Subject: Visualising SMILES string
Posted by amorrison on Thu, 18 Mar 2021 09:55:31 GMT
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Hi Thomas,

I have a smiles string with an attachment point that has been created in another application, e.g. C1CCC([*:1])CC1. Datawarrior fails to identify it as a valid smiles either on paste or convert structure to name. I'm assuming it's the '*:1' that is the issue. Can I modify the smiles so it can be interpreted by Datawarrior?

many thanks in advance,

Angus