Subject: Copy and paste from Chemdraw to Datawarrior structure Posted by JZhang on Fri, 13 Nov 2020 23:53:38 GMT View Forum Message <> Reply to Message

Hello,

I am having trouble pasting structures from chemdraw19.1 2 to Datawarrior. When I click on the structure and paste (command+V) nothing happens. My ChemDraw file is in ChemDraw XML format and I am using MacOS Mojave 10.14.6. Can you help me with this? Thank you.

Subject: Re: Copy and paste from Chemdraw to Datawarrior structure Posted by thomas on Sat, 14 Nov 2020 16:43:22 GMT View Forum Message <> Reply to Message

The problem is that the binary ChemDraw clipboard format is not passed to the Java environment. Thus, DataWarrior sees an empty clipboard, if you just use 'Copy'.

I suggest to use 'Copy As->Mol Text' or 'Copy As->Mol V3000 Text'. Then ChemDraw is creating and pushing a molfile to the clipboard, which is text data, is passed to the Java runtime environment and is seen and converted by DataWarrior. I tried and confirmed with the current development version.

Subject: Re: Copy and paste from Chemdraw to Datawarrior structure Posted by JZhang on Sat, 14 Nov 2020 20:15:02 GMT View Forum Message <> Reply to Message

Thank you. I can paste the molecule onto DataWarrior now. A follow-up question: When I paste the structure there are many bonds showing up with the ESR Tools(abs and R and S), but I don't want them to show up. Is it possible to get rid of them and just show white bonds without the labels?

Subject: Re: Copy and paste from Chemdraw to Datawarrior structure Posted by thomas on Sun, 15 Nov 2020 19:43:50 GMT View Forum Message <> Reply to Message

This can only be done in the Structure view. The popup menu in the structure view that you get after a right mouse click contains two submenus: 'Set Structure COlor Display Mode' and 'Set Structure Stereo Display Mode'. Both contain various options to define which stereo decorations you see and where color is used. These modes are then also used when copying the view, saving a view image or printing it.