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 287 times
2) ligand_5.png, downloaded 256 times