
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 !.

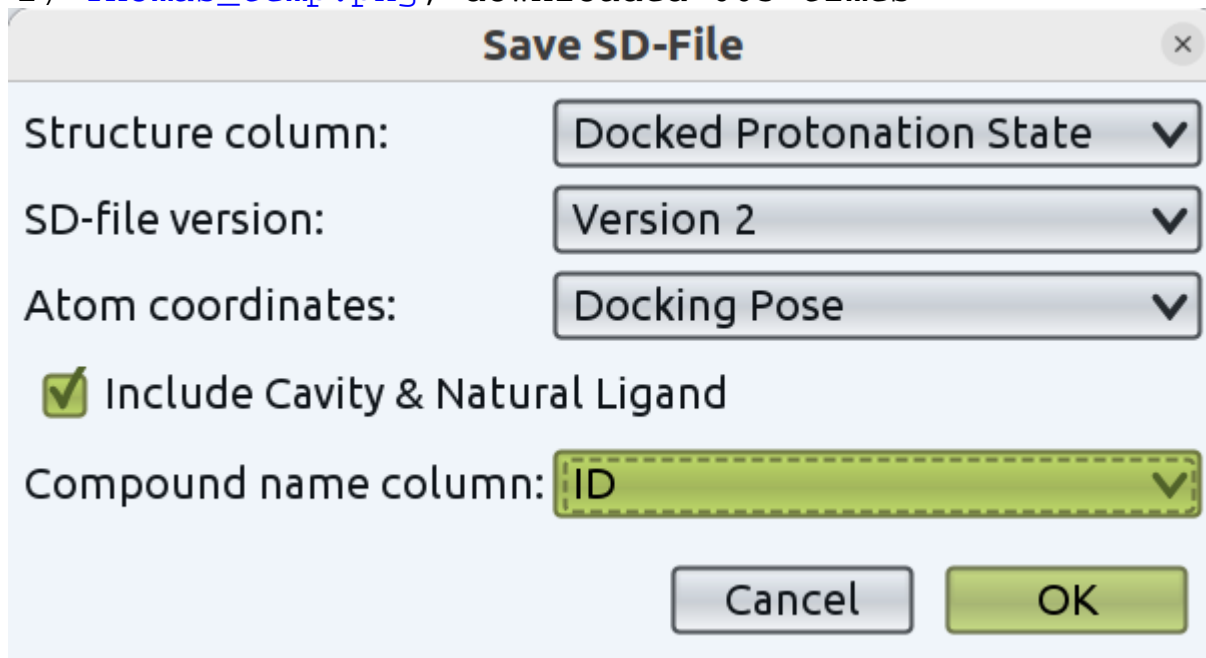
It still needs some fine-tuning and I do not know if it would work on other OSs.

Hope it helps!

julio

File Attachments

- 1) [DW to PyMOL.Table.docx](#), downloaded 683 times
- 2) [Thomas_temp.png](#), downloaded 663 times



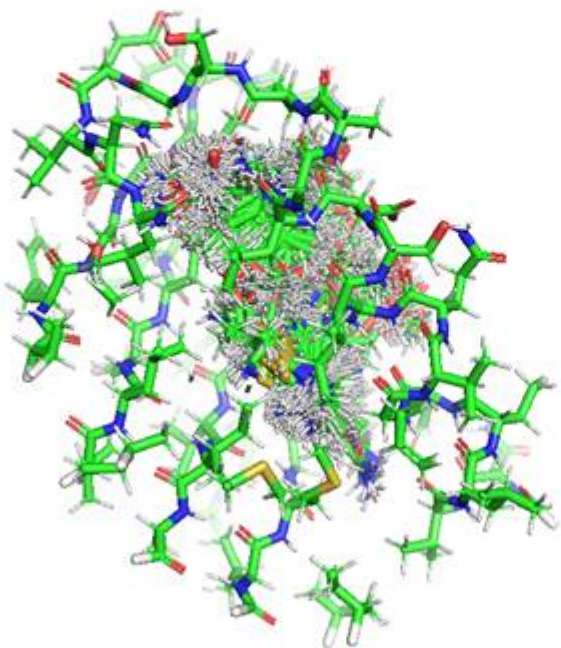
- 3) - [BuildEvolutionaryLibrary.docx](#), downloaded 954 times
- 4) [Figure1.PyMol protein cavity+ligands.jpg](#), downloaded 792 times

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>
```



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DblCl
Select
State

5) [Figure2.PyMol protein cavity+ligands+protein.jpg](#),
downloaded 1576 times

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2999Evolutionary_Library<--

PyMOL>split_states 299Evolutionary_Library

Warning: Invalid characters in 'Protein_Cavity' have been replaced or stripped

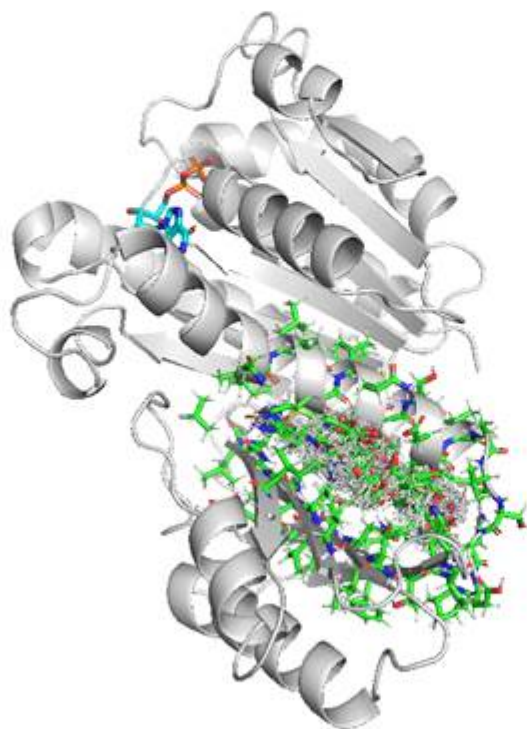
Warning: Invalid characters in 'Natural_Ligand' have been replaced or stripped

Setting: seq_view set to off.

ObjectMolecule: Read crystal symmetry information.

CmdLoad: "" loaded as "4dx".

PyMOL>



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