Subject: Re: question about 'analyse similarity/activity cliffs' function
Posted by thomas on Tue, 09 Jul 2019 12:12:52 GMT
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Hi Avril,
the easiest way would be to use a structure filter: right mouse click on a molecule marker of the view, then select 'New Structure Filter From -> this structure'. Then you may adjust the similarity slider in the filter and see the similar molecules in the Table view. To avoid always creating new filters, you may within a view do a right mouse click and 'Copy->Structure as->2D-Structure' and in an existing structure filter double-click the structure and use 'paste' in the editor.

You may also sort the Table/Structure view by a right mouse click on a structure, then 'Sort by->XXX-similarity to this molecule.

Tip: If you calculate the SkeletonSpheres descriptor from your chemical structures with 'Chemistry->From Chemical Structure->Calculate Descriptor->SkelSpheres', you may use this for all chemical similarity functionality, which usually gives better results than the FragFp descriptor.

Hope this helps, Thomas