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 1357 times

