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 470 times

Murcko Skeleton

Murcko Skeleton