

Subject: Re: Use of calculated column functions
Posted by [nbehrnd](#) on Wed, 11 Mar 2020 21:25:50 GMT
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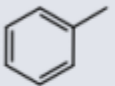
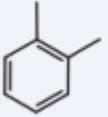
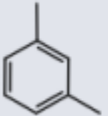

To showcase this function with a minimal working example (attached below), I set up a new file with benzene, toluene, and the xylenes in the first column, and their then molecular masses calculated by DW in the second column. Subsequently, a third column was generated (Data -> Add Calculated Values). 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 $(\text{TotalMolweight} < 80) == 1$ 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

| | 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 |

Add Calculated Values

Please enter a formula:

Add Variable Structure

New column name:

Help Cancel OK