Subject: Re: Bug in how stereochemistry is reported
Posted by richards99 on Thu, 11 Mar 2021 08:26:49 GMT
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Hi Thomas,
Below is a text file of the SMILES I mention in the previous post. When I load this directly into DataWarrior, the carbon with the alcohol attached correctly shows a wedge bond indicating its chirality, whilst the carbon which has the nitrile attached only shows flat bonds with a ? label to indicate unknown stereochemistry. I am using the Dev build of DataWarrior. Other colleagues can reproduce the problem I am seeing also.

With regards the chiral flag issues of mol files, the solution you propose would be very useful as there seems to be multiple tools which are not setting the chiral flag, and therefore when importing into DataWarrior the stereochemistry is getting scrambled. Whether it is in the dialog box for opening an SDF, or a setting in the preferences, I do not mind, so long as an option is available.

Thanks,

Simon.

File Attachments

1) temp.txt, downloaded 820 times