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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

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- 1) [my\\_interests.dwar](#), downloaded 385 times
  - 2) [larger\\_group.dwar](#), downloaded 366 times
  - 3) [removed\\_these.dwar](#), downloaded 394 times
  - 4) [keep\\_these.dwar](#), downloaded 364 times
  - 5) [GUI\\_entries-or8.png](#), downloaded 649 times
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