Subject: Re: Errors calculating flexophore-based similarity/activity cliff of certain molecules
Posted by user on Thu, 13 May 2021 04:39:49 GMT
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Edit: the windows version of dev patch works now, but not for the linux version.

Thanks for the quick response Thomas! Flexophore analysis of the dataset is now working with the dev patch (for windows).

Those molecule examples were part of the smiles generated by an open source de novo fragment-based virtual screening code that I'm currently playing with. That code has a feature of automatically generating multiple tautomers and protonation states of a compound, I guess that's where those weirdly defined structures come from.

Datawarrior make it much easier to visualize the screening results with minimal scripting, and the 2D structure of smiles in datawarrior looks nicer than the figures generated with rdkit especially for those bulky and more complicated structures. Really appreciate all your hard work developing this software and making it publicly available.