
Subject: Re: Count # scaffolds by plate ID
Posted by [chemtv](#) on Wed, 05 May 2021 21:23:11 GMT
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Starting with: 500K smiles, cpdID, plateID
Here's what I'm ultimately trying to get to...

plateID	Num Scaffolds	Scaffolds (smiles of scaffold)
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abc01	5	phenyl, pyridine, indole, thiazole, naphthyl
abc02	3	phenyl, pyrimidine, naphthyl
abc03	2	indole, oxazole

Actually the 1st two columns are what I need.

Greg
