Subject: Bug in how stereochemistry is reported
Posted by richards99 on Fri, 08 Jan 2021 10:52:09 GMT
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Hi,
When a molecule has had its 3D coordinates generated in other software packages, and then these are loaded into DataWarrior as an SDF, it seems the stereochemistry representation in the table is not always correct or defined.

Not knowing how this works so I am only speculating, but I suspect DW may be picking up flags just from a 2D representation and not looking at the 3D representation. Is it possible for DW to look and see if 3D coordinates have been generated, and if they have, then to display the stereochemistry defined in the 3D conformation.

It has been causing a lot of problems, in that when generating smiles in DW of molecules with 3D coordinates, it is sometimes returning the wrong stereochemistry or undefined stereochemistry.

Thanks,

Simon.