
Subject: 3D coordinates lost during "Paste Special>Paste with header row"

Posted by [zhentg](#) on Tue, 10 Mar 2020 15:20:23 GMT

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Aim: I want to save a subset into a new SDF file with 3D coordinates

Here is my workflow:

1. Load an SDF containing molecules with 3D coordinate.
2. Select some rows, then "Paste Special>Paste With Header Row", and a new DataWarrior file is created

In the new DataWarrior window, 3D coordinates is missing.

Please check the attached screenshot and example DataWarrior file.

Thanks.

File Attachments

1) [Screenshot](#), downloaded 470 times

2) [cHex.dwar](#), downloaded 455 times

Subject: Re: 3D coordinates lost during "Paste Special>Paste with header row"

Posted by [thomas](#) on Tue, 10 Mar 2020 21:55:21 GMT

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For creating a subset it is easier to use "File->New From->Selected Rows" after selecting some rows.

This replicates all other settings, e.g. filters and views.

Of course, ideally copy/paste should also recreate 3D-coordinates. As described in my other answer, copy and 'paste into table' now support structures/reactions and coordinates, but paste from the main menu doesn't do that yet. It will come...

Thank you for pointing this out and the example file.

Subject: Re: 3D coordinates lost during "Paste Special>Paste with header row"

Posted by [zhentg](#) on Wed, 11 Mar 2020 01:05:10 GMT

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Thanks a lot for your reply.

"File->New From->Selected Rows" works great! And it really solved my problem.

And looking forward to the "Paste special" enhancement coming!
