Subject: Export Options

Posted by MedChemProf on Sat, 12 Mar 2016 16:36:25 GMT

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Dear DataWarrior Forum,

Is there a way to export the data in the table view to something other than a data warrior, text or sdf format? I simply want to export the information in the table to view it in excel. I do not need the molecular information (if the SMILES is there that is fine). Ideally I would like to export it into a csv file which I can then open in excel.

I am using a Mac with the latest OS X. Thank you in advance for any help.

@MedChemProf

Subject: Re: Export Options

Posted by thomas on Tue, 15 Mar 2016 16:21:55 GMT

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Dear MedChemProf,

there are two ways to achieve that. txt-exports are TAB delimited and can be imported into Excel.

However, still easier is to use "Select All" and "Copy" from the "Edit" menu, go to Excel and select "Paste".

DataWarrior uses TAB delimited text as standard clipboard format, which Excel then correctly puts into cells.

Thomas

Subject: Re: Export Options

Posted by MedChemProf on Sun, 20 Mar 2016 15:25:50 GMT

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Thanks, but neither suggestion seems to work for me. The text export seems to be broken and only saves a blank .txt file or makes Datawarrior freeze. When I try and copy and paste into excel, I get the error - 'java.lang.NullPointerException'.

I am running MacOSX 10.11.3 El Capitan (iMac 21.5-inch, Mid 2011; 2.7 GHz Intel Core i5; 4 GB 1333 MHz DDR3) using Java 8 Update 73 Java Runtime Environment 1.8.0_73.

Thanks, Chase

Subject: Re: Export Options Posted by thomas on Wed, 23 Mar 2016 11:32:35 GMT

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Dear Chase,

I am also using El Capitan on one machine with JRE 1.8.0_66 and don't see any issues.

If your file does not contain confidential information, you may send it to my mail address shown on the openmolecule.org -> about page. Provided that this is caused by a bug, I will then make sure that the next version won't have the problem.

Sorry for that, Thomas

Subject: Re: Export Options

Posted by MedChemProf on Sat, 26 Mar 2016 12:55:18 GMT

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Dear Thomas,

Thank you for your help. I created a smaller, new list of compounds and I encountered the same issues. I will send the new file to the email address that you indicated.

Thanks again, Chase