Subject: Category Filter logic
Posted by chemtv on Wed, 18 Nov 2020 20:01:52 GMT
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From the behavior of using several category filters together it seems the combination of filters uses AND logic? Can this be switched to OR logic?

ie. I get the union of the exact match of filters rather than all the rows with at least one filter being met.

Thanks for the hard work keeping datawarrior running so well!
Greg

Subject: Re: Category Filter logic
Posted by nbehrnd on Wed, 18 Nov 2020 20:55:02 GMT
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Hello Greg,

once the properties are stored in DW's main table, both Boolean .or. and .and. may be used for further analysis. In the example below, I extended the initial query for molecular weights greater than 110 (yielding mesitylene) to one that would accept molecules with a molecular weight of either less than 80 .or. greater than 110 by the instruction

if((TotalMolweight<80) || (TotalMolweight>110), "True", "False")

in an additional column (Data -> Add Calculated Values). As expected, the second query yields both benzene and mesitylene now.

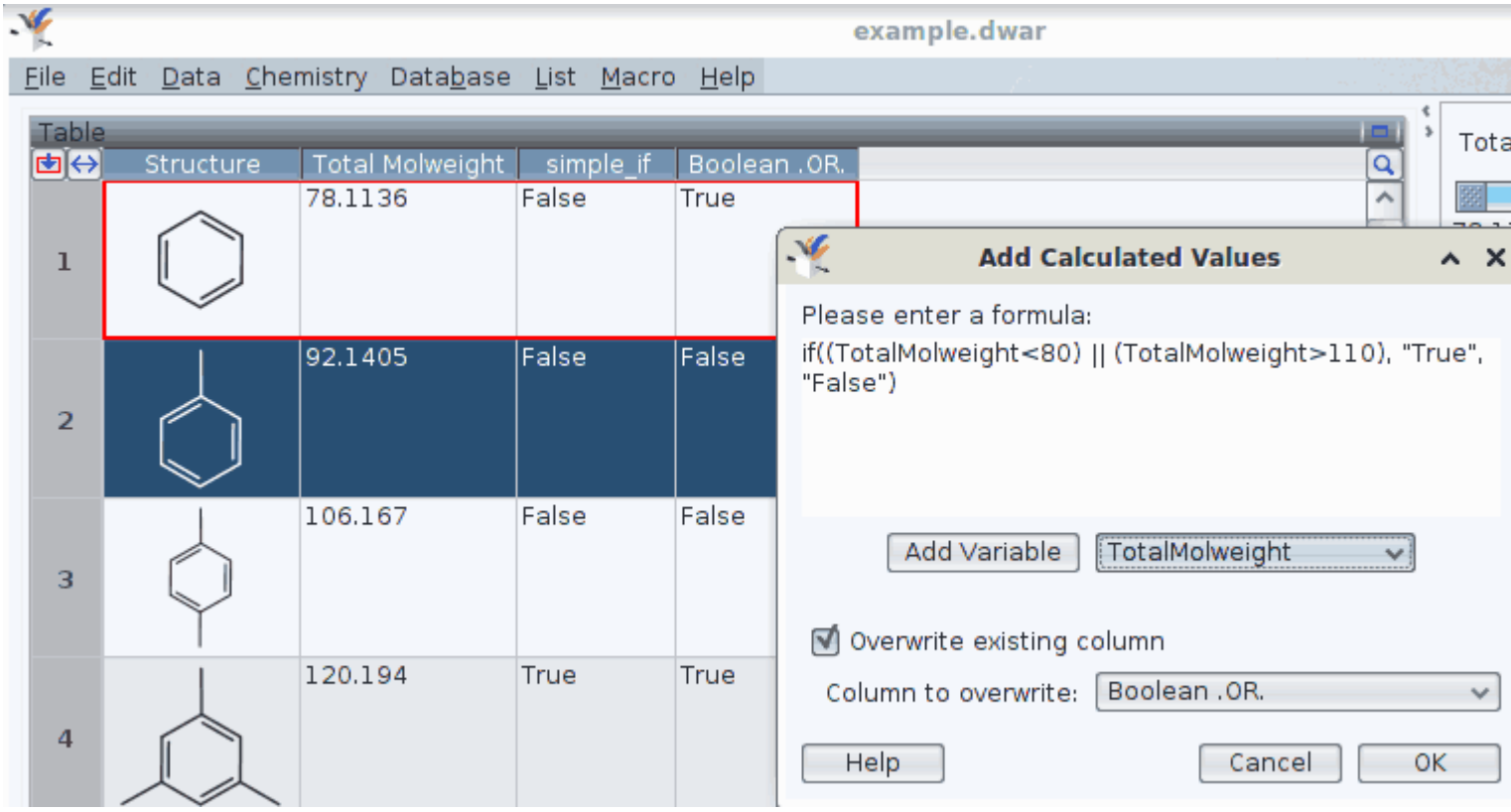
It is possible to use multiple properties of different columns, too. DW's mathematics, including logic expressions, which may be used are presented on

http://www.openmolecules.org/help/jep.html

Norwid

File Attachments

1) example.dwar, downloaded 809 times
2) boolean_or.png, downloaded 1846 times



Subject: Re: Category Filter logic
Posted by thomas on Fri, 20 Nov 2020 21:51:11 GMT
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Multiple filters are always AND, which means that a row to be shown must meat all filter's criteria. Nevertheless, logical OR filtering often can be achieved by one of these ways:
- Use a single filters for logical OR, e.g.
  - a text filter with multiple comma separated items
  - an 'ALL COLUMNS' text filter that searches all columns at once
  - category filters use a natural OR
  - use a multi structure filter hitting if at least one of the provided query structures match
- Using multiple filters with 'inverse' settings allows to model OR to some extend

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Subject: Re: Category Filter logic
Posted by jeusamio on Mon, 04 Sep 2023 15:33:52 GMT
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Hi, is there a way of applying an OR filter that matches a given structure for a specified set of columns?

i.e. Columns 1, 2, and 3 contain chemical structures. I would like to apply a filter to return any row which contains the specified structure in any of the three columns.

Would this kind of behavior be possible?

Thanks,

Javier

Subject: Re: Category Filter logic
Posted by nbehrnd on Mon, 04 Sep 2023 19:36:57 GMT
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Dear Javier,

the program's internal documentation, chapter «working with data» briefly describes `chemsim(descriptor, idcode)` and `chemsim(descriptor1, descriptor2)` as if one could run build a new column of computed (Boolean) values line of `chemsim(PP3DMM2_of_Structure,"gFx@@eJf`@@@")` «check if column PP3DMM2_of_Structure contains the 3D motif of pyridine. I'm not aware if there either is a sketcher/converter to yield the DW's (2D) idcodes other than by access of a .dwar file with a text editor, or if/how e.g., a SMILES/SMARTS string could serve for a (sub) structure search. (Possibly, «descriptor» refers to the ones via Chemistry -> From Chemical Structure -> Calculate Descriptor.) Once identified, an extension to logical .and. and .or. would a next consequent step.

Norwid

Subject: Re: Category Filter logic
Posted by thomas on Thu, 07 Sep 2023 13:10:43 GMT
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Dear Javier and Norvid,

another way would be to merge your three structure columns into one new column and use a sub-structure-filter on the new column.

Norvid's suggestion reminds me to add a new chemsss() function, which would be more useful in this context than the chemsim() function.

Thomas

Subject: Re: Category Filter logic
Posted by nbehrnd on Thu, 07 Sep 2023 20:31:10 GMT
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Dear Thomas,

chemsim() attracted attention because of a recent find that openbabel's not only can retrieve molecules sharing a structural motif as a filter criterion, yet equally can highlight substructures, e.g. (discounting the backticks / accents graves) `obabel -:"c1ccncc1CCOC" -O example.png -s "c1ccncc1 blue"` in visual outputs.

Thank you,

Norwid
