Subject: Viewing 3-D structures from an imported SDF in DW.
Posted by timritchie on Sun, 27 Jan 2019 11:23:45 GMT
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Hello,
I've loaded a SDF into DataWarrior containing several molecules with 3-D conformations
superimposed on a common substructure (generated externally in MOE).
I can see the 3-D structure in the panel bottom right, but only when I hover over a structure in the
table or structure view. Is it possible to keep the 3-D structure visible in order to rotate it for a
selected molecule?
Also I like the 3-D conformer viewer. Is it possible to use this to view the imported conformers but
without first running any conformer generation within DW?
Thanks and regards,
Tim.

Subject: Re: Viewing 3-D structures from an imported SDF in DW.
Posted by timritchie on Sun, 27 Jan 2019 12:03:36 GMT
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Hello again,
Just realised that the 3-D molecule stays in the RHS panel only when a molecule is selected in a
2-D or 3-D visualisation...
It would still be nice to be able to overlay them in the Conformer Explorer using the originally
imported conformers.
Regards,
Tim.
PS. This is in version 5.0.0 by the way.

Subject: Re: Viewing 3-D structures from an imported SDF in DW.
Posted by thomas on Tue, 12 Feb 2019 17:49:45 GMT
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Hallo Tim,
thank you for the suggestions. I have some conformer super-positioning functionality on the
agenda for this year. Whether it will be part of DataWarrior or part of a new project (fxmolviewer
on github) is not yet decided. Possibly it will be both, because the conformer viewer in
DataWarrior is based on fxmolviewer.
Best wishes, Thomas