Subject: Docking score and Datawarrior
Posted by Jo W on Fri, 23 Dec 2022 13:23:47 GMT
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The docking score in DW seems to be very, very useful but there appears to be no information on it in the manual or in the forum.

Could we have some more information here – even just a brief paragraph on how it works in DW would be greatly appreciated. I am referring to the feature of “dock structures into the protein”.

Is this a flexible/static/mixed docking process?

Also what forcefields are used in the minimisation?

It seems to only work if you upload a protein combined with a ligand rather than just the protein alone from PDB – why is that?

Can it be adapted to work with other structures (ie not just proteins) for example, such as the modeling haem complexation with various metal ions such as K+ instead of Iron?

Is it possible to include the export of a protein/ligand docking as a pdb or sdf file Mol filer (ideally all three!) after docking in DW?– this does not seem possible at the moment and would be very useful for example for looking in more detail within an external 3D visualization software such as Pymol?

If there is any chance of even a brief answer to any of the above before xmas it would be very much appreciated as I would like to play with this more over the xmas break

Many thanks in advance

Subject: Re: Docking score and Datawarrior
Posted by nbehrnd on Thu, 29 Dec 2022 09:46:08 GMT
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Dear Jon,

> Also what forcefields are used in the minimisation?

In chapter Chemistry 3D, section minimize energy, the documentation shipped with DW lists MMFF94s+, MMFF94s, and Idorsia forcefields.

Because Joel Wahl is mentioned as contributor to MMFF94s+ for «A peer-reviewed publication is in process.», maybe «Accuracy evaluation and addition of improved dihedral parameters for the MMFF94s» by 2019 is the corresponding literature reference[1] to address problems in MMFF94s. DW as distributed here possibly is not on the white list for Idorsia's forcefield.

Norwid

[1] https://jcheminf.biomedcentral.com/articles/10.1186/s13321-0 19-0371-6 It is an open access publication; by today, there are 15 citations of this work the journal identified.

Subject: Re: Docking score and Datawarrior
Posted by Jo W on Wed, 04 Jan 2023 14:35:50 GMT
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Many thanks Norwid. Could you and/or Thomas comment on my other points?
Happy new year

Subject: Re: Docking score and Datawarrior
Posted by Jo W on Tue, 17 Jan 2023 14:05:41 GMT
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Within the "dock structures into protein cavity" feature, is it possible to include the ability to export a protein/ligand docking as a pdb or sdf file / Mol filer (ideally all three) after docking in DW?– this does not seem possible at the moment and would be very useful for example for looking in more detail within an external 3D visualization software such as Pymol.

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 !.

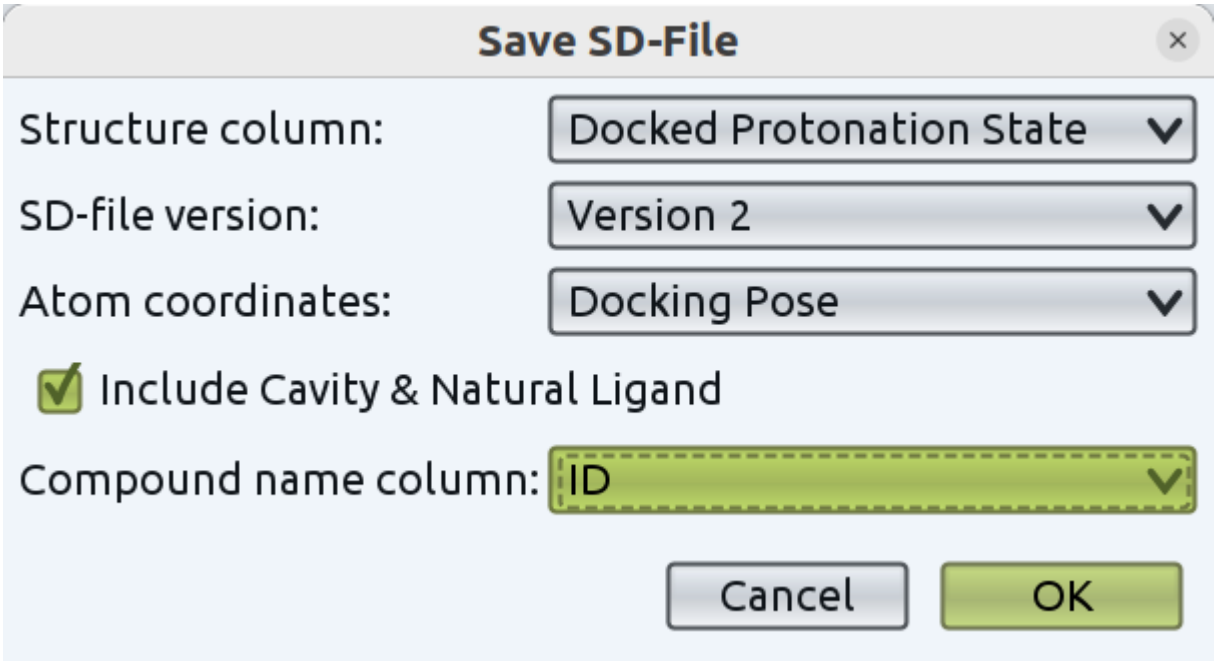
It still needs some fine-tunning and I do not know if it would work on other OSs.

Hope it helps!

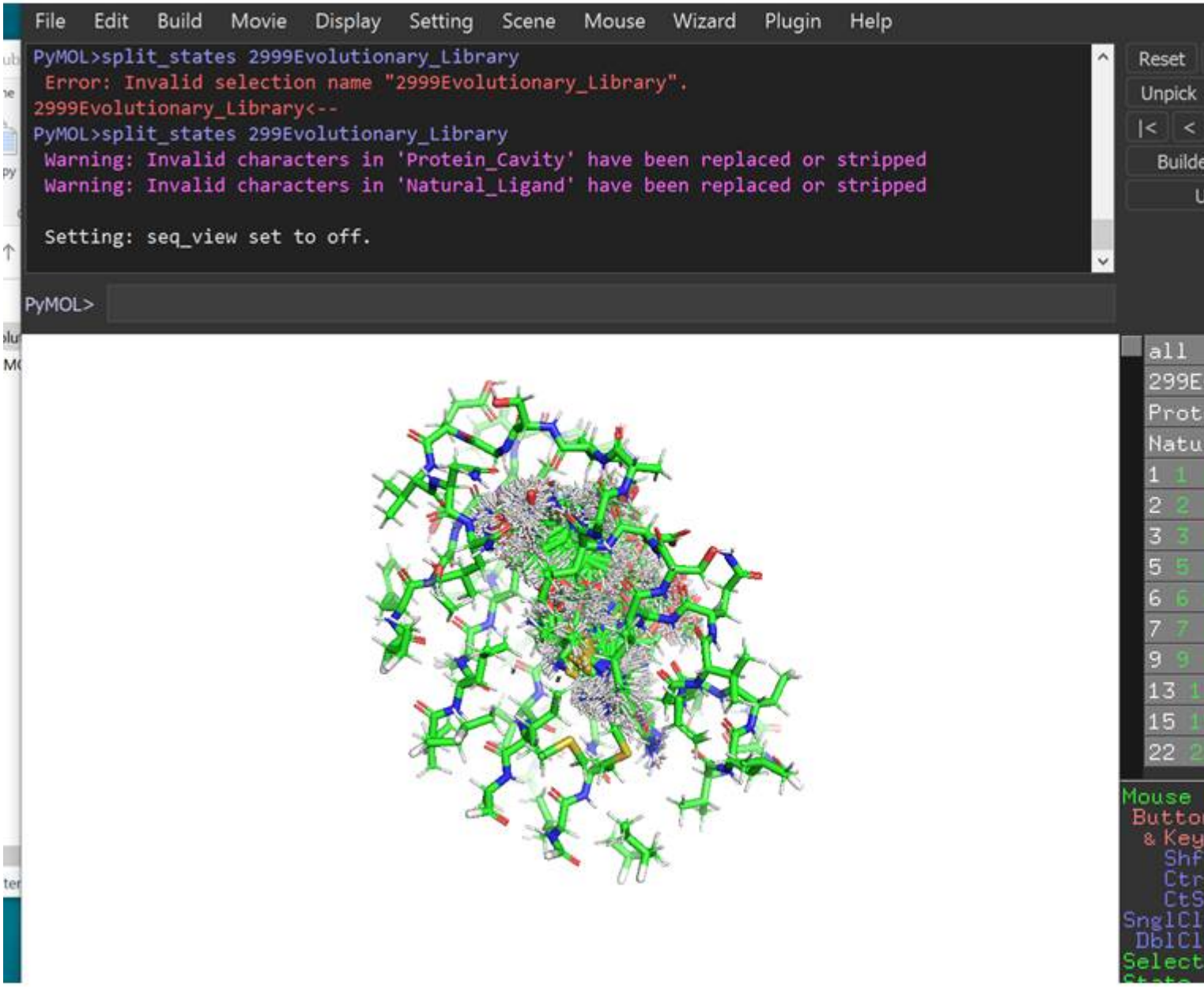
julio

File Attachments

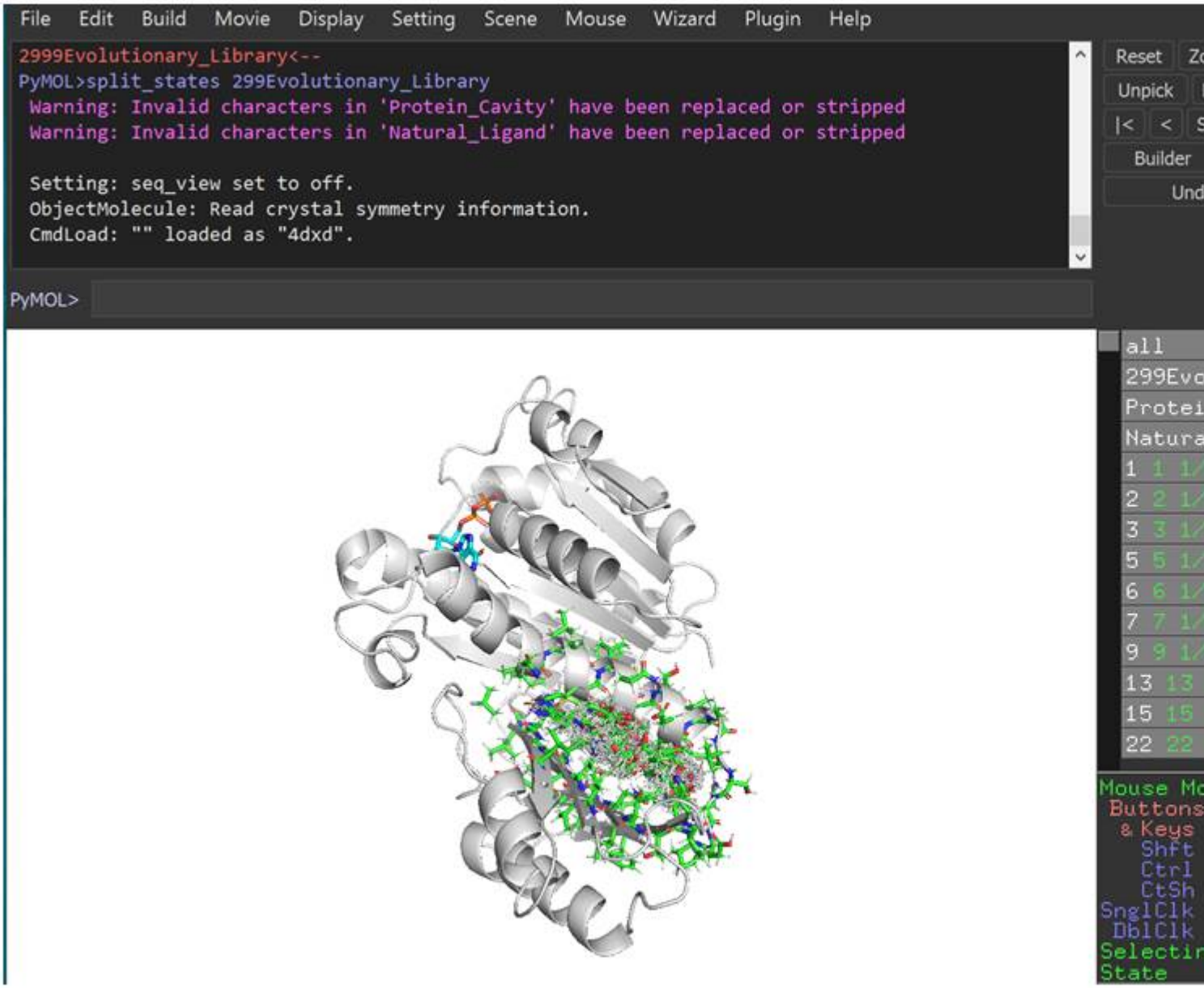
1) DW to PyMOL.Table.docx, downloaded 652 times
2) Thomas_temp.png, downloaded 596 times



3) - BuildEvolutionaryLibrary.docx, downloaded 934 times
4) Figure1.PyMOl protein cavity+ligands.jpg, downloaded 656 times



5) Figure2.PyMOl protein cavity+ligands+protein.jpg, downloaded 1417 times



Subject: Re: Docking score and Datawarrior
Posted by Jo W on Sat, 04 Feb 2023 18:22:58 GMT
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Julio
There was some information I was missing, but you have solved it and the exporting out of DW now works.

Many thanks for your and Thomas's efforts
Jon