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 947 times
2) photo.png, downloaded 1866 times

