
Update: Manual Docking Module - Advanced Docking with Custom Parameters

Introduction

This update introduces the *Manual Docking* module, a powerful new feature that provides users with enhanced flexibility and control over the docking process. Unlike the standard docking approach, which automatically assigns grid boxes and parameters, *Manual Docking* allows users to specify exact configurations for each receptor. This is especially useful for cases where predefined pockets or non-standard docking conditions are required.

With this update, users can upload multiple receptor structures and corresponding parameter files, ensuring that each docking run adheres to precise experimental or computational requirements. The module is fully integrated into the **Streamlit GUI**, enabling a seamless experience without requiring manual file management.

How Manual Docking Works

1. Uploading Receptor and Parameter Files

- Users can upload multiple receptor files (**.pdbqt**) into the *receptors* folder.
- Each receptor must have a corresponding parameter file (**.csv**) stored in the *parameters* folder.
- The CSV file defines docking parameters such as:
    - Grid center coordinates
    - Grid size in each dimension (x, y, z)
    - Exhaustiveness of the search
    - Number of docking modes
    - Energy range
    - Random seed

Example CSV file format:

parameter,value

exhaust,40

energy_range,1

num_modes,5

seed,1988

grid_center_x,107

grid_center_y,114

grid_center_z,143

grid_size_x,17

grid_size_y,20

grid_size_z,35

Each receptor file **must** have a matching CSV file, named identically (except for the extension).

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2. Selecting the Ligand File

- Users must upload a single ligand file (**.sdf** or **.mol2**) containing all the ligands they wish to dock.
- The system will automatically read and process all ligands in the file.

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3. Running the Docking Process

- The docking process is initiated directly from the GUI.
- The system will:
    1. Read all receptor files and locate corresponding parameter files.
    2. Convert ligands to **.pdbqt** format for compatibility with AutoDock Vina.
    3. Perform docking for each ligand-receptor pair using the defined parameters.
    4. Generate output files for results analysis.

Output Files and Results

1. Individual Docking Results

For each receptor, a separate folder is created containing:

- **Docked ligand files** (**.pdbqt**) – The final docking results.
- **Images and visualizations**:
    - PNG images of docking poses generated using PyMOL.
    - PyMOL session files (.pse) for interactive visualization.
- **A CSV summary file** (receptor_name_results_in_CSV.csv), containing:
- name,affinity,smiles
- ligand_001,-5.23,C[NH2+]C[C@@H]1OCCc2ccsc21
- ligand_002,-5.37,C[NH2+]C[C@@H]1OCCc2ccsc21

This file records ligand names, binding affinities, and molecular SMILES representations.

- **A full docking log file** (receptor_name_results.txt), listing all docking poses and their corresponding binding energies.

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2. Global Summary of Receptors

A new summary file (receptors_manual.csv) is created in the *receptors* folder. It contains a simple list of all receptor names that were used in the docking process. This file is essential for result visualization.

Integration with the GUI

- The *Manual Docking* module has been added to the **Streamlit GUI**.
- Users no longer need to manually place files in specific directories.
- The GUI automatically detects available receptors, ligands, and parameter files.
- Results can be downloaded directly from the interface.

When viewing results in the **SHOW RESULTS** module:

- If a *standard docking* session was performed, results are loaded from receptors.csv.
- If a *Manual Docking* session was performed, the system will detect receptors_manual.csv and load results accordingly.

This ensures that both standard and manual docking workflows are seamlessly integrated.

Why Use Manual Docking?

Key Benefits

✓ Allows **custom grid settings** for each receptor.
✓ Supports **multiple receptors and ligands** in a single session.
✓ Enables **precise control** over docking parameters for advanced experiments.
✓ Fully integrated into the **Streamlit GUI**, requiring no manual file handling.
✓ Provides **detailed output files** for post-processing and analysis.

This module is ideal for cases where researchers need absolute control over docking conditions, such as:

- Studying different binding sites on a receptor.
- Comparing ligand interactions under different conditions.
- Refining docking parameters for improved accuracy.

Conclusion

The *Manual Docking* module extends the capabilities of the docking workflow, making it more flexible and suited to complex research needs. By supporting multi-receptor docking with precise parameter control, it provides a robust tool for computational chemistry and molecular docking studies.

Users can now easily configure, execute, and analyze docking simulations with **fully customized receptor-ligand interactions** – all from within the **Streamlit GUI**.

This update represents a significant improvement in docking efficiency and usability, further enhancing the capabilities of our platform.