■ Docking Pipeline User Guide

Linux/Ubuntu Edition – Simplified `~/docking` Version

Overview

This guide describes how to run the AutoDock Vina docking pipeline from the `~/docking` directory. The workflow automates receptor preparation, ligand combination, conversion, docking, and result summarization. Each run creates a timestamped subdirectory (e.g., `docking_run_2025-10-23_14-30-00`) to store outputs, keeping your workspace clean and reproducible.

Prerequisites

• Ubuntu or other Linux system • Miniconda installed • Open Babel and AutoDock Vina available • Python 3.8+ environment with dependencies installed (`PyYAML`, `requests`)

Setup Instructions

1. Clone or unzip the provided `docking` directory into your home folder.
2. Open a terminal and create the environment: `conda env create -f environment.yml`
3. Activate it each session with: `conda activate docking_env`
4. Change into the docking directory: `cd ~/docking`

Configuration File (`docking_config.yml`)

The YAML file defines all key settings. Use either a PDB ID **or** a pre-prepared receptor file.

Example minimal config:

pdb_id: 4DIU receptor: "" chains: "A" keep_cofactors: false ligand_dir: ligands/ combined_sdf: combined_ligands.sdf pdbqt_dir: pdbqt_files/ results_dir: results/ residues: "A:22" padding: 6 config_out: vina_config.txt

If you already have a prepared receptor:

pdb_id: "" receptor: "4DIU_prepped.pdbqt"

Running the Pipeline

1. Ensure your ligands are in `~/docking/ligands/` as `.sdf`, `.mol`, or `.mol2` files.
2. Edit `docking_config.yml` if needed.
3. Run the full pipeline: `python3 run_pipeline.py docking_config.yml | tee docking_run.log`
4. All results are saved under a timestamped folder (e.g., `~/docking/docking_run_2025-10-23_14-30-00`).

Output Summary

Each run directory contains: • Cleaned and prepared receptor file (`*_prepped.pdbqt`) • Combined ligand file (`combined_ligands.sdf`) • Converted ligand files (`pdbqt_files/`) • Docking results (`results/`) • `binding_scores.csv` summary table • `view_top_ligands.cxc` ChimeraX command file

Viewing Top Ligands in ChimeraX

After the pipeline finishes, run:

chimerax @results/view_top_ligands.cxc

If the preset line causes issues, remove it from the `.cxc` file (last line) and re-run.

Sharing with Others

To share the project: 1. Zip the entire `~/docking` folder. 2. Others can unzip it anywhere, `cd` into it, and run as above. Paths are automatically managed internally, so no hardcoding is required.

Troubleshooting

• If Open Babel errors occur, ensure all `.sdf` files are valid 3D molecules. • If the receptor already exists, it will be reused automatically. • The YAML config file is copied into each run folder for reproducibility.