Subject: Re: Suggestion: add molecular weight calculation for individual compound
Posted by nbehrnd on Fri, 30 Jan 2026 19:02:33 GMT
View Forum Message <> Reply to Message

Hello Laurent

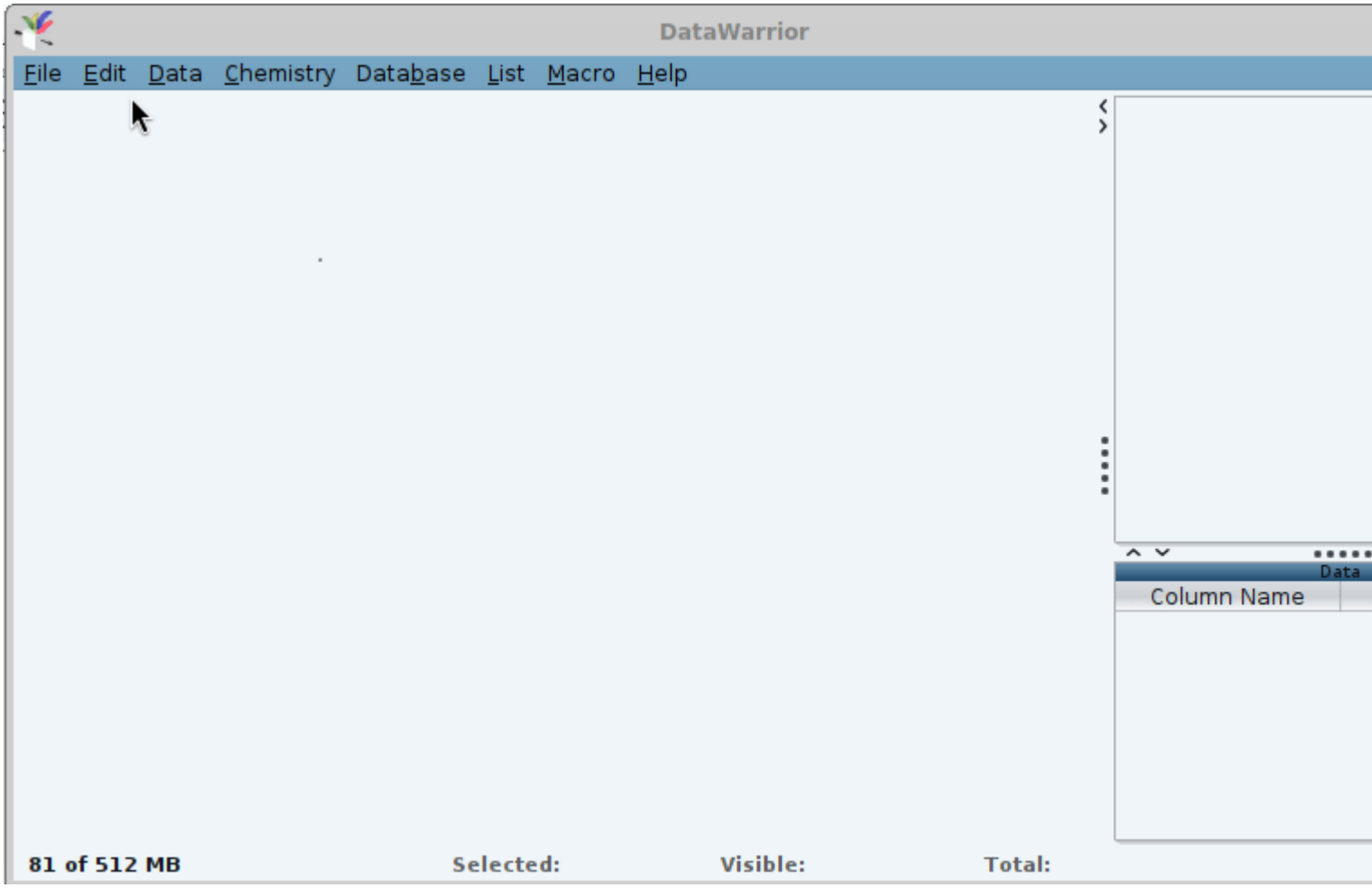
Contrasting to molecule editors like ACD ChemSketch, or Biovia Draw which monitor and continuously monitor and if necessary automatically update the display of the molecular weight of a structure, such a check and revision in DataWarrior has to be initiated manually, explicitly. Click with the right-hand button on the column's head to open a pull-down menu to select "Re-calculate". This causes DW to the reference field (here: the potentially updated structure) and populate the dependent field about the molecular weight with the newly calculated value if necessary. This is quite similar to the deployment of user defined columns (data -> add calculated values) which later equally cause this pull-down menu to feature a re-calculate of this very column (and if there multiple, an entry to re-calculate all columns at once, too).

The .gif attached illustrates this for the molecular weight of an empty structure, then of benzene, and naphthalene with DW 06.05.02 (published by September 2025).

Regards,
Norwid

File Attachments

1) 2026-01-30_DW_update_value_by_re-calculate.gif, downloaded 506 times


DataWarrior
File Edit Data Chemistry Database List Macro Help
Data
Column Name
81 of 512 MB
Selected:
Visible:
Total: