Subject: Re: Docking score and Datawarrior Posted by Jo W on Tue, 17 Jan 2023 14:05:41 GMT View Forum Message <> Reply to Message

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.

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