
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.
