Subject: Re: Docking score and Datawarrior
Posted by juliocoll on Fri, 03 Feb 2023 12:24:55 GMT
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dear Jo,
I can share with you my recent protocol I now follow to link DW sdf to PyMOL images. I attached all-related files. Thomas kindly help is greatly appreciated !.

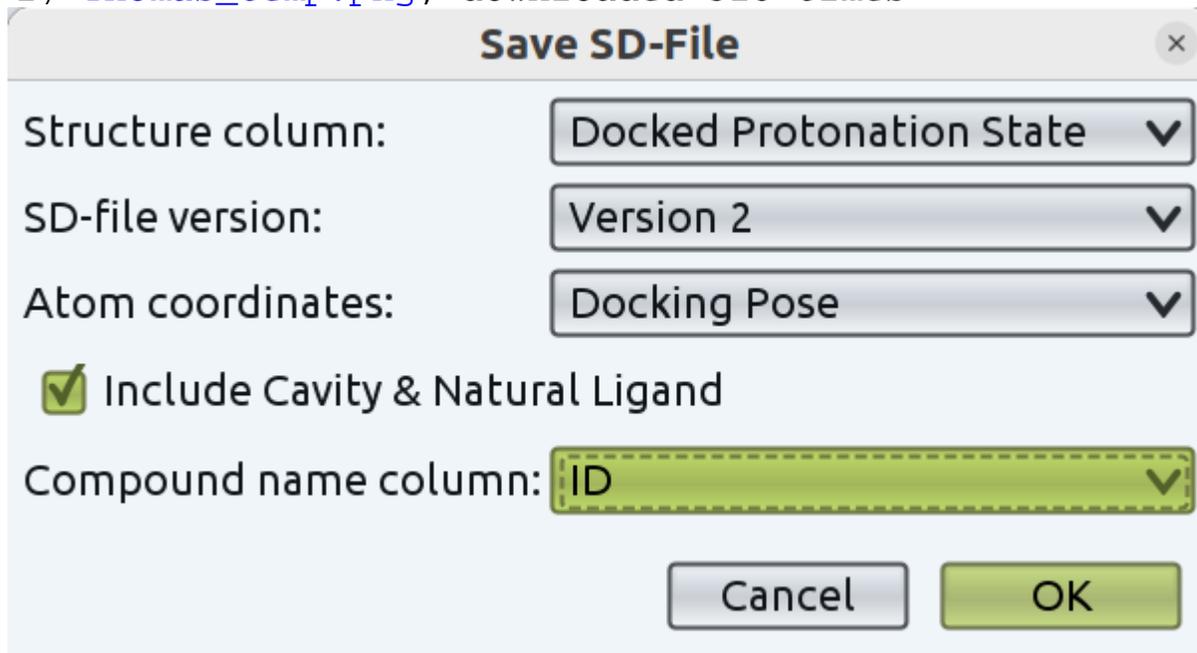It still needs some fine-tunning and I do not know if it would work on other OSs.

Hope it helps!

julio

## File Attachments

1) DW to PyMOL.Table.docx, downloaded 624 times
2) Thomas_temp.png, downloaded 528 times



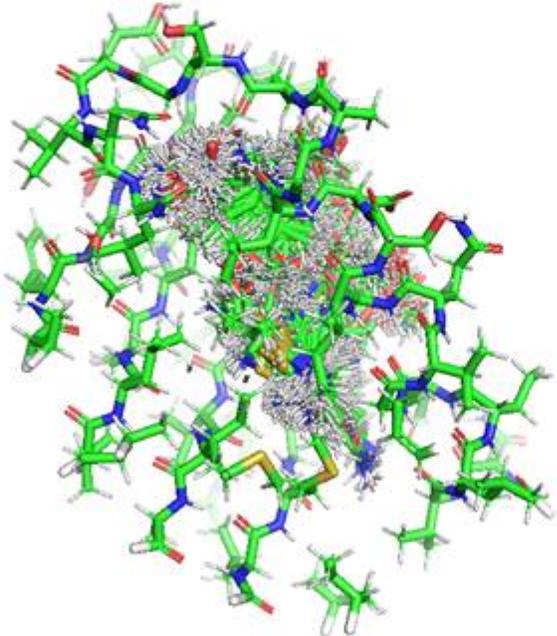3) - BuildEvolutionaryLibrary.docx, downloaded 918 times
4) Figure1.PyMOl protein cavity+ligands.jpg, downloaded 548 times

5) Figure2.PyMOl protein cavity+ligands+protein.jpg, downloaded 1301 times

File  Edit  Build  Movie  Display  Setting  Scene  Mouse  Wizard  Plugin  Help

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2999Evolutionary_Library<--
PyMOL>split_states 299Evolutionary_Library
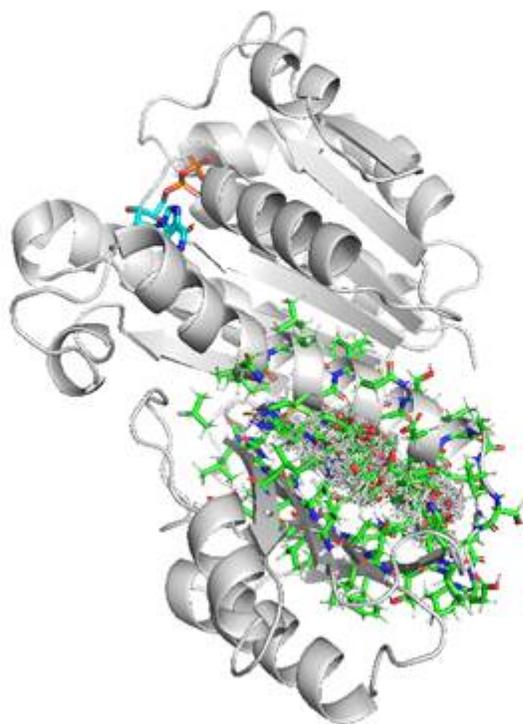 Warning: Invalid characters in 'Protein_Cavity' have been replaced or stripped
 Warning: Invalid characters in 'Natural_Ligand' have been replaced or stripped

 Setting: seq_view set to off.
 ObjectMolecule: Read crystal symmetry information.
 CmdLoad: "" loaded as "4dxd".

PyMOL>

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