Subject: Re: Visualising SMILES string
Posted by amorrison on Sun, 21 Mar 2021 04:00:31 GMT
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Thanks Thomas,

I've tried this. Doing a find and replace my smiles string becomes - C1CCC([*])CC1. If try a structure to name this is still not recognised as a valid smiles. If I remove the square bracket - C1CCC(*)CC1. I get the structure but lose the attachment point.

Sorry if this trivial I'm a med chemist and not so familiar with smiles syntax.

Thanks,

Angus