Subject: Structures not visible on 2D-axis Posted by amorrison on Fri, 27 Dec 2019 03:57:38 GMT

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Hi,

For 2D-graphical views, if I select a structure column (say from a r-grp decomposition), the structures no longer show on the axis. If I select the same r-group column in a 3d-view the r-groups show correctly.

Thanks,

Angus

Subject: Re: Structures not visible on 2D-axis Posted by thomas on Sun, 29 Dec 2019 14:05:11 GMT

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Hi Angus,

I assume that this was a bug in an earlier version. You may check in the current pre-release, which is available as zip archive containing some files that replace older ones in the installation folder of the official 5.0.0 version. You may download the patch files from openmolecules.org/datawarrior/dw500win.zip (Windows) or openmolecules.org/datawarrior/dw500x.zip (Linux and OSX).

Thomas

Subject: Re: Structures not visible on 2D-axis
Posted by amorrison on Mon, 30 Dec 2019 06:19:00 GMT
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Thanks Thomas, I've looked at my file again in more detail and noticed something odd. If the view is small, I can see the r-grps (attached image rgrp_minimised) but only the vertical lines of the grid (view set to show full grid). If I maximise this window the r-grps disappear and I lose the whole grid (rgrp_maximised). I've included an example dwar file from ChemBL where this behaviour occurs with R5 on the x-axis. Any thoughts how to deal with this?

Thanks,

Angus

File Attachments

- 1) CB2_example_r5.dwar, downloaded 336 times
- 2) rgrp_maximised.png, downloaded 350 times
- 3) rgrp_minimised.png, downloaded 365 times

Subject: Re: Structures not visible on 2D-axis Posted by thomas on Tue, 31 Dec 2019 17:33:18 GMT Angus, thank you very much for posting files and reproducibly showing the issue. I have updated the logic when showing structures on axes on the 2D-view and hopefully fixed the issue. The dw500 zip files are updated.

Subject: Re: Structures not visible on 2D-axis Posted by amorrison on Fri, 03 Jan 2020 08:21:33 GMT View Forum Message <> Reply to Message

Thanks Thomas, very much appreciated. Angus