
Subject: Re: Use of calculated column functions
Posted by [nbehrnd](#) on Wed, 11 Mar 2020 21:25:50 GMT
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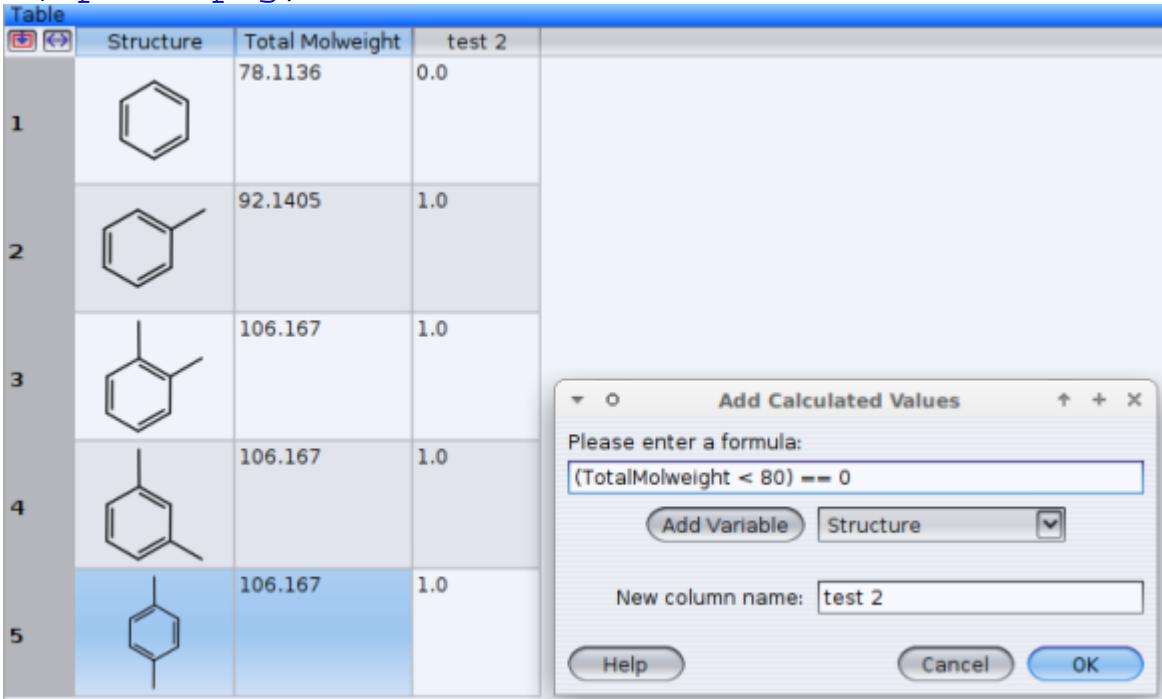
To showcase this function with a minimal working example (attached below), I set up a new file with benzene, toluene, and the xylenes in the first column, and their then molecular masses calculated by DW in the second column. Subsequently, a third column was generated (Data -> Add Calculated Values). Instead of an IC50 value, the MW was used as threshold criterion -- available from the pull-down menu next to «Add Variable» -- which was combined into (TotalMolweight < 80) == 1 as test condition.

Page <http://www.openmolecules.org/help/jep.html> offers additional insight about the functions and syntax available.

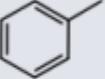
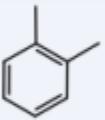
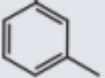
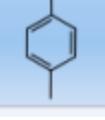
File Attachments

- 1) [minimum_test.dwar](#), downloaded 769 times
- 2) [photo.png](#), downloaded 1302 times

Table



The screenshot shows a software interface with a table and a dialog box. The table has three columns: 'Structure', 'Total Molweight', and 'test 2'. The dialog box is titled 'Add Calculated Values' and contains a formula input field with '(TotalMolweight < 80) == 0', an 'Add Variable' button, a 'Structure' dropdown, a 'New column name' input field with 'test 2', and 'Help', 'Cancel', and 'OK' buttons.

	Structure	Total Molweight	test 2
1		78.1136	0.0
2		92.1405	1.0
3		106.167	1.0
4		106.167	1.0
5		106.167	1.0