Subject: Re: Comparing Structure Files
Posted by nbehrnd on Thu, 13 Jan 2022 22:44:47 GMT
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Dear Oliver,

your question contains little material to replicate your finding. Thus, it is difficult to identify a plausible cause for your observation.

On the other hand, I created two tiny libraries of drug-like molecules (chemistry -> generate random molecules) where the defaults were modified slightly (instead of 1000, I opted for 100 molecules each). Subsequently, while reading set_b.dwar, I selected set_a.dwar for a comparison. With a structureFp threshold lowered to 70%, DW identified 13 molecules as similar enough. Raw data, set up of the parameters, and result files in the attachement below. Perhaps the threshold set by you was too high? The criterion «structure exact» isn't a restraint, it is meant as a constraint*); any variation in the molecule to check vs. the reference molecule and the test assigns the two as dissimilar.

*) which may be weakened in regard of stereochemistry, tautomers, or application on the largest fragment only.

Norwid

File Attachments

1) set_a.dwar, downloaded 281 times
2) set_b.dwar, downloaded 265 times
3) parametres.png, downloaded 177 times
4) Similar Compounds.dwar, downloaded 255 times
5) Dissimilar Compounds.dwar, downloaded 255 times