Subject: Use of calculated column functions
Posted by sansun on Wed, 11 Mar 2020 10:09:56 GMT
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I have a file with the bioactivity column for several molecules.

I want to create a new column so that molecules with IC50 less than value 'x' are annotated as '1' while those with more than 'y' value labelled as '0'.

I understand that it can be done bey 'Calculated column' but I am not able to figure out the exact formula.
Any help is appreciated.

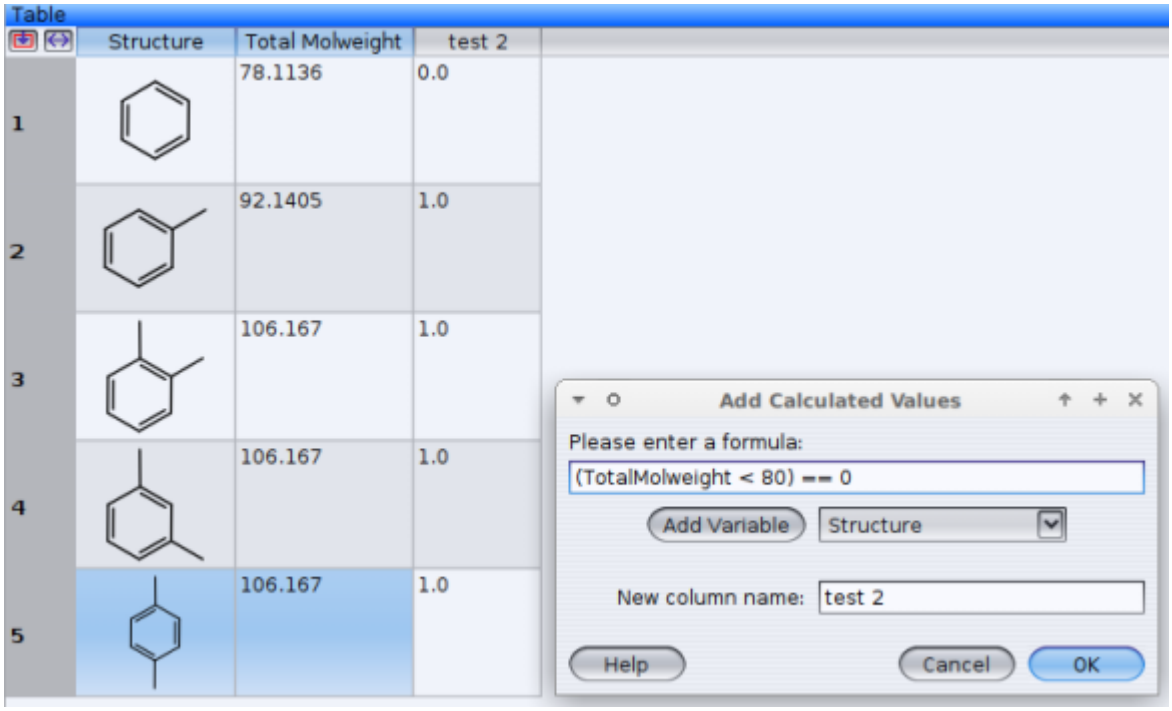
Subject: Re: Use of calculated column functions
Posted by nbehrnd on Wed, 11 Mar 2020 21:25:50 GMT
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To showcase this function with a minimal working example (attached below), I set up a new file with benzene, toluene, and the xylenes in the first column, 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 940 times
2) photo.png, downloaded 1832 times




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Subject: Re: Use of calculated column functions
Posted by sansun on Thu, 12 Mar 2020 10:43:21 GMT
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Thanks a lot.

However, with your example molecules with Mwt = 80 are labelled as 0 but all others are labelled as 1.

My problem is slightly different. For example, I want '1' only for the molecules with Mwt > 100.

I don't want any value (or want some distinct value e.g. '3' for molecules with Mwt between 80-100.

I am trying to find other ways. Let me know if you get some idea.

Thanks again!

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Subject: Re: Use of calculated column functions
Posted by nbehrnd on Thu, 12 Mar 2020 21:03:52 GMT
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Your observation is true because I understood your question as aiming for a (Boolean) on/off or True / False categorical two-level criterion.  Please clarify if this was misunderstood by mine.

So far, I did not mind that instead categorical "1" and "0" strings the calculated column reads like floating numbers "1.0", and "0.0" instead and seems to be limited to two levels. To label molecules of molecular weight greater than 100, the computation would be adjusted to (TotalMolweight > 100 ) == 1. If searching for molecules with a molecular weight either below 80 .OR. greater 100, a plausible instruction were (TotalMolweight > 100 || TotalMolweight < 80) == 1; and the toluene molecule as an example for the range of 80 < MW < 100 is identified by (TotalMolweight > 80 && TotalMolweight < 100) == 1.

I see that attributing a string as a result of such a computation may be useful, or to extend the Boolean two-level perspective for, e.g. annotating members of a compound list as basic / neuter / acidic. Even more so as such an attribution by Add Calculated Values may consider multiple criteria from multiple columns at once. For both however, I do not know if DW contains such a functionality.

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Subject: Re: Use of calculated column functions
Posted by thomas on Wed, 18 Mar 2020 18:19:26 GMT
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This assigns molweights into three different string categories:

if(Molweight<200, "low", if(Molweight>400, "high",""))

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Subject: Re: Use of calculated column functions
Posted by sansun on Sun, 10 May 2020 04:00:29 GMT
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nbehrnd and Thomas, thanks a lot for your useful replies.

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