Subject: Managing Columns
Posted by ELFritzen on Sat, 29 Aug 2020 15:17:10 GMT
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I'm looking for some tips to help me manage columns in Datawarrior. I've been maintaining our small corporate database using Datawarrior for almost a year now tracking molecules' structure, ADME data, and biological activity. Eventhough I have tried to only add the most important and relevant data in columns, I still have a large number of columns. I've written macros to display selected columns which helps in displaying subsets of the data. There are so many columns, that they all cannot be displayed when right clicking on a column header. This is a problem, especially using a laptop computer, since I can't right click on a column header to select a column that might be hidden because the contextual menu is much larger than the screen and can't display all the hidden columns. I can't scroll to the hidden column that I might want to display. Is there a way around this? Is there a limit to the number of columns one can have in a Datawarrior file? I would think that this would be a big problem with some much larger corporate databases. My current Datawarrior file contains 246 molecules and 63 columns of data. I could create smaller Datawarrior files with only selected data, but it's easier to maintain one 'master' file which contains all the data in one file. I'd be interested in any tips on how others manage this.

Thanks,
Ed Fritzen

Subject: Re: Managing Columns
Posted by thomas on Thu, 03 Sep 2020 08:10:54 GMT
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As a short term remedy I have changed the table popup menu: Instead of having a 'Show column x' entry for every hidden column, it now has one submenu 'Show Column', which contains the names of all hidden columns. Since the sub-menu is scrollable, small screen sizes are not an issue. The update can be downloaded as development patch from the download page after clicking the 'Read and understood' checkbox. The link is in the small print.

Would it be useful to be able to define column sets, which can be hidden or shown en bloc from the table popup menu?

Thomas

Subject: Re: Managing Columns
Posted by ELFritzen on Mon, 07 Sep 2020 15:48:38 GMT
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Hi Thomas,
Thank you for your reply. I think I downloaded the correct file. It was a zip file with the name "datawarrior521Source.tar.gz". I unzipped the file but I'm not sure which files should be copied and to where they should be copied. I run Datawarrior both on an iMac and a Windows Laptop

So far I've only tried to update Datawarrior on my iMac. I'm not sure on the iMac where the Datawarrior Installation Directory is located.

I think defining sets of columns would be great addition and very useful to me.
Thanks again for all your help.

Ed

Subject: Re: Managing Columns
Posted by thomas on Sun, 13 Sep 2020 09:22:01 GMT
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Hi Ed,

sorry for the late reply. You downloaded the source code, which you cannot directly use to patch.

For Mac/Linux you need: http://www.openmolecules.org/dw521x.zip
If you unpack the zip, you find a 'datawarrior.jar'. On the Mac in a Finder window open the Application folder. Then, over the DataWarrior icon make a right mouse click and choose 'Show Package Contents' (The DataWarrior application is actually a directory, which can be opened this way). Open 'Contents', then 'Java'. Replace the old 'datawarrior.jar' in the 'Java' folder with the new one from the zip. Then you are done.

For Windows: http://www.openmolecules.org/dw521win.zip
The zip contains a 'DataWarrior.exe' which goes into 'C:\Program Files\DataWarrior\' replacing an old file there.

Thomas

Subject: Re: Managing Columns
Posted by thomas on Sun, 13 Sep 2020 17:06:56 GMT
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I have just added three new items in the table popup menu:
- Group Selected Columns -> defines a named(!) column list of all currently selected columns
- Show Column Group -> shows all columns in a given named column group and hides columns not in the group
- Ungroup Columns -> removes a named column list

this is part of todays development patch update.

Subject: Re: Managing Columns

Posted by ELFritzen on Sun, 13 Sep 2020 18:30:03 GMT
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Hi Thomas,

Sorry to bother you with this, but neither of the hyperlinks you provided work. I get a message saying "Not Found: The requested URL was not found on this server." I also get the same message in trying to download from the "download" page after checking the "Read and Understood" checkbox and clicking on the link provided in the fine print as you first suggested.

Ed

Subject: Re: Managing Columns
Posted by nbehrnd on Mon, 14 Sep 2020 11:41:48 GMT
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Hi Ed,

based on previous posts relating to «see the development version», possibly the addresses intended are
http://www.openmolecules.org/datawarrior/dw521win.zip for Windows, and
http://www.openmolecules.org/datawarrior/datawarrior/dw521x. zip for MacOS and Linux. Note the
insert of «datawarrior».

Even if downloaded today (2020-09-14), extracting these archives yields files time stamped by yesterday's date, 2020-09-13 16:59:59.

Norwid

Subject: Re: Managing Columns
Posted by ELFritzen on Mon, 14 Sep 2020 18:24:55 GMT
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Thanks for the information, Norwid. Once I got the correct URL, everything worked. The updates provided by Thomas are just what I'm looking for. Thanks to Thomas as well for his responses, and help.

Ed Fritzen

Subject: Re: Managing Columns
Posted by thomas on Tue, 15 Sep 2020 09:19:48 GMT
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sorry for the wrong links and thanks, Norwid and Ed for pointing me to the problem. I have corrected the links in the download page.