AutoSite- binding Site identification and predicting ligand atoms

Overview

AutoSite requires a receptor in PDBQT format. Here we will help you get started with the command line execution of the program to obtain binding sites for streptavidin (pdb:1STP), represented as fill points, and the corresponding predicted ligand atoms for each binding pocket identified. To get started go to the Downloads section and install the package following the installation instruction.

Step 1: Download 1STP.pdbqt.

All the water molecules, ions and ligands are removed from the receptor and converted to PDBQT format using AutoDockTools by adding hydrogens and charges.

Step 2: Execute AutoSite in command line.

Linux command:

> $WHERE_YOU_INSTALLED/MGLTools2-latest/bin/pythonsh $WHERE_YOU_INSTALLED/MGLTools2-latest/MGLToolsPcks/AutoSite/bin/AS.py –r 1STP.pdbqt

MacOSX command:

> /Library/MGLTools2/latest/bin/pythonsh /Library/MGLTools2/latest/MGLToolsPckgs/AutoSite/bin/AS.py –r 1STP.pdbqt

Step 3: Results.

The results include every binding site with fill points greater than or equal to 50 in PDB format. All the results have the prefix "1STP" from the receptor filename, followed "_cl_<rank>.pdb" for the fills and "_fp_<rank>.pdb" for the predicted ligand. The rank is based on the default AutoSite score computed as,

$$\frac{\text{(No. of fill points x buriedness}^2\text{)}}{\text{(Radius of gyration)}}$$