Subject: Re: Racemates showing as chiral
Posted by thomas on Tue, 25 Jun 2019 11:30:42 GMT

Hi Dave,

DataWarrior consequently uses the 'enhanced stereo representation' that MDL has introduced with the molfile version 3. Unluckily, many software packages still write molfiles and sd-files version 2, which lack support for proper stereochemistry encoding. When DataWarrior exports a racemate with multiple stereocenters into a molfile 2, then up- and down-bonds are written in order to not loose the relative configuration between the stereo centers. And the 'chiral' flag is not set to indicate that it is a racemate. In the special case, where we have exactly one stereo center, DataWarrior still writes an up- or down-bond. If it would not do that, the undefined stereo center could be interpreted as unknown, either R or S, or as racemate.

With the SMILES encoding there has been the problem that you describe, but it is fixed since some months. In case of a racemate with one stereo center, the stereo symbols '@' are not included in the SMILES anymore. You may download a DataWarrior patch with the fix from openmolecules.org/datawarrior/dw500win.zip (for linux or mac use dw500x.zip), then open the zip archive and move the obtained files into the original installation folder.

Best wishes,

Thomas