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