Installation

Decompress PocketPicker_1.0.zip and store the contents into the following folder:

$PYMOL_DIRECTORY\modules\pmg_tk\startup

$PYMOL_DIRECTORY stands for the installation folder of your PyMOL distribution. For example, the standard PyMOL installation-path for German users is:

C:\Programme\DeLano Scientific\PyMOL

Furthermore the absolute path to the PocketPicker-Plugin folder has to be entered in the PocketPocker_Plugin.py file in line 42 (Linux) or line 45 (Windows). Preset are the paths of the standard English installation (C:\Program Files\DeLano Scientific\PyMOL\modules\pmg_tk\startup) as well as the German installation (C:\Programme\DeLano Scientific\PyMOL\modules\pmg_tk\startup).

(If you run PyMOL from a server, you might also include the full path to PyMOL in line 31 in 'PocketPickerScript\LigandKicker.py'.)

Usage of PocketPicker

After successful installation the PocketPicker plugin can be accessed via the `Plugin` menu of PyMOL.

To begin load your PDB-File into PyMOL. PyMOL provides the PDB-Loader-Plugin (PDB online access) for this purpose:

--> Plugin --> PDB Loader Service

If the PocketPicker Plugin is installed correctly, you can start calculations by selecting

--> Plugin --> PocketPicker Plugin --> Pocket Prediction

You can now choose from a selection which ligands ought to be removed prior to computation.

WARNING: The implementation of this sophisticated pocket detection algorithm causes considerable long runtimes. The calculation runtime of a reference molecule PDB 121P may take up to 22 minutes on a 1.73 GHz Intel Pentium machine.

The five largest predicted pockets are visualized by colored CGOs (compiled graphics objects) in PyMOL. Colorings indicate buriedness of grid probes. Pockets are sorted by size and can be selected by respective buttons placed in the PyMOL window.

Usage of SessionRestore

Prediction results of former computations can be restored by selecting

--> Plugin --> PocketPicker Plugin --> Restore Session

You will be asked to

1. reload the respected PDB-File into PyMOL (e.g. 121P)
2. enter 'cgoload <NAME OF PDB>' (e.g. 'cgoload 121P')

Result Files

Results of PocketPicker are stored in a folder **/results** in PyMOL (a new subfolder named after the actual PDB-name is added to this folder). Three new files will be created for one computation:

1. **clusterinfo.txt**: tab-separated file holding pocket-index, xyz-coordinates and buriedness of each grid probe
2. **descriptor420.txt**: 420 dimensional shape descriptors for five biggest pockets (one descriptor per line)

3. **`info.txt`**: settings of the computation

Note: Please contact modlab.de for python scripts calculating Euclidean distances of shape descriptors of different pockets.