Molecular Docking Services

Chemspace Virtual Screening Services

CHEMSPACE
Delivering Discovery Solutions®

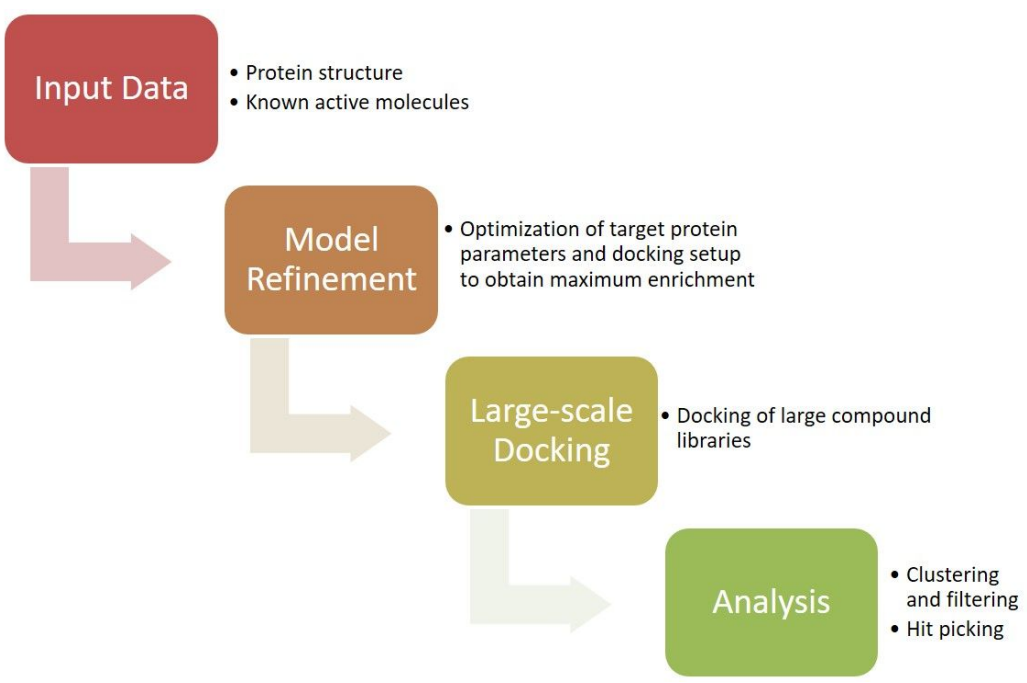
INPUT

What do we expect as Input?

- Desired target of interest
- Availability of actual X-ray structure is beneficial
- If the structure of the selected protein was not determined, it can be modeled based on the structure of similar proteins
- Known active compounds (optional)
- Preferred ligand chemotype (optional)
- Additional biochem criteria for candidates (optional)

PIPELINE

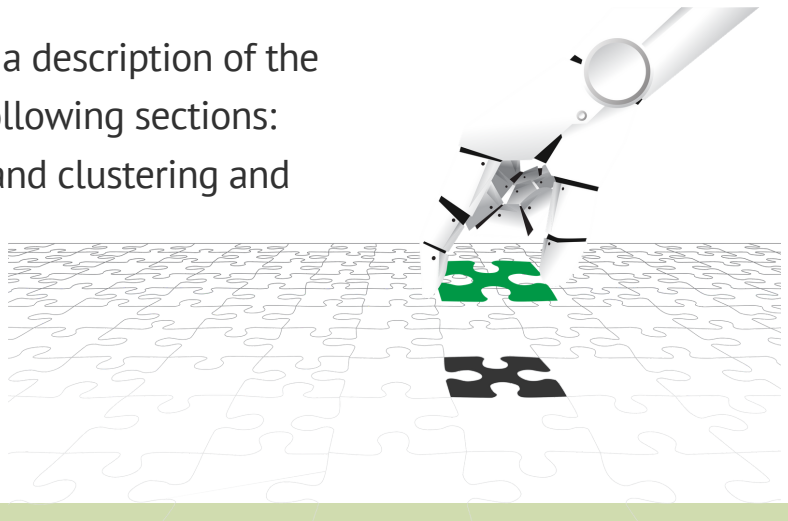
Docking Pipeline



OUTPUT

RESULTS

- List of perspective hit compounds, having the highest affinity to the selected receptor and preferred or diversified chemotypes
- A report containing a description of the workflow and the following sections: ligand filtration, ligand clustering and ligand docking



MISSION OF MOLECULAR DOCKING

- Investigation of protein-ligand interactions
- Prediction of ligand binding affinity
- Most importantly: Finding biologically active molecules that show activity against a specific protein
- Also applicable for fast screening of multi-million compound libraries