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Subject: Re: Copy and Paste 3D Pose

Posted by [nbehrnd](#) on Tue, 10 Jan 2023 07:27:13 GMT

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I think you refer to the (interactive) structure display which shows e.g., the superposition of conformers. One can pick one molecule at a time from this one (right click on the molecule of interest when it no longer uses the CPK colors, but is uniform turquoise), however the representation (possibly) is the 2D/3D idcode string only (the format equally used internally in the .dwar file. To best of my current knowledge, this window does not yet allow the direct export of one, or about all the molecules displayed as .sdf. I'm going to perform some additional tests during the day.\*)

Norwid

\* I once suggested to openbabel to add reading/exporting DW's idcodes. So far, the incentive was not convincing / attractive enough (<https://github.com/openbabel/openbabel/issues/2311>).

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