Quick Start Guide: AutoDock Tools on Linux

Launch AutoDock Tools

type “adt” in bash

Copy the following files to your Working Directory:

- protein.pdb

- ligand.pdb

- autogrid4

- autodock4

PDB File Preparation

Protein Preparation:

1. File → Read Molecule → Select protein.pdb

2. Edit → Hydrogens → Add (Parameters: All hydrogens, Method:

nonbondorder, Click Yes)

3. File → Save → Write PDB (Check "Sort nodes", Click Yes to overwrite)

Ligand Preparation:

4. Ligand → Input → Open (Select ligand.pdb → OK)

5. Select ligand from Dashboard

6. Edit → Hydrogens → Add (Parameters: All hydrogens, Method: nonbondorder, Click Yes)

7. File → Save → Write PDB (Check "Sort nodes", Click Yes to overwrite)

---

8. Edit → Delete → Delete All Molecules → Continue

PDBQT File Generation

Ligand Processing:

9. Ligand → Input → Open (Select ligand.pdb → OK)

10. Ligand → Torsion Tree → Detect Root

11. Ligand → Torsion Tree → Show Root Expansion

12. Ligand → Torsion Tree → Show/Hide Root Marker

13. Ligand → Torsion Tree → Hide Root Expansion

14. Ligand → Torsion Tree → Choose Torsions → Done

15. Ligand → Torsion Tree → Set Number of Torsions → Dismiss

16. Ligand → Output → Save as PDBQT (Save as ligand.pdbqt)

Protein Processing:

17. Grid → Macromolecule → Open (Select protein.pdb → OK → OK, Save as protein.pdbqt)

---

18. Edit → Delete → Delete All Molecules → Continue

Search Space Setup & AutoGrid Execution

19. Grid → Macromolecule → Open (Select protein.pdbqt → No → OK → OK)

20. Grid → Set Map Types → Open Ligand (Select ligand.pdbqt)

21. Grid → Grid Box (Adjust grid points and center coordinates) → File → Close Saving Current

22. Grid → Output → Save GPF (protein.gpf)

23. Run → Run AutoGrid → Launch

Docking Setup & AutoDock Execution

24. Docking → Macromolecule → Set Rigid Filename (Select protein.pdbqt)

25. Docking → Ligand → Choose (Select ligand → Accept)

26. Docking → Search Parameters → Genetic Algorithm → Accept

27. Docking → Output → Lamarckian GA (Save as ligand.dpf)

28. Run → Run AutoDock → Launch

View and Analyze Conformations

29. Analyze → Docking → Open (Select ligand.dlg)

30. Analyze → Macromolecule → Open (Select protein.pdbqt)

31:Analyze → Conformations → Load

- Select your desired conformation from the list

- The structure will be displayed in the AutoDock viewer

- A new window will open showing binding energy and other detailed parameters

32. Analyze → Clustering → Show (To view the clusters and select one)

32. Analyze → Docking → Show Interactions