Subject: Veiwing PDB Binding Sites in DataWarrior
Posted by MedChemProf on Sun, 12 Jan 2025 19:56:00 GMT
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Dear All,

There are downloadable files on the Open Molecules website under the section "All Non-Covalent Binding Sites From the PDB-Database (Dec 2024)" where you can view the binding of a ligand to a protein. There is some description of how the file was created, but I have been unable to reproduce it.

Are there any detailed instructions on how to view or add the information from a PDB into DataWarrior to allow similar viewing? Any help woudl be appreciated.

Subject: Re: Veiwing PDB Binding Sites in DataWarrior
Posted by nbehrnd on Tue, 14 Jan 2025 22:30:01 GMT
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For a recreation of a similar illustration, there must be at least one molecule on the spreadsheet. I took water (cf. screen cast concept.gif attached) before heading to chemistry -> dock structures into protein cavity. With a click on the right button of a mouse, the pull down menu opens; for similarity with the illustration you refer to, the option to load 7L7P from the PDB database was selected (which obviously requires a connection to the internet). After completed download, it was possible to select one (already known) ligand; for simplicity, the first one selected here. After completion of the computation, the interactive 3D window was resized; for greater similarity with the reference picture, the look-and-feel of DW's GUI was changed to "graphite".

The advertising picture includes a couple of dotted lines, likely to indicate hydrogen bonding, pi stacking, close contacts. The docking with fifth ligand molecule known to L7LP exhibits this more prominently (see the screen photo attached). As usual, moving the mouse while pressing the right hand button allows to tilt/rotate the molecule/scene depicted in the 3D window.

Regards,

Norwid

File Attachments
1) concept.gif, downloaded 146 times
2) ligand_5.png, downloaded 130 times

Subject: Re: Veiwing PDB Binding Sites in DataWarrior
Posted by thomas on Thu, 16 Jan 2025 10:15:20 GMT
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Currently, you can download and browse through these binding site files, but DataWarrior cannot

create such files itself from e.g. a set of PDB entries. These files were created with a separately developed Java program using OpenChemLib functionality. The mid-term goal is to analyze ligand-protein interaction geometry of different ligand and protein substructure combinations to better visualize and quantify individual interactions, similar to the Rf-interaction concept published by Roche, where they 'forgot' to add the geometry statistics to the papers making it a challenge to reproduce.