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.

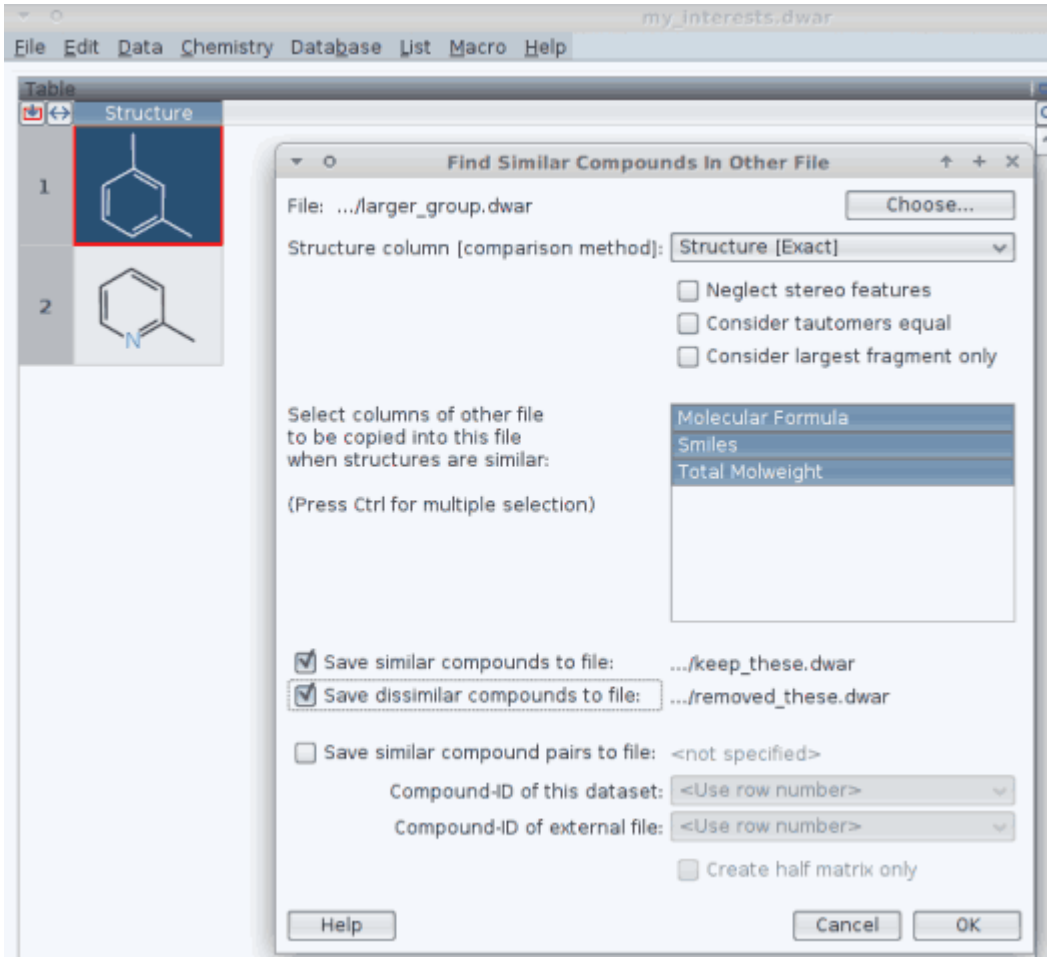
A second file was defined to contain only the structures of o-xylene, and 2-methyl pyridine (my_interests.dwar). From this file, I accessed chemistry -> Find Similar Compounds In File to encounter a new menu shown below. The file to scrutinize was indicated in the first field (larger_group.dwar), and 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 652 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 1032 times


my_interests.dwar
File Edit Data Chemistry Database List Macro Help
Table
Structure
1
2
Find Similar Compounds In Other File
File: .../larger_group.dwar
Choose...
Structure column [comparison method]:
Structure [Exact]
Neglect stereo features
Consider tautomers equal
Consider largest fragment only
Select columns of other file
to be copied into this file
when structures are similar:
(Press Ctrl for multiple selection)
Molecular Formula
Smiles
Total Molweight
Save similar compounds to file:
.../keep_these.dwar
Save dissimilar compounds to file:
.../removed_these.dwar
Save similar compound pairs to file:
<not specified>
Compound-ID of this dataset:
<Use row number>
Compound-ID of external file:
<Use row number>
Create half matrix only
Help
Cancel
OK