
Subject: Deuterium in property calculations

Posted by [jenninaj2019](#) on Fri, 12 Apr 2019 14:19:33 GMT

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All,

I was surprised that datawarrior's clogP calculator treats a deuterated molecule differently than a protium analog.

A simple example of benzene vs. hexadeuterobenzene:

Total Molweight: 78.11 vs. 84.15 (which is correct)

clogP: 1.66 vs. 0 (which is weird)

clogS: -1.616 vs. -0.53 (which I guess comes from the clogP)

Total Surface Area: 73.26 vs. 32.76 (I agree D is effectively smaller than H but I'm surprised by the magnitude)

Relative PSA 0 vs. 0 (which is correct, although with polar molecules this number differs between the two...which likely comes from the Total Surface Area)

Looking at other methods of calculating logP I see that they ignore the D vs. H and produce identical results. I would fix this myself but I figured this is significant an issue to raise with the community.

Lastly, thanks to everyone involved in the development and support of DW: it's an outstanding piece of work.

Best,
Andy
