Subject: Re: Count # scaffolds by plate ID
Posted by nbehrnd on Tue, 04 May 2021 17:06:16 GMT
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I think I grasp your intent. By running the scaffold analysis, you aim for a table which either separates the entries by category like

scafffold	frequency	plate addresses	individual label
isoxazolone	2	12, 91	cmpd18, cmpd13
antipyrine	4	18, 19, 20, 21	cmpd23, cmpd24, cmpd25, cmpd26
...	...	...	...

or one where the number in the plate (plate address) and the compound label are next to each other like

scafffold	frequency	plate address / individual label
isoxazolone	2	12, cmpd18; 91, cmpd13
antipyrine	4	18, cmpd23; 19, cmpd24; 20, cmpd25; 21, cmpd26
...	...	...

Here, «plate address» is used just as alias for the number of the well in the plate == entry line in the initial .dwar file to process.

Norwid