

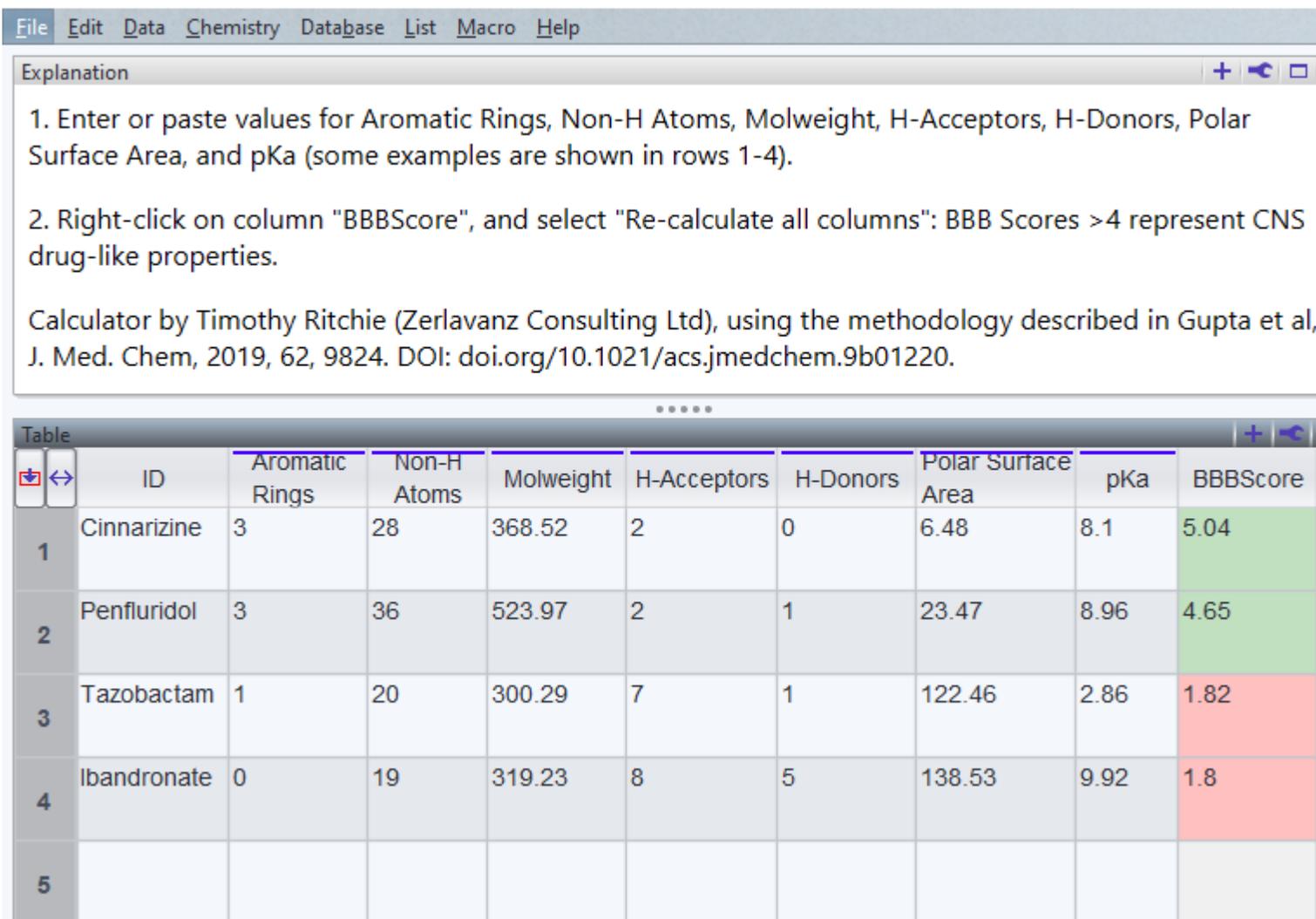
Subject: Re: Functionality request: MPO score
Posted by [timritchie](#) on Mon, 21 Feb 2022 12:30:27 GMT
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Hi,
If it's of use, I have created a formula in DataWarrior that calculates the BBB Score using the methodology from the original published article.
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 2079 times

 [BBBScore1.dwar](#)



The screenshot shows the DataWarrior interface with a menu bar (File, Edit, Data, Chemistry, Database, List, Macro, Help) and a toolbar. The main window is titled "Explanation" and contains the following text:

1. Enter or paste values for Aromatic Rings, Non-H Atoms, Molweight, H-Acceptors, H-Donors, Polar Surface Area, and pKa (some examples are shown in rows 1-4).

2. Right-click on column "BBBScore", and select "Re-calculate all columns": BBB Scores >4 represent CNS drug-like properties.

Calculator by Timothy Ritchie (Zerlavanz Consulting Ltd), using the methodology described in Gupta et al, J. Med. Chem, 2019, 62, 9824. DOI: doi.org/10.1021/acs.jmedchem.9b01220.

Below the text is a table with 10 columns: ID, Aromatic Rings, Non-H Atoms, Molweight, H-Acceptors, H-Donors, Polar Surface Area, pKa, and BBBScore. The table contains 5 rows of data, with rows 1 and 2 highlighted in green and rows 3 and 4 highlighted in red.

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									