Subject: Re: Count # scaffolds by plate ID
Posted by amorrison on Wed, 05 May 2021 04:23:35 GMT
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Hi Greg,
Would either of these achieve what you are aiming to do.

a) Generate Murcko scaffolds then calculate 'Frequency of same value in same category' - frequencyInCategory(category-column, value-column). Where the category-column is the plateID and the value-column is the Murcko.

b) Generate Murcko scaffolds then merge rows on both Murcko and PlateID. This would give you the list of compoundIDs with the same Murcko in one cell which you could then do a valueCount to get the number of compounds.

Best,

Angus