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

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