

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 482 times
 - 2) [larger_group.dwar](#), downloaded 454 times
 - 3) [removed_these.dwar](#), downloaded 478 times
 - 4) [keep_these.dwar](#), downloaded 450 times
 - 5) [GUI_entries-or8.png](#), downloaded 797 times
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