

The pymol plugin is composed of few files:

- `cavite.py` :
this file contains the definition for the cavity class.
- `ligands.py`
this file contains the definition for the `ligands` class.
- `canva.py`
this file contains the definition for the canvas class. It is the display of fingerprints. Clicking on fingerprints displays the residue and the ligand implicated in the current fingerprint in pymol viewer.
- `launcher.py`
This file contains the definition of the window for input files.
- `pymolFP.py`
This file contains the main part of the plugin.
- `CustomManager.py`
this file contains the definition of the manager at the right bottom of the canvas. By clicking, you can scroll the fingerprints.

INSTALL:

First, you have to configure `PYTHONPATH` at the place you want to install the plugin.

ex : `export PYTHONPATH=/usr/local/pymol-plugin/src`

Secondly, you have to copy all files from the tar file to this directory.

ex: `tar xvf pymolFP.tar`
 `cp pymolFP/*.py $PYTHONPATH`

Finally, you have to set the plugin in pymol. Pymol-> plugin-> install plugin:
give the file `pymolFP.py`

restart pymol.

USE:

You have to generate few files:

- the cavity in `pdb` format (generate from the `mol2` by Sybyl)
- the list of ligands (same input given to IFP)
- the list of Fingerprints in the same order as the list of ligands

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