Subject: Re: Errors calculating flexophore-based similarity/activity cliff of certain molecules
Posted by thomas on Tue, 11 May 2021 15:35:58 GMT
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Thank you for sending these strange, but correctly defined molecule examples. The charge normalization did indeed make a mistake with these 1,2-hydrogen shifted 1,2 dipolar input structures. The problem in the charge normalization is fixed and another issue with the flexophore not working in case of one pharmacophore point only is fixed as well. You can download the update as development patch from the DataWarrior download page after clicking the 'read and understood' checkbox. Note, that the download link for this dev update is in the fine print.