Subject: question about 'analyse similarity/activity cliffs' function
Posted by alc@sanger.ac.uk on Thu, 04 Jul 2019 09:44:23 GMT

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