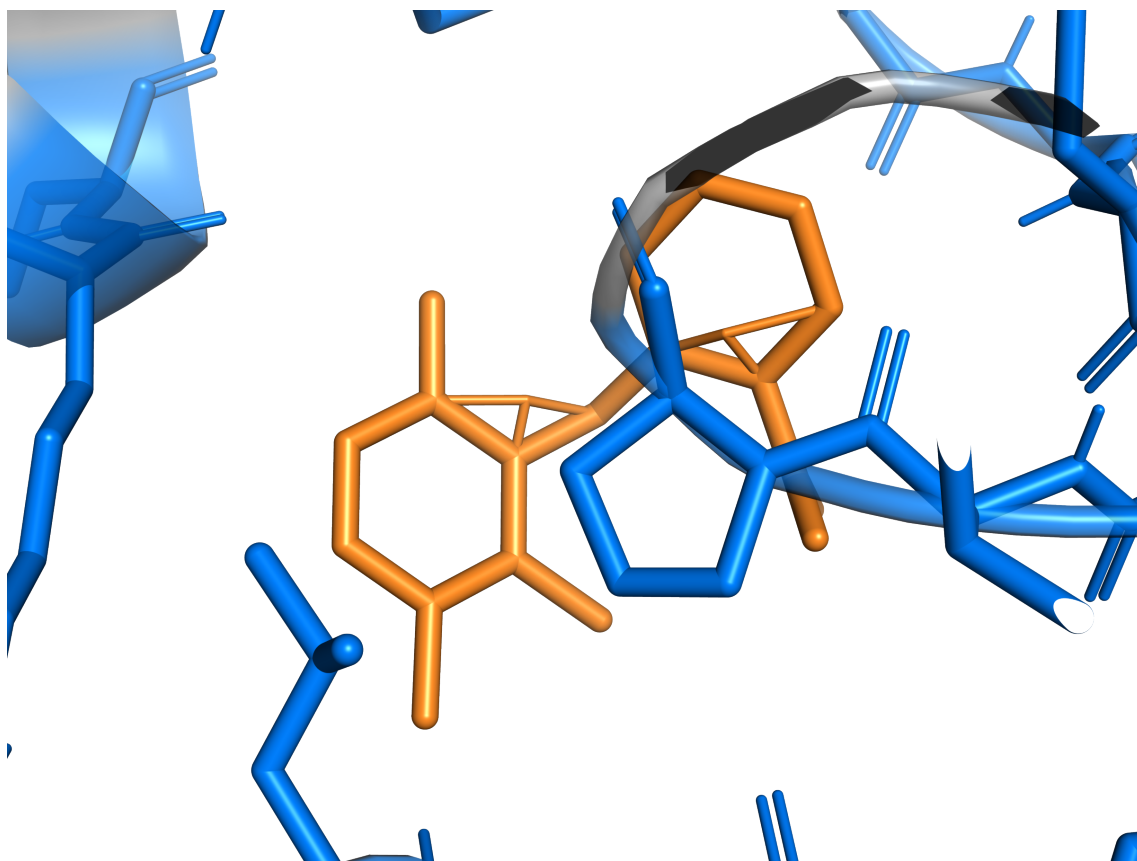
Build a reproducible pipeline that prepares ligands, converts structures to PDBQT, runs batch docking with AutoDock Vina, ranks candidates, and visualizes top binding poses.

## 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.