Subject: fewer digits when hovering over plots
Posted by mcmc on Thu, 22 Jul 2021 09:36:32 GMT
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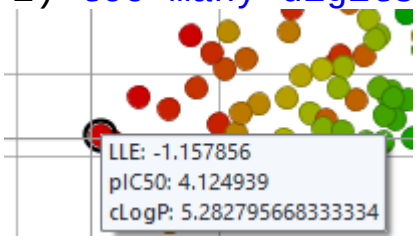
See attached image. Would be nice if the number of digits there would be either
* reduced to max 3, or,
* follow the rounding that can be specified in the respective columns

The current number of digits makes little scientific sense, makes it harder to quickly grasp the values, and clutters the window.

(I realise this is a nice to have, but it would help my eternal battle to free the world of useless digits :))

File Attachments

1) too many digits.png, downloaded 913 times



Subject: Re: fewer digits when hovering over plots
Posted by nbehrnd on Thu, 22 Jul 2021 20:41:09 GMT
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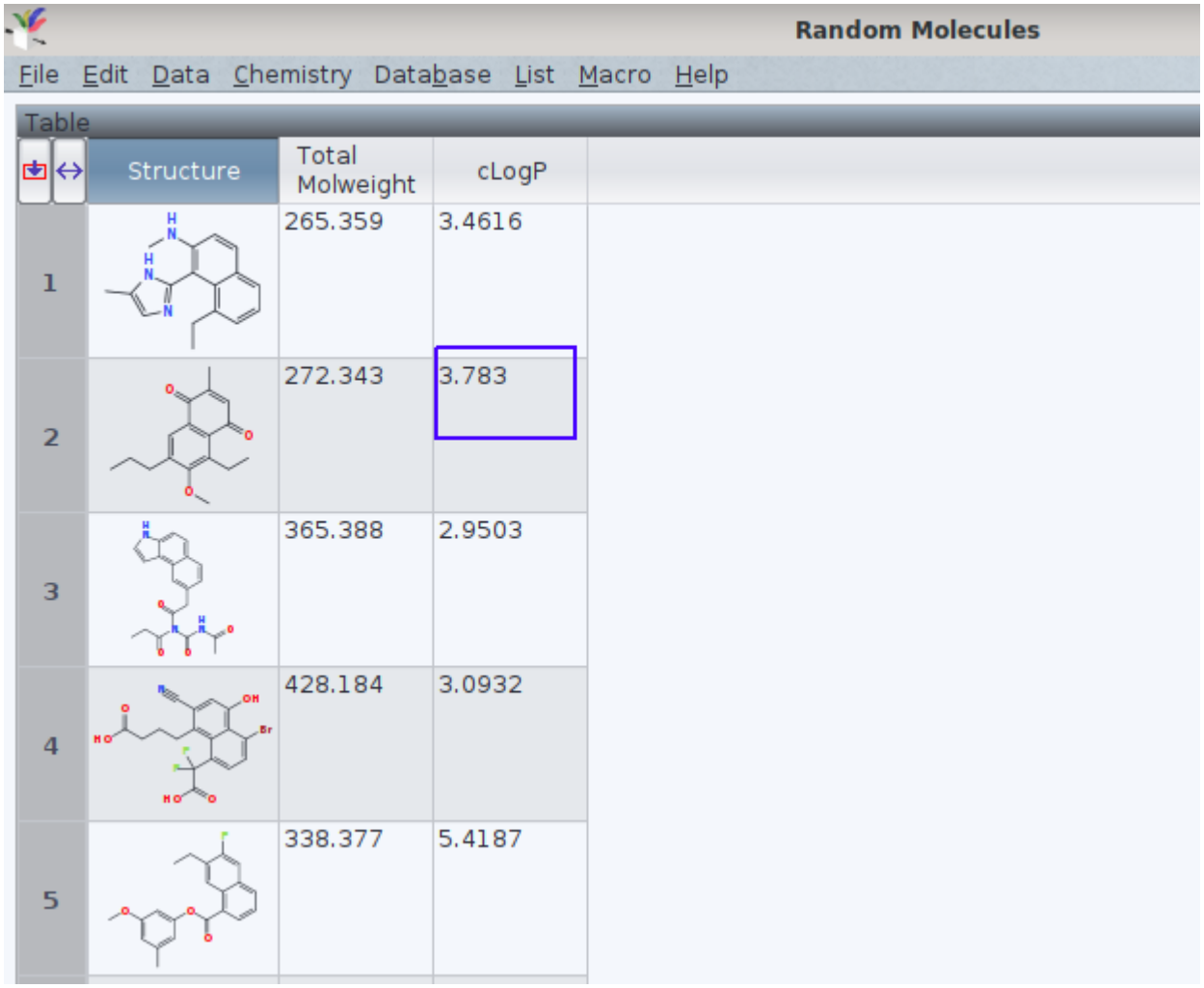
If the representation of numerical results is revised, I would welcome if the data were presented in a fixed precision which might be user defined (e.g., f8.4). Present computations look like decimals are dropped if not leading .and. equal to zero. As an example, a set of random molecules with clogP:

This actually points to the question, does DW internally perform the computations at single / double precision (if there is such an equivalent of Fortran's parlance in Java)?

Norwid

File Attachments

1) decimals.png, downloaded 1205 times



Subject: Re: fewer digits when hovering over plots
Posted by thomas on Thu, 19 Aug 2021 17:08:05 GMT
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no discussion needed: I now changed the code to use the rounding settings from the table. Will be in the next dev update...

DataWarrior uses single and double precision (float or double) for calculations. This depends on location and whether amount of data used. For very large data precision is reduced for the sake of smaller memory footprints.
