Subject: Re: Similarity analysis using "find similar compounds..." - slow analysis of libraries

Posted by SM2020 on Sun, 29 Nov 2020 14:07:13 GMT

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That great Thomas! Thanks very much.

I've installed and it seems to be working well, including using other descriptors as the basis for the similarity comparison.

I played around with workflows in Knime to achieve similar results but now that this is incorporated into the DW development version, it so much more straightforward(!. Brilliant.

Thanks again.