
Subject: Re: Functionality request: MPO score
Posted by [timritchie](#) on Mon, 21 Feb 2022 12:30:27 GMT
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Hi,
If it's of use, I have created a formula in DataWarrior that calculates the BBB Score using the methodology from the original published article.
One has to enter or paste values for 'Aromatic Rings', 'Non-H Atoms', 'Molweight', 'H-Acceptors', 'H-Donors', 'Polar Surface Area', and 'pKa', and then update the formula and re-calculate the score.
Regards,
Tim Ritchie.

File Attachments

1) [BBBScore.png](#), downloaded 1524 times
