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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 624 times

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misleading...

Thomas

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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 629 times

