Subject: Viewing 3-D structures from an imported SDF in DW. Posted by timritchie on Sun, 27 Jan 2019 11:23:45 GMT

View Forum Message <> Reply to Message

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,

Thanks and regar

Tim.