Subject: Aligning molecules to a common substructure
Posted by sbembenek18 on Sat, 05 Oct 2019 01:05:26 GMT
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Is it possible to align all the molecules to a common substructure?

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):

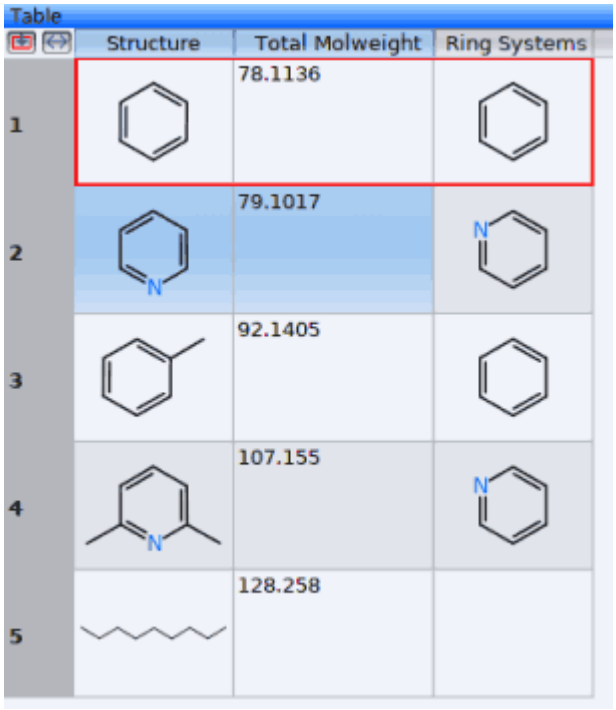
by a sorting according to the Murcko scaffold (here the third column):

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).

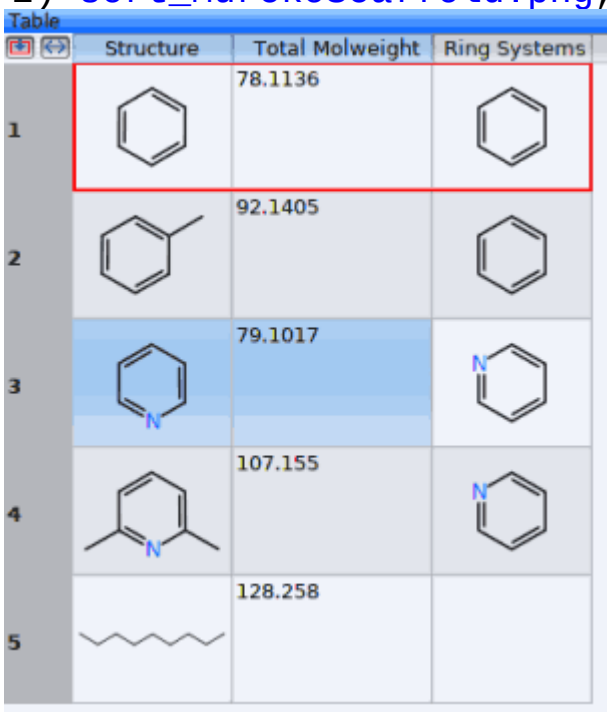
Norwid

File Attachments

1) sort_structure.png, downloaded 1702 times



2) sort_MurckoScaffold.png, downloaded 1858 times



Subject: Re: Aligning molecules to a common substructure
Posted by thomas on Wed, 09 Oct 2019 21:17:38 GMT
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You can generate new atom coordinates with:

"Chemistry -> Generate 2D Atom Coordinates"

Then check

"Automatically detect scaffolds and unify their orientation"
and select a scaffold detection method: "most central" should be fine

When clicking OK, DataWarrior will rearrange your 2D-structures such that the most central ring system, where multiple molecule share the same scaffold, this scaffold is always drawn the same way.

For more flexibility, you may provide scaffolds with defined coordinates in the same dialog.

Subject: Re: Aligning molecules to a common substructure
Posted by sbembenek18 on Fri, 11 Oct 2019 16:48:00 GMT
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thanks!
