Subject: Re: Drug score
Posted by thomas on Thu, 05 Nov 2020 12:29:38 GMT
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Dear Sergio,

the contribution factor for the druglikeness part is: *(1-0.5/(1+exp(Druglikeness))).
Thus, if druglikeness increases, then the sum (1+...) grows, 0.5/sum gets smaller and 1-0.5/sum grows towards 1.
Currently, I don't see a problem here. Do you refer to a different formula?

Best wishes, Thomas