Subject: Structure Copy generates errors
Posted by richards99 on Mon, 05 Dec 2022 09:28:25 GMT

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Hi,
If you draw a structure in the right hand filter panel, and then in the right hand filter panel right click on the structure and choose "Copy Structure" (So copying it from the filter panel, not from the sketcher).
If you now create a new substructure filter in the panel and right click on it and choose "Paste Structure or Name", it generates an error which says "Uncaught Exception: 0".
Alternatively if I go to Generate 2D atom Coordinates and paste it in there, it generates the same error.

Additionally, if from the main data SAR table I right click on a structure and choose "Copy Structure as 2D Structure". If I then try and paste this in the same way described above I get the same error. Note if I copy structure as SMILES or MolFile etc, then it works fine.

Also sometimes the error shows "Uncaught Exception: 0", but sometimes it also says "Java Heap Space Error".

I am using the latest DEV version of DataWarrior 5.5.0, and the issue has been present for a while now. I am using a MacBook Intel machine with 16Gb RAM.

Thanks,

Simon.