
Subject: Possible to create substructure SMILES column?

Posted by [jowi](#) on Thu, 25 Aug 2016 12:37:16 GMT

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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

Subject: Re: Possible to create substructure SMILES column?

Posted by [thomas](#) on Sat, 27 Aug 2016 07:08:05 GMT

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Hi Jowi,

I don't see a straightforward solution. What may come close are any of these two procedures:

1: make a core-based or interactive (this is faster to use, because you select scaffolds rather than drawing them) SAR analysis to split the molecule structures into scaffold and substituent columns. Then you can use e.g. 4 substituent columns as labels decorating the actual marker. The marker itself could be colored or shaped by scaffold class.

2: Use 'Add Largest Fragment' to create a new column to be used for scaffold replacement

The for every scaffold:

1 - Use a filter on the original Structure column to show only molecules with that scaffold

2 - Copy scaffold in filter and open 'Search and replace' dialog

Select the new(!) Structure column, paste scaffold in 'Search' field, attach R-groups at every substituted position

In the 'Replace' field draw one C atom, change the C to a distinguishable atom e.g. V that supports higher valences

Attach the same R-groups to V, which you use in the 'Search' field.

Select 'Visible rows only' and click OK.

This way you replace all selected scaffold by a pseudo atom (V), which should result in smaller labels

Since the whole procedure is a little cumbersome, you may create a macro out of it if scaffolds don't change and you do this often.

Hope this helps,
Thomas

Subject: Re: Possible to create substructure SMILES column?
Posted by [jowi](#) on Mon, 29 Aug 2016 06:10:59 GMT
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Hi Thomas,

Many thanks for your quick help. Much appreciated!

Cheers,
Jowi
