Subject: Re: Aligning molecules to a common substructure
Posted by nbehrnd on Sun, 06 Oct 2019 22:02:30 GMT
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Please indicate if I'm wrong, but I understand your case like aiming to sort molecules featuring the same core substructure in groups together. If so, I suggest to try Chemistry -> Analyse Scaffolds -> Murcko scaffold. This will add a new column which equally allows sorting of the data set, e.g. to alter a sort by structure (here, the first column):

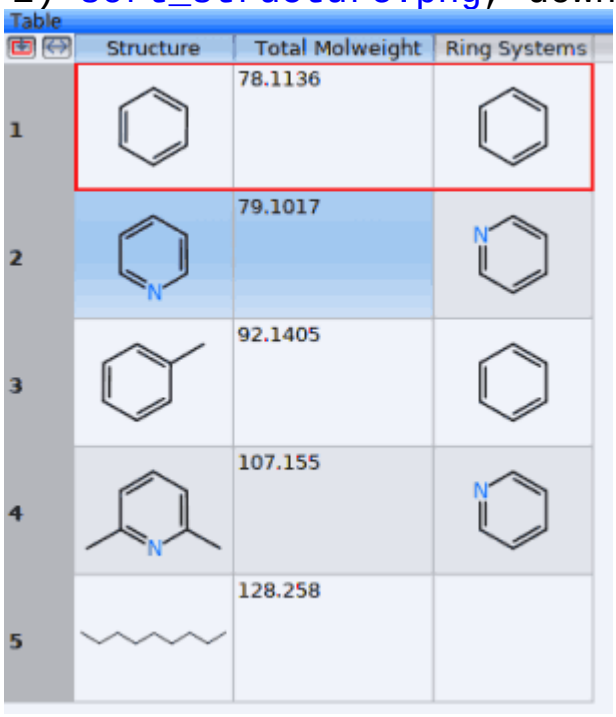
by a sorting according to the Murcko scaffold (here the third column):

As usual, the header of the column (e.g., the third one) may be renamed to your needs. Note, the manual includes an illustrated definition about different scaffold criteria available to you (http://www.openmolecules.org/help/chemistry.html#ScaffoldAna lysis).

Norwid

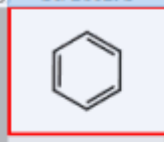
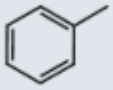
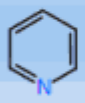
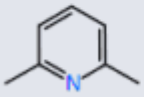
File Attachments

1) sort_structure.png, downloaded 1373 times



2) sort_MurckoScaffold.png, downloaded 1468 times

Table

	Structure	Total Molweight	Ring Systems
1		78.1136	
2		92.1405	
3		79.1017	
4		107.155	
5		128.258	