Subject: Re: Suggestion: add molecular weight calculation for individual compound
Posted by thomas on Sun, 22 Mar 2026 10:45:27 GMT
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Hello Laurent and Norvid,

I indeed see the usefulness of an automatic re-calculation of values, structures, descriptors, SMILES, etc. whenever an interactive change of a value or structure occurs that was used as input to a formula, descriptor calculation, SAR-table generation, docking, ...

That would, however, require to change the DataWarrior architecture and its file format substantially, because all operations that take table data as input to calculate something out of it, would need to be traced. The total history would need to be part of any dwar files. Merging and appending of files would break this mechanism. Some algorithms (e.g. chemical space visualisations) need to know and process the entire table before calculating the position of an individual compound. An interactive change of a structure could cause a cascade of potentially expensive re-calculations of order-dependent calculations, which still would fail in certain cases, e.g. if rows have been deleted. Thus, the complete solution is impossible.

Currently, there is an event mechanism that triggers recalculation of structure descriptors when a structure is changed. This could be extended to also trigger repeating some other simple 'from chemical structure' tasks like property calculations. This would already require extending the file format, because DataWarrior currently does not know, whether a numerical value column contains calculated compound properties nor which structure column was used to create it. I will look into this...

Thomas