Subject: Re: Functionality request: MPO score
Posted by mvamos on Tue, 28 Apr 2020 22:57:20 GMT
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Thanks!
Wanted to update this posting with an improved CNS-related score: BBB Score. Apparently this one is better at predicting brain penetration.

BBB Score paper: https://doi.org/10.1021/acs.jmedchem.9b01220
A Vortex script to calculate the Blood-Brain Barrier (BBB) SCORE:
https://www.macinchem.org/reviews/vortex/tut48/scripting_vor tex48.php