Subject: Re: calculated props after file merge/append Posted by thomas on Mon, 09 Apr 2018 19:22:48 GMT

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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