Subject: bar graph Murcko Skeleton and count
Posted by khom on Thu, 13 Oct 2022 19:46:05 GMT
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Dear fellow users,
I am trying to plot a bar graph with the Murcko Ring systems (Chemistry --> Analyze Scaffold --> Murcko Skeleton) on the x-axis and with the number of molecules belonging to a particular ring system as the value for the vertical bars. The scheme I used with a file of 97 entries worked, but failed for a file with 2000 entries. The error message was: "A bar chart is not shown because an axis is assigned to a column that does not contain categories". My troubleshooting attempt of excluding the entries without a Murcko Skeleton did not succeed; however, reducing the number of entries to about 200 worked. Is this a (my) computer issue ? Thank you.

File Attachments
1) Screenshot_2022-10-13_15-38-53.png, downloaded 302 times

Subject: Re: bar graph Murcko Skeleton and count
Posted by thomas on Fri, 14 Oct 2022 17:42:11 GMT
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Dear Khom,

the number of allowed categories in a bar (and pie) chart is limited to 256. This does not depend on your computer's resources. It was a design decision because depicting thousands of bars is simply not possible. One could argue to increase the limit. And admittedly, the error message is misleading...

Thomas

Subject: Re: bar graph Murcko Skeleton and count
Posted by khom on Wed, 19 Oct 2022 14:56:27 GMT
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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 288 times