Subject: Updating columns
Posted by ChristerW on Thu, 16 Jun 2022 03:53:28 GMT

Hi!

Can one update internally calculated columns in DataWarrior and if so how does one do that? For example if you have a column with calculated Log P and add some new compounds, how do you update the LogP column for the new new compounds.

ChristerW

Subject: Re: Updating columns
Posted by thomas on Sat, 25 Jun 2022 10:47:26 GMT

If a column was calculated with 'Add Calculated Values...', then the formula is stored in the file. In this case the column's values can be re-calculated. Calculated chemical properties are different: The procedure here would involve deleting the old column and freshly generating a new one. Of course, one can do that as a macro. Especially, if multiple columns shall be recalculated, a macro would be a convenient ways to do that: start macro recording, delete property columns manually, calculated the same columns freshly, stop macro recording, export the macro into a file. You may then move the macro file into the datawarrior/macro folder, which would create an entry in the 'Macro' menu, which allows to run the macro from any DataWarrior window any time.

Subject: Re: Updating columns
Posted by ChristerW on Mon, 27 Jun 2022 07:22:57 GMT

Thanks so very much for the answer Thomas and the description of the procedure for creating a macro for doing this. I must say though, that it would have been much easier to to be able to recalculate also these type of calculated columns. Now the new column ends up at the end and one has to move it manually to the place where the old column was and also change background coloring and such again for the new column. Perhaps one could do that with a macro also, but I don't see why there couldn't be a function to just recalculate the values in these columns also.

ChristerW

Subject: Re: Updating columns
Posted by thomas on Thu, 30 Jun 2022 14:26:25 GMT

I just have released an development update that allows to re-calculate chemical properties of an existing column from the column header popup menu. Thanks for being persistent.

Subject: Re: Updating columns
Posted by sansun on Sat, 16 Jul 2022 12:22:22 GMT
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Hi Thomas

I have the latest development update but don't see this option. Can you please explain where is this exactly located?

SS

Subject: Re: Updating columns
Posted by thomas on Sun, 17 Jul 2022 20:30:26 GMT
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Hi Sansun,

after calculating a new chemical property column, e.g. cLogP, then you find in the column header popup menu of that new column in the table view (right mouse click on the column name) a new menu item, e.g. 'Re-Calculate cLogP'.

Subject: Re: Updating columns
Posted by sansun on Tue, 19 Jul 2022 03:43:33 GMT
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Yes, I found it. This feature is really helpful

Thanks a lot!