Subject: Re: Functionality request: MPO score
Posted by thomas on Sun, 10 May 2020 18:48:22 GMT
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thank you for the suggestion. I will be happy to implement it. The problem is that the BB score needs a pKa value as input and most DataWarrior installations don't include a pKa-prediction. DataWarrior still uses the ChemAxon pKa prediction, if licensed and installed, which typically is not the case outside Idorsia. This reiterates the need for an open-source pKa prediction...