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