Subject: Count # scaffolds by plate ID
Posted by chemtv on Mon, 03 May 2021 14:35:28 GMT
View Forum Message <> Reply to Message

Hi folks,
I am looking at some plated cpds where I have individual IDs and the assay plate IDs that I am trying to analyze. I want to calculate Murcko scaffolds then count the number of different scaffolds on each plate, (rough estimate of diversity). For datawarrior I suspect this is where macros can be your friend but I'm not familiar with writing macros. Has anyone else tried something like this? Even in Knime I'm not sure how to get to counts of a previous "aggregation". Any thoughts?
Thanks,
Greg