
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 file (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/s13321-019-0371-6> 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-tuning 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 679 times
- 2) [Thomas_temp.png](#), downloaded 655 times

Save SD-File ✕

Structure column: ▼

SD-file version: ▼

Atom coordinates: ▼

Include Cavity & Natural Ligand

Compound name column: ▼

3) - [BuildEvolutionaryLibrary.docx](#), downloaded 948 times

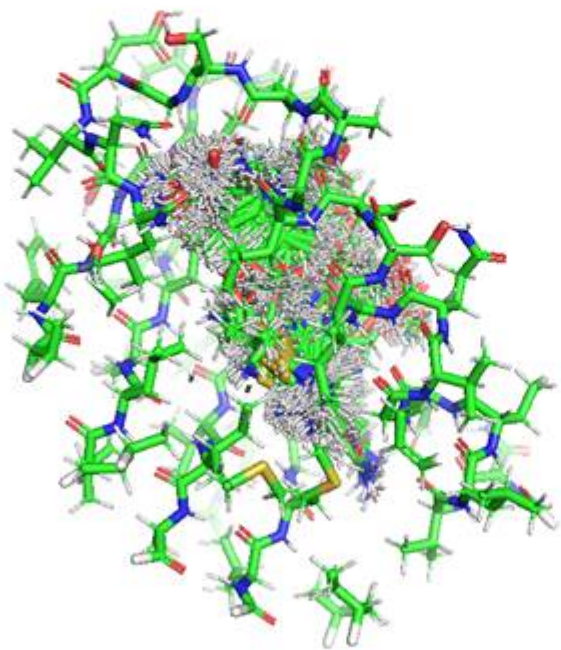
4) [Figure1.PyMol protein cavity+ligands.jpg](#), downloaded 774 times

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

```
PyMOL>split_states 2999Evolutionary_Library
Error: Invalid selection name "2999Evolutionary_Library".
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.

PyMOL>
```



all
299E
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2 2
3 3
5 5
6 6
7 7
9 9
13 1
15 1
22 2

Mouse
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& Key
Shf
Ctr
CtS
SnglCl
DblCl
Select
State

5) [Figure2.PyMol protein cavity+ligands+protein.jpg](#),
downloaded 1556 times

File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

```
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>
```



all
299Evo
Protei
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1 1 ✓
2 2 ✓
3 3 ✓
5 5 ✓
6 6 ✓
7 7 ✓
9 9 ✓
13 13
15 15
22 22

Mouse Mo
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& Keys
Shift
Ctrl
CtSh
SnglClk
Db1Clk
Selectir
State

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
