Subject: Re: bar graph Murcko Skeleton and count
Posted by khom on Wed, 19 Oct 2022 14:56:27 GMT
View Forum Message <> Reply to Message

Dear Thomas,
Thank you for your quick response. My original goal of plotting the frequencies of a structure in a bar graph for a large dataset, is not efficient at all. Upon searching the DataWarrior forum (which is what I should have done initially), I learned that I should first calculate the frequency with the function frequencyInCategory("PlateID","Murcko"), and then display the results in a scatter plot. I was able to display the frequency of interest for over 3000 Murcko structures AND still get a readable information, as in attached. Thank you to you and fellow warriors.

File Attachments
1) Screenshot_2022-10-19_10-52-00_a.png, downloaded 464 times