Subject: Racemates showing as chiral
Posted by DaveS on Mon, 24 Jun 2019 13:11:38 GMT

Hi,

I have recently discovered an issue that I have traced back to the use of DataWarrior. I was sent sdf files containing a subset of compounds that are racemic. When imported into DW they show as chiral with a wedge/hashed bond and when I export, this is carried in the export file so when I upload into my database, the pure enantiomers are uploaded rather than the racemates. I noticed that the chiral flag is rightly marked as zero but in the SMILES field, a specific stereochemistry is shown.

When i import the exported sdf into any other software, the racemates are defined as chiral so I'd like to know how to avoid the chirality being added where it is not wanted and how to display without the wedge/hashed bonds.

Any suggestions are gratefully received.

Thanks,

Dave