Subject: Loss of stereochemical information when importing sdf file
Posted by Mike Parker on Fri, 08 Feb 2019 20:11:31 GMT
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I have a database file in sdf file format. It includes chemical compounds with a single stereocenter in which stereochemistry is drawn explicitly. Compounds are either the (S)-enantiomer or the (R)-enantiomer. When I open the file in Datawarrior, each is depicted as a racemate. The stereochemical information appears to have been lost. However, when I copy the SMILES string for each structure I can see that a stereochemical designator is still present (@ or @@) - but the structures that were R and S in the original sdf file have both become S in the SMILES string. So, in fact, the stereochemical information appears to have actually been altered in some cases, not lost.

Any ideas about what might be going on or suggestions on how to avoid the issue?