Subject: calculated props after file merge/append
Posted by mcmc on Mon, 09 Apr 2018 14:41:11 GMT
View Forum Message <> Reply to Message

First post, so let me start of by saying what an awesome piece of software Datawarrior is.

But there is a little hiccup in my workflow that maybe I can get help with here. Or maybe it will turn into an improvement suggestion.

I have a .dwar file with compounds, experimental data, and a bunch of calculated properties (eg cLogP). I get new data in an SD file every week, that I merge into the .dwar file. When the merge is done, the new compounds do not have calculated properties. There is an empty field in the cLogP column for those new compounds.
I cannot find an easy way to populate those empty fields. I end up recalculating the properties, which creates new columns (eg cLogP 2). Was kind of hoping right clicking on the cLogP column header would give me the option to recalculate or something like that.

Am I missing something obvious, or am I using the best workaround already?

kind regards
Rutger

Subject: Re: calculated props after file merge/append
Posted by thomas on Mon, 09 Apr 2018 19:22:48 GMT
View Forum Message <> Reply to Message

Thanks for the praise. Multiple times is was considering to store the calculation history of data columns in order to allow fresh calculation of values for updated or new structures. The problem is, that this may get quite complex with columns recursively depending on other columns alphanumerical content or on chemical structures or on descriptors. A change may trigger cascades changes on other columns. Therefore I finally have chosen not to provide that kind of feature.

However, you should be able to solve the issue in a different way: Just create a macro that deletes all calculated property columns, then merges the new file, and then freshly calculates the property columns. If you export the macro into a dwam file and put it into the 'macro' folder in the DataWarrior installation directory, the macro is always directly accessible from the 'Macro' menu.

Hope this helps,

Thomas