Subject: calculated props after file merge/append
Posted by mcmc on Mon, 09 Apr 2018 14:41:11 GMT
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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