Subject: Re: defining molecule clusters after similarity analysis
Posted by thomas on Tue, 05 Apr 2022 13:03:11 GMT

Hi Xènia,

you are not the first to ask for that. Thus, I have updated the similarity/activity-cliff-analysis to generate two more columns: a cluster number and the cluster member count. You can download the updated DataWarrior file (dev version) from the link in the fine-print that appears when clicking the 'read and understood' checkbox on the DataWarrior download page.

Hope this solves the issue for you,

Thomas