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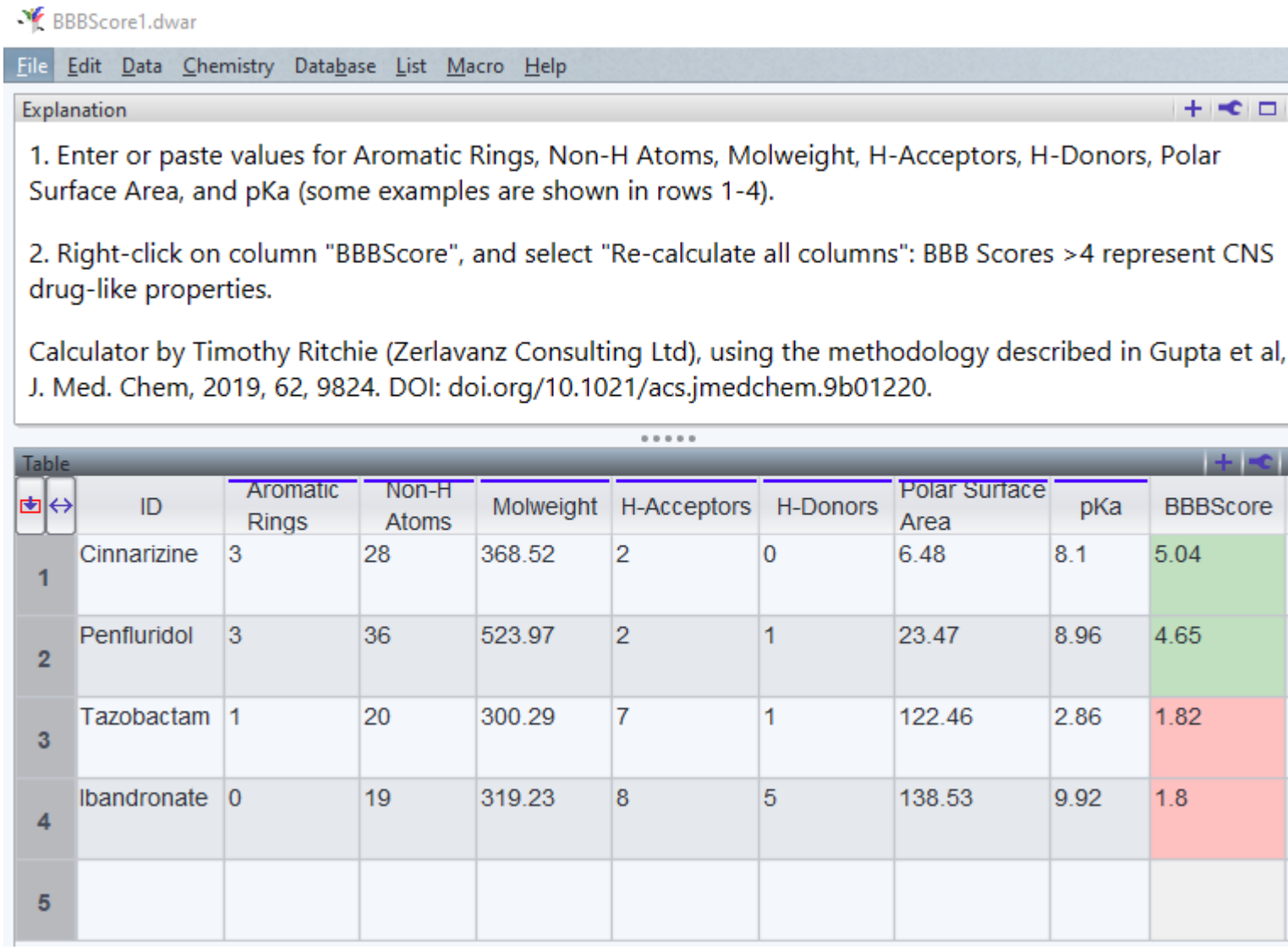
Hi,
If it's of use, I have created a formula in DataWarrior that calculates the BBB Score using the methodology from the original published article.
One has to enter or paste values for 'Aromatic Rings', 'Non-H Atoms', 'Molweight', 'H-Acceptors', 'H-Donors', 'Polar Surface Area', and 'pKa', and then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

File Attachments

1) BBBScore.png, downloaded 2366 times



	ID	Aromatic Rings	Non-H Atoms	Molweight	H-Acceptors	H-Donors	Polar Surface Area	pKa	BBBScore
1	Cinnarizine	3	28	368.52	2	0	6.48	8.1	5.04
2	Penfluridol	3	36	523.97	2	1	23.47	8.96	4.65
3	Tazobactam	1	20	300.29	7	1	122.46	2.86	1.82
4	Ibandronate	0	19	319.23	8	5	138.53	9.92	1.8
5									