Subject: Re: Count # scaffolds by plate ID
Posted by nbehrnd on Mon, 03 May 2021 16:02:16 GMT
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Once the structures are read by DW, you may launch via chemistry -> analyze scaffolds the assignment of the Murcko scaffold. If you like, DW may write a new .dwar file with a frequency count of these common denominators, too:

In these files, the idcode of the identified scaffold is separated by a tabulator from the integer, as documented in the archive attached below. Is this the direction of analysis you would like to automate?

If so, it suffices to identify the pathway you would go to process the data manually, and to document this by recording a macro (`macro -> start recording` to initiate, `macro -> stop recording` to complete DW's «training»). You may export then export the macro as a file as an individual .dwam file, a plain ASCII file.

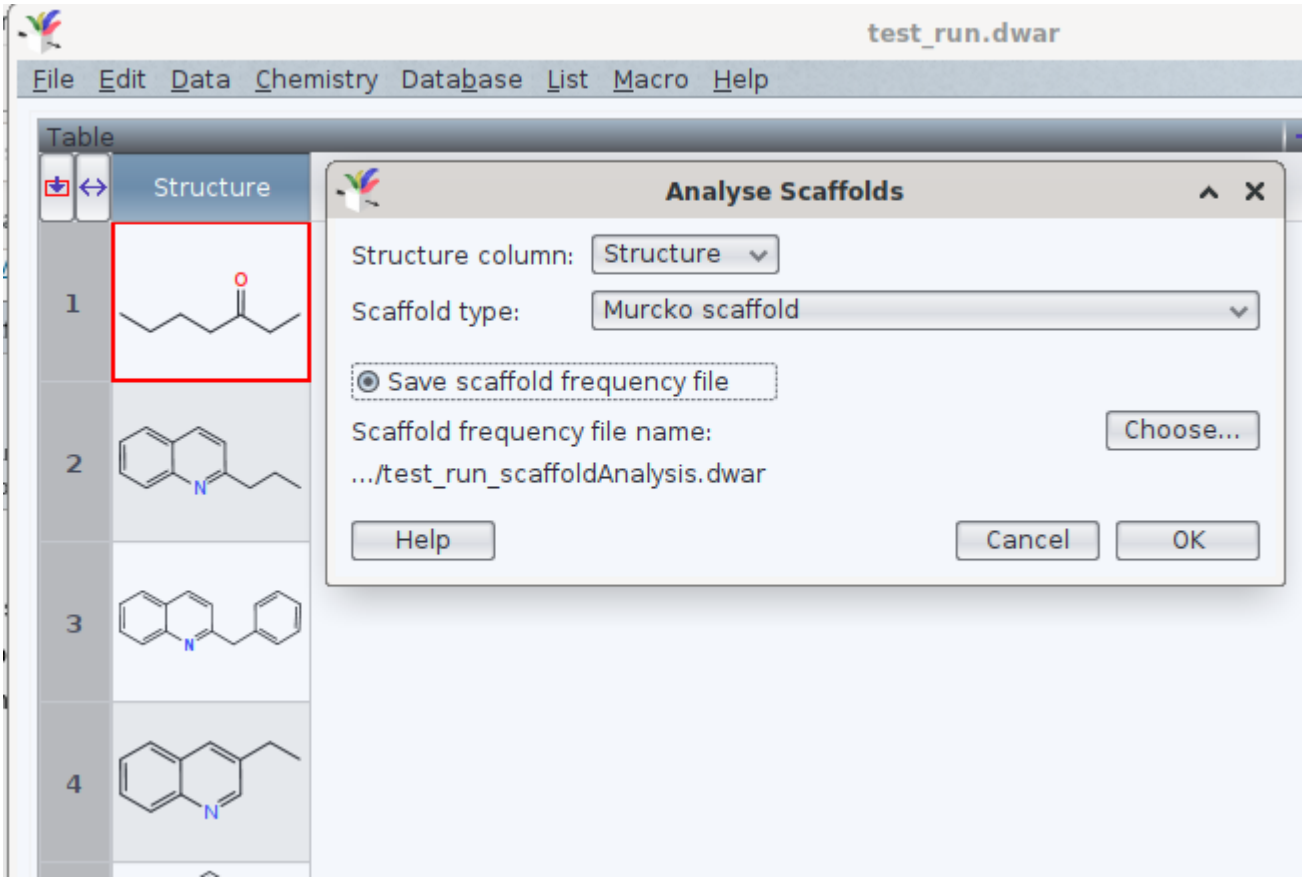
The one attached below as example requires some adjustment in line #5 about the path and file name for the new .dwar (about the frequency count) to be written by you. This edit has to happen outside DW. Then, DW already working, load this macro adjusted .dwam file (macro -> import macro) and let it run (macro -> run macro, then select export_scaffold). As set up by now, it will write murcko_scaffolds.dwar as permanent record.

Note, regardless of your .dwar processed, above macro will yield a file murcko_scaffolds.dwar with the frequency count. Because of the static file name of the output it is possible you accidental overwrite the results of a precedent analysis.

Norwid

File Attachments

1) murcko_scaffold.png, downloaded 1294 times



2) scaffold.zip, downloaded 609 times
3) export_scaffold.dwam, downloaded 636 times