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) |
|---|---|---|
| abc01 | 5 | phenyl, pyridine, indole, thiazole, napthyl |
| abc02 | 3 | phenyl, pyrimidine, napthyl |
| abc03 | 2 | indole, oxazole |

Actually the 1st two columns are what I need.

Greg