rDOCK Tutorial

rDock is a fast and universal open source docking program that can be used to dock small molecules with proteins and nucleic acids. It is designed for high-throughput virtual screening (HTVS) and combined model prediction research. rDock is mainly written in C++. The complete rDock software package requires less than 50 MB of hard disk space and can be compiled on all Linux computers.

Features

Docking preparation

Define cavities using known binders or with user-supplied 3D coordinates. Allow -OH and -NH2 receptor side chains to rotate. Add explicit solvent molecules and structural waters. Supply pharmacophoric restraints as a bias to guide docking.

Pre-processing of input files

Define common ligand structure for performing tethered docking (requires OpenBabel python bindings). Sort, filter or split ligand files for facilitating parallelization. Find HTVS protocol for optimizing calculation time. Pre-calculate grids to decrease subsequent calculation times.

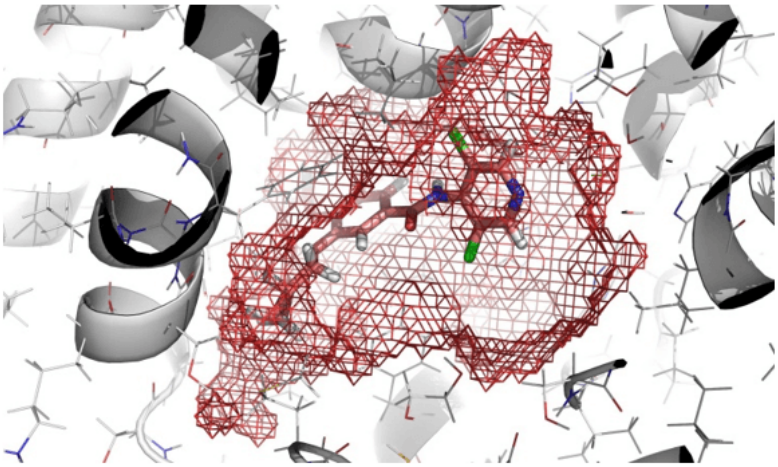

Figure 1 Software picture

Post-processing and analysis of results

Summarize results in a tabular format. Sort, filter, merge or split results files. Calculate RMSD with a reference structure taking into account internal symmetries (requires OpenBabel python bindings).

Binding mode prediction

Predict how a ligand will bind to a given molecule. The ASTEX non-redundant test set for proteins and DOCK and rDock test sets for RNA have been used for validating and comparing rDock with other programs.

HTVS

Run for millions of compounds in short time by exploiting the capabilities of computer calculation farms. Ease of parallelization in relatively unlimited CPUs to optimize HTVS running times. The DUD set has been used for validating rDock and comparing its performance to other reference docking programs.