Subject: Possible to create substructure SMILES column?
Posted by jowi on Thu, 25 Aug 2016 12:37:16 GMT

Hi,

I have a collection of compounds with molecular weights of approx 400 Da, all with SMILES structures.
To visualize the effect of certain structural decorations on my parameter of interest, I would like to use the 2D plot and the structure as a label. However, the plot becomes rather messy with only a few compounds. Therefore, I would like to only use sub-structures in the plot.

If I first filter my compound list on the shared common structure, is there any way to automatically create a new column with SMILES describing the rest of the molecules?

To increase the level of complexity, all my SMILES structures are not written in the same way.

Any input is appreciated.

Thanks,
Jowi