
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

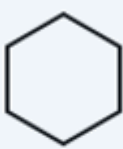
1) [Screenshot](#), downloaded 812 times

File Edit Data Chemistry Database List Macro Help

Table			
	Structure	Molecule ...	chiralLabel
1		cHex	noChiralCenter

Untitled Form View

Structure:



3D-Structure:

Untitled Form View



Edit Data Chemistry Database List Macro Help

- Cut Ctrl+X
- Copy Ctrl+C
- Paste Ctrl+V
- Paste Special >
- 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

- Paste With Header Row
- Paste Without Header Row

2) [cHex.dwar](#), downloaded 660 times