Subject: Re: Bug in how stereochemistry is reported
Posted by richards99 on Thu, 04 Mar 2021 08:50:12 GMT
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There also seems to be issues with it accepting chiral atoms next to Nitrile groups. For example, if you paste this made up structure into DataWarrior, it should have two chiral atoms, as defined in the SMILES, but it does not create two chiral atoms:

CC[C@H](O)[C@@H](CC1=CC=CC=C1)C#N

Thanks,
Simon.