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

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

[View Forum Message](#) <> [Reply to Message](#)

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 810 times

The screenshot shows the cHex.dwar software interface. At the top, there is a menu bar with options: File, Edit, Data, Chemistry, Database, List, Macro, Help. Below the menu bar is a table with the following columns: Structure, Molecule ..., and chiralLabel. The first row of the table contains a hexagonal chemical structure, the text 'cHex', and 'noChiralCenter'. A red box highlights this row. A red arrow points from this row to a context menu that is open over the table. The context menu includes options: Cut (Ctrl+X), Copy (Ctrl+C), Paste (Ctrl+V), Paste Special (with a submenu), Delete, Select All (Ctrl+A), Select Rows Randomly..., Invert Row Selection, Find And Replace... (Ctrl+H), New Filter..., Disable All Filters, Enable All Filters, Reset All Filters..., and Remove All Filters. The 'Paste Special' submenu is open, showing 'Paste With Header Row' and 'Paste Without Header Row'. In the background, there is a window titled 'Untitled Form View' which contains a 'Structure:' label and a hexagonal chemical structure. Another window titled 'Untitled Form View' is partially visible on the right, showing a '3D-Structure:' label and a ball-and-stick model of a molecule.

2) [cHex.dwar](#), downloaded 659 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
[View Forum Message](#) <> [Reply to Message](#)

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
[View Forum Message](#) <> [Reply to Message](#)

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!
