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