Subject: Feature Request: Reference List Filter
Posted by richards99 on Sat, 30 May 2020 21:43:47 GMT
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Hi,
It would be really useful if with a dataset loaded, you can open up another dataset and use this dataset as a filter against the original data table (based on a specified column such as Structure). So besides the Append File.. option, maybe a Filter From File.. option.

Thanks,

Simon.

Subject: Re: Feature Request: Reference List Filter
Posted by nbehrnd on Tue, 02 Jun 2020 18:18:06 GMT
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Hi Simon,

might the merge/append and merge/replace function of DW an option for you?
http://www.openmolecules.org/help/import.html#MergeData

Norwid

Subject: Re: Feature Request: Reference List Filter
Posted by richards99 on Tue, 02 Jun 2020 19:06:00 GMT
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I'm not sure this will do the function I want.
As an example, I have a data table with structures and data and I want to remove rows with specific structures which I have contained in a separate data file.

Simon.

Subject: Re: Feature Request: Reference List Filter
Posted by nbehrnd on Thu, 04 Jun 2020 12:54:12 GMT
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Hi Simon,

assuming both .dwar files contain a column of structures, DW's function «find similar compounds in file» possibly may perform the kind of sort you seek.

As a minimal example, I created a library of a few compounds around benzene and pyridine with some data computed by DW like molecular weight.  This file (larger_group.dwar, attached below) was closed.

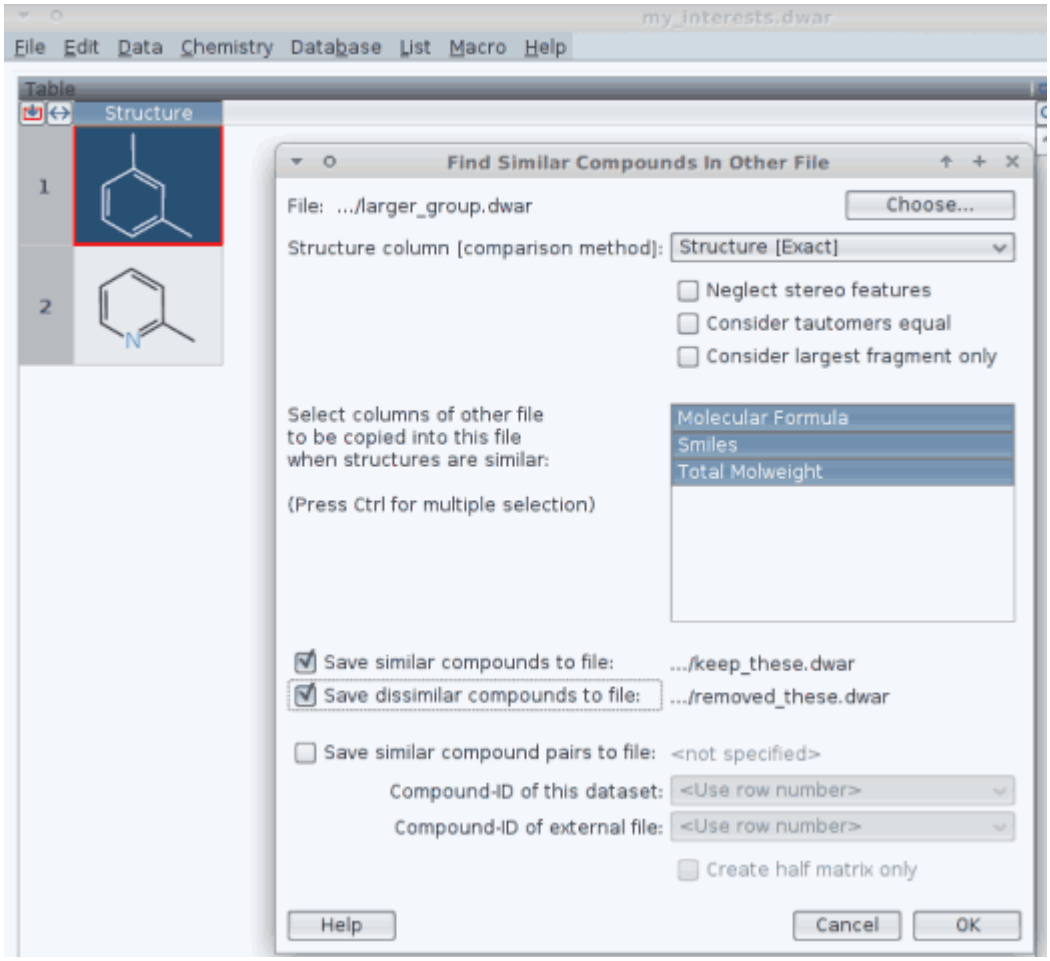
A second file was defined to contain only the structures of o-xylene, and 2-methyl pyridine (my_interests.dwar).  From this file, I accessed chemistry -> Find Similar Compounds In File to encounter a new menu shown below.  The file to scrutinize was indicated in the first field (larger_group.dwar), and the structure criterion was set to be exact.  It is possible to use a less strict, and adjustable structure comparison, which is the one suggested by default, though.

Then, I opted to retain all of the data already computed in larger_group.dwar to be transmitted to either the new file about matching structures (keep_these.dwar), or to export the entries not needed now (file removed_these.dwar).

The scope of structures of the two files newly written is complementary to each other, and adds up to the set of structures in the initial file, larger_group.dwar.

## File Attachments

1) my_interests.dwar, downloaded 651 times
2) larger_group.dwar, downloaded 621 times
3) removed_these.dwar, downloaded 642 times
4) keep_these.dwar, downloaded 598 times
5) GUI_entries-or8.png, downloaded 1030 times

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Subject: Re: Feature Request: Reference List Filter
Posted by thomas on Sun, 07 Jun 2020 18:45:14 GMT
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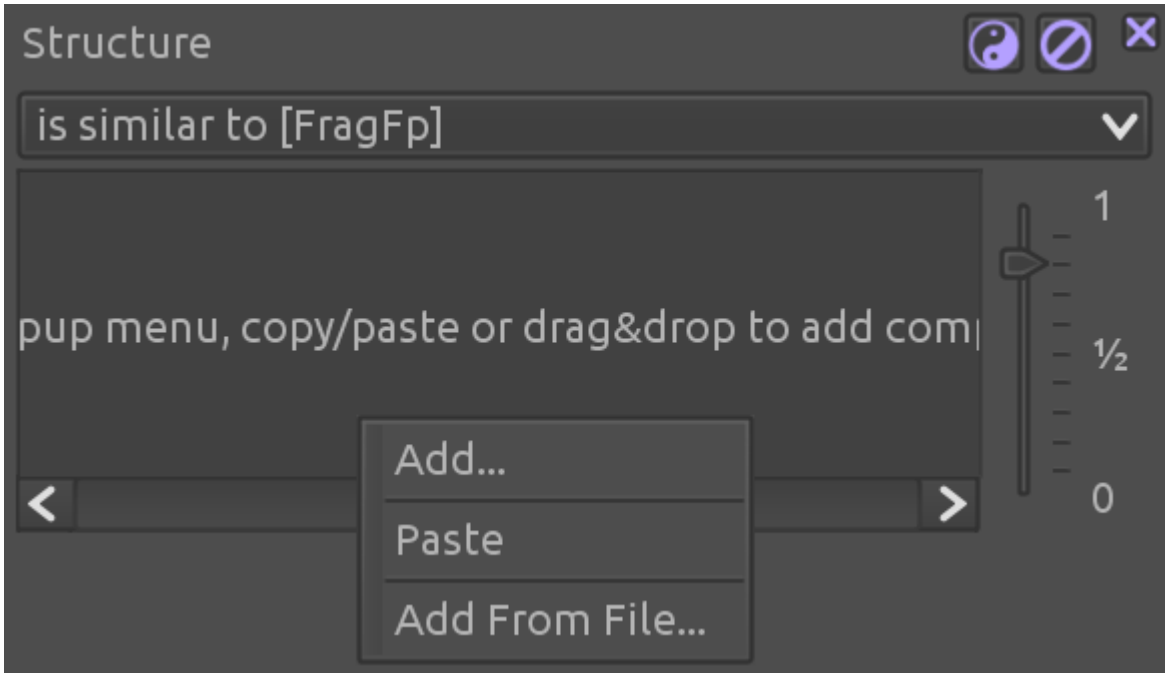
You also could add a structure list filter (substructure of similarity) and open the other file from within the filter structure list with a right mouse click:

## File Attachments

1) msf.png, downloaded 913 times


Structure
is similar to [FragFp]
pup menu, copy/paste or drag&drop to add com
1
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Add...
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Add From File...