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)                , downloaded 579 times
2) cHex.dwar, downloaded 572 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!