Subject: question about 'analyse similarity/activity cliffs' function
Posted by alc@sanger.ac.uk on Thu, 04 Jul 2019 09:44:23 GMT
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Hello,
I'm new to DataWarrior and finding it very nice.
I've tried the 'Analyse similarity/activity cliffs' function, and it has made a nice plot showing the molecules as dots.
I can select a molecule and see other similar molecules coloured according to how similar they are to my molecule of interest, using the FragFP score (green: very similar, red: not similar).
I'm wondering is there a way to list the other molecules by their FragFP score from my molecule of interest? The plot I've made contains thousands of molecules, so it's a little hard to see ones that are a bit greenish in the huge plot.
Any advice will be much appreciated!
Regards,
Avril

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

Subject: Re: question about 'analyse similarity/activity cliffs' function
Posted by alc@sanger.ac.uk on Wed, 04 Sep 2019 07:40:42 GMT
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Dear Thomas,
I'm sorry for the delay in my reply.

Thank you so much for your helpful reply to my question. I will try out hte SkeletonSpheres descriptor, that ones sounds very interesting to me.
Thank you for making DataWarrior available, it has helped me so much in my work,
Kind Regards,
Avril

Subject: Re: question about 'analyse similarity/activity cliffs' function
Posted by pmallard on Mon, 30 Sep 2019 12:18:06 GMT
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Dear Thomas,

I have some issue with the structure similarity filter.
I have a large set of structures (>10M) which I imnported from csv and FragFp has been automatically calculated.
Most of the structures display well. I am able to a "contain" search and look for molecules containing the structure I just drawed.
However the "is similar to [FragFp]" function doesn not work.
No error message is returned however the search is not working and the filter is automatically switched to the "disable filter" mode when I run it ....

Any clue ?
Many thanks for this excellent software !

PM

Subject: Re: question about 'analyse similarity/activity cliffs' function
Posted by thomas on Thu, 03 Oct 2019 21:22:06 GMT
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Dear PM,

I am not sure, whether your problem is related to an embarrassing bug related to structure filtering in large files. There is a download link of a datawarrior development version with new functionality and bug fixes, which may have solved your issue: openmolecules.org/datawarrior/dw500win.zip (dw500x.zip for Linux or Mac). These archives contain some files to be placed into the datawarrior installation folder. Some replace earlier files of the official 5.0.0 version and some are new. I assume, your problem is solved with the update, but if not then please send me a short not and I will invetigate further.

Sorry for the inconvenience,

Thomas

Subject: Re: question about 'analyse similarity/activity cliffs' function
Posted by pmallard on Sun, 06 Oct 2019 14:10:39 GMT
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It's working !
A thousand thanks !!!

PM