Subject: Re: Round numbers by decimal places?
Posted by nbehrnd on Sun, 07 Dec 2025 11:46:40 GMT
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Hello Santora

As an example for a small set of 10 molecules, the dwam macro attached proceeds in a sequence to

- compute the molecular weight, like one would click over Chemistry -> From Chemical Structure -> Calculate Propeties -> Total average molweight, to create a temporary new column. DW 06.0.5.02 populates this one with three decimals if the third one is 1-9, a 0 leads to truncation
- creates a new column `MW_rounded` of calculated values (here: to round the molecular weight to 0 decimals)
- deletes the earlier, now no longer needed column of molecular weights with up to 3 decimals.

The .dwam is the result of recording the macro (macro -> start recording, later macro -> end recording and export macro). In the step to create the column about rounded molecular weights, during recording the macro, one can opt-in to directly overwrite the already existing column about molecular weight, too (see the second macro). This simplifies the macro file; using one, or the other route depends on your preferences.

Best regards

Norwid

File Attachments

1) Random_Molecules.dwar, downloaded 30 times
2) MW_rounded.dwam, downloaded 29 times
3) rounded_overwrite.dwam, downloaded 30 times