LIQUID - PyMOL Plugin 1.0 Manual

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Installation

To install the LIQUID plugin copy all files and folders of this archive in following directory:

```
$PYMOL_DIRECTORY\modules\pmg_tk\startup
```

where `$PYMOL_DIRECTORY` points to the path of your PyMOL program directory. PyMOL can be found her: http://www.pymol.org

Usage

After successful installation of the plugin it can be found in the `Plugins`-Menu of PyMOL. Please load a desired molecule or molecular ensemble and compute its pharmacophore model by clicking on the respective button in the `LIQUID-Plugin`-Menu. The calculated model will be directly shown in the OpenGL area of PyMOL. The shown potential pharmacophore points are color-coded as follows:

```
GREEN:     LIPOPHILIC
BLUE:      H-BOND DONOR
RED:       H-BOND ACCEPTOR
```

Notice

The default cluster radius is 2.0 Å for each potential pharmacophore point type. To change the cluster radii afterwards, please type the following command in PyMOL's command line:

```
changeCR [cr_lipos], [cr_donors], [cr_acceptors]
```

where cr_lipos, cr_donors and cr_acceptors are to be exchanged by your desired radii.

Reference

Tanrikulu Y, Nietert M, Scheffer U, Proschak E, Grabowski K, Schneider P, Weidlich M, Karas M, Goebel M, Schneider G. Scaffold hopping by "fuzzy" pharmacophores and its application to RNA targets.*ChemBioChem* **2007** Nov 5;8(16):1932-6.