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.
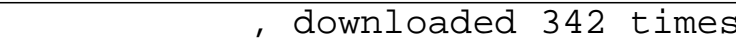2. Select some rows, then "Paste Special>Paste With Header Row", and a new DataWarrior file is created

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

Please check the attached screenshot and example DataWarrior file.

Thanks.

File Attachments
1)   , downloaded 342 times
2) cHex.dwar, downloaded 301 times