Subject: Re: Visualising SMILES string
Posted by thomas on Tue, 23 Mar 2021 15:38:22 GMT
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Dear Angus,

I have extended the SmilesParser within OpenChemLib and used by DataWarrior to support '*' and '?' as pseudo atom symbols. Both symbols can be used inside or outside square brackets. While '*' is inline with the opensmiles.org standard, '?' is not. Nevertheless, because of the missing distinction in the smiles syntax between query fragments and full molecules, I believe that '?' makes sense.

'*' creates a wild card atom, which is an atom query feature and only allowed in query fragments. Therefore, a smiles containing a '*' is atomatically perceived as a query structure rather than a full molecule. Its free valences are not considered as being filled with hydrogen.

'?' is converted into an atomicNo=0, which DataWarrior uses as attachment point, e.g. in R-groups after a SAR deconvolution. These atoms are meant to not exist. Their sole purpose is to carry the bond sticking out of the R-group.

If you paste the these 6 rows of smiles:

C1CCC([*:1])CC1O
C1CCC([*])CC1O
C1CCC(*)CC1O
C1CCC([?:1])CC1O
C1CCC([?])CC1O
C1CCC(?)CC1O

into a new DataWarrior Window (newest dev release), then you get the following table:
Note that I have added an oxygen atom. If you see an 'H' at the oxygen, the structure is considered a molecule. If not, the structure is a query fragment with open valences.

File Attachments

1) t.png, downloaded 1033 times