Subject: Murcko scaffold
Posted by sansun on Tue, 13 Aug 2024 05:54:59 GMT
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In the case of 'Scaffold Analysis, ' we have options for determining Murcko scaffolds/skeletons.

There is an option to save a new file with the structures of scaffolds/rings and corresponding frequencies. However, it would be helpful to be able to select more columns from the existing file. For example, in some cases I'd like to carry compound IDs or dataset name columns from the original file from which scaffolds are generated.

Or it would be useful to get the frequency column in the original file it self.

Thank you
Sansun