Subject: Re: Drug score

Posted by Sifontes on Thu, 29 Oct 2020 13:56:11 GMT

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Dear Thomas,

I installed the macro successfully and performed some test calculations. It worked fantasticly. So far, I had run the calculations in a dedicated excel spreadsheet. Thanks for that new contribution!!! However, I have a doubt. In the formula for the calculation of the drug score, the coefficients for drugability are 1 and 0. That results in and inversely proportional contribution of druglikeness to the drug score, ie. the higher the druglikeness, the lower the drug score. Please, correct me if I'm wrong.

Best wishes,

Sergio