

---

Subject: Re: Count # scaffolds by plate ID  
Posted by [nbehrnd](#) on Mon, 03 May 2021 16:02:16 GMT  
[View Forum Message](#) <> [Reply to Message](#)

---

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 805 times
  - 2) [scaffold.zip](#), downloaded 312 times
  - 3) [export\\_scaffold.dwam](#), downloaded 364 times
-