Subject: sp3 count
Posted by mvamos on Mon, 09 Aug 2021 22:22:08 GMT
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I'm curious about the sp3-Atoms count from the Calculate Properties->Atom Counts section. Generally for fraction sp3 calculations, it's # of sp3 carbon atoms divided by total carbon atoms. The sp3-Atoms count from DW seems to over-count, just not sure what else it's including.

In the attached photo, for the compound I count 3 sp3 carbon atoms, but DW returns 5.

Feature request: it might be more useful for users if it calculated the fraction of sp3 carbons instead of just # of sp3 atoms, as it's common to report the fraction for druglike compounds. https://pubs.acs.org/doi/10.1021/jm901241e

Thanks and keep up the good work!

File Attachments
1) Untitled9.png, downloaded 373 times

Subject: Re: sp3 count
Posted by nbehrnd on Tue, 10 Aug 2021 20:24:10 GMT
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Dear mvamos,

based on the SMILES string generated by DW for this very structure, yet submitted to RDKit (2020.09.4) suggests different programs assign sp3-hybridization differently. In the case of RDKit, including fluorine [sic!], a total of 6.

Norwid

File Attachments
1) test_case.zip, downloaded 347 times

Subject: Re: sp3 count
Posted by thomas on Thu, 19 Aug 2021 19:23:57 GMT
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Dear Mvamos,

DataWarrior considers C,N,O,P,S as potential sp3 atoms. In your case the 2 oxygen atoms are considered to be sp3 in addition to the 3 obvious carbon atoms. I agree that an ether-oxygen doesn't contribute much to the 3D-shape of a molecule, but the same is true for an (sp3) methyl group. It is a formal number. sp3 fraction in carbon atoms is simple and I will add it...

Thomas

Subject: Re: sp3 count
Posted by thomas on Fri, 20 Aug 2021 10:05:19 GMT
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I just deployed an update with 'sp3-Carbon Fraction', which is the count of sp3 carbons devided by all carbons as proposed in the 'Escape from flatland' paper.