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

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

Subject: Re: Racemates showing as chiral
Posted by DaveS on Tue, 02 Jul 2019 12:57:42 GMT
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Thanks Thomas,

So where exactly to I place the files I downloaded? I am working on a Mac so I was going to place them in the the Applications folder, within which I keep the datawarrior app.

Is this correct?

Thanks,

Dave

Subject: Re: Racemates showing as chiral
Posted by thomas on Tue, 09 Jul 2019 11:51:12 GMT
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Sorry Dave for the late reply. I somehow missed the question. These files replace the original ones in "/Applications/DataWarrior.app/Contents/Java/". You may use a terminal to copy them there or you can do it interactively within the Finder: Open the 'Application' folder and perform a right mouse click over the DataWarrior application icon. Then select something like 'Open Package Contents'. A Finder window opens and lets you navigate into Contents and Java, where you need to replace datawarrior.jar and put the other file(s) as well.

Thomas