

---

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 741 times

File Edit Data Chemistry Database List Macro Help

Table	Structure	Molecule ...	chiralLabel
1		cHex	noChiralCenter

Untitled Form View

Structure:



3D-Structure:



Edit Data Chemistry Database List Macro Help

- Cut Ctrl+X
- Copy Ctrl+C
- Paste Ctrl+V
- Paste Special >
  - Paste With Header Row
  - Paste Without Header Row
- 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...
- Remove All Filters

2) [cHex.dwar](#), downloaded 630 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!

---