Subject: update/recalculation of all computed array data
Posted by nbehrnd on Tue, 13 Sep 2022 09:38:43 GMT
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Dear Thomas,

DW offers integrated functions to compute, e.g. the molecular formula for a structure in the first column. In a current installation, I observe one can change the structure formula, yet this does not not affect Hill formula. This contrasts with user-defined calculations where the program offers to recalculate
the result of the selected column in question. In the illustrative example below, I use a macro which reads-out a string -- so there is an update of the third column possible, yet it appears to be constrained to this column only:

Assuming the first column contains the data used for computations in all subsequent columns, does DW offer assistance to re-run/update the computations all across the the data sheet by single click to ensure consistency of the data?

Norwid

Observations refer to a native installation of DW 5.5.0 for Linux including updates packaged by 2022-09-02 15:00 running in Linux Debian 12/bookworm (branch testing).

File Attachments
1) feature_suggest_table_update_b.gif, downloaded 723 times

Subject: Re: update/recalculation of all computed array data
Posted by thomas on Tue, 13 Sep 2022 20:02:27 GMT
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Dear Norwid,

originally, DataWarrior did not allow to change any cell content, just deleting rows and columns or adding calculated columns or adding columns from merging. Its file format does not include life-links or the complete history of columns created, calculated, updated, merged, etc, which would be needed to recalculate the chain of sometimes dependent calculations in the original order. Recalculating one column is a convenient feature that can/must be triggered by the user. For DataWarrior a column containing molecular formulas is just a text column. There is no link to a parent structure column not does DataWarrior know that the content was generated by creating a molecular formula. Of course, I can add that automatism, but this will never be complete, especially in regard to multi-step calculations. Invisible columns are different: descriptors are kept up-to-date automatically.

Thomas