Subject: Re: fewer digits when hovering over plots
Posted by nbehrnd on Thu, 22 Jul 2021 20:41:09 GMT
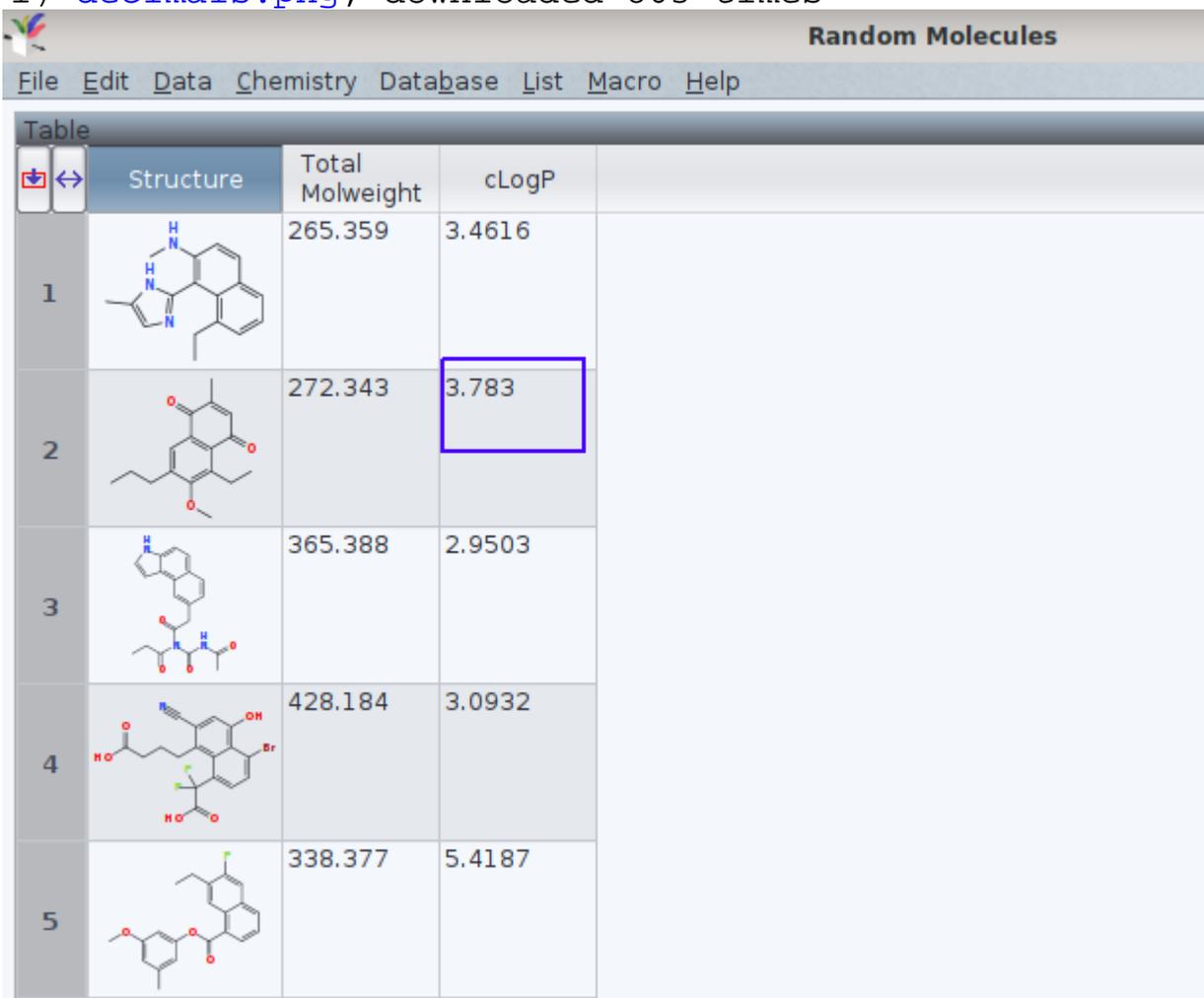
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If the representation of numerical results is revised, I would welcome if the data were presented in a fixed precision which might be user defined (e.g., f8.4). Present computations look like decimals are dropped if not leading .and. equal to zero. As an example, a set of random molecules with clogP:
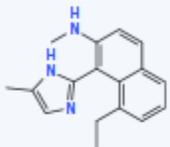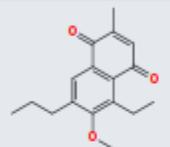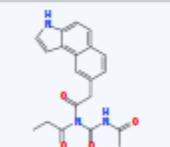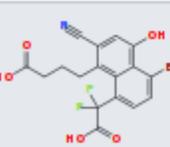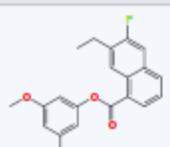
This actually points to the question, does DW internally perform the computations at single / double precision (if there is such an equivalent of Fortran's parlance in Java)?

Norwid

File Attachments
1) decimals.png, downloaded 863 times

	Structure	Total Molweight	cLogP
1		265.359	3.4616
2		272.343	3.783
3		365.388	2.9503
4		428.184	3.0932
5		338.377	5.4187