Subject: Re: > and < signs not interpreted in 6.0.0
Posted by nbehrnd on Sat, 13 Jan 2024 19:18:59 GMT
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In continuation with DW 06.00.00, I created a new array: the first column with three random molecules (DW generated), the second column added with Data -> Add empty columns, where I selected "text" as category. Manually, I added the strings `>2000`, `55.6`, and `20` to the cells as a test property (cf. attached .dwar and `dw_screenphoto_01.png`). The subsequent addition of a third column by Data -> Add Calculated Values used a function of

if(test_property>20, "big", "small")

proceed smoothly. In your case application, do you equally have the automatic assignment of the column type enabled? This is based on the observation the intended computation is going to fail if the second column (still/accidentally) is set to the level of `text` -- regardless if `force categories` is activated, or not. Subsequent adjustment of the second column, then re-run by right-click on the third column and "update formula and recalculate" adjusted the results.

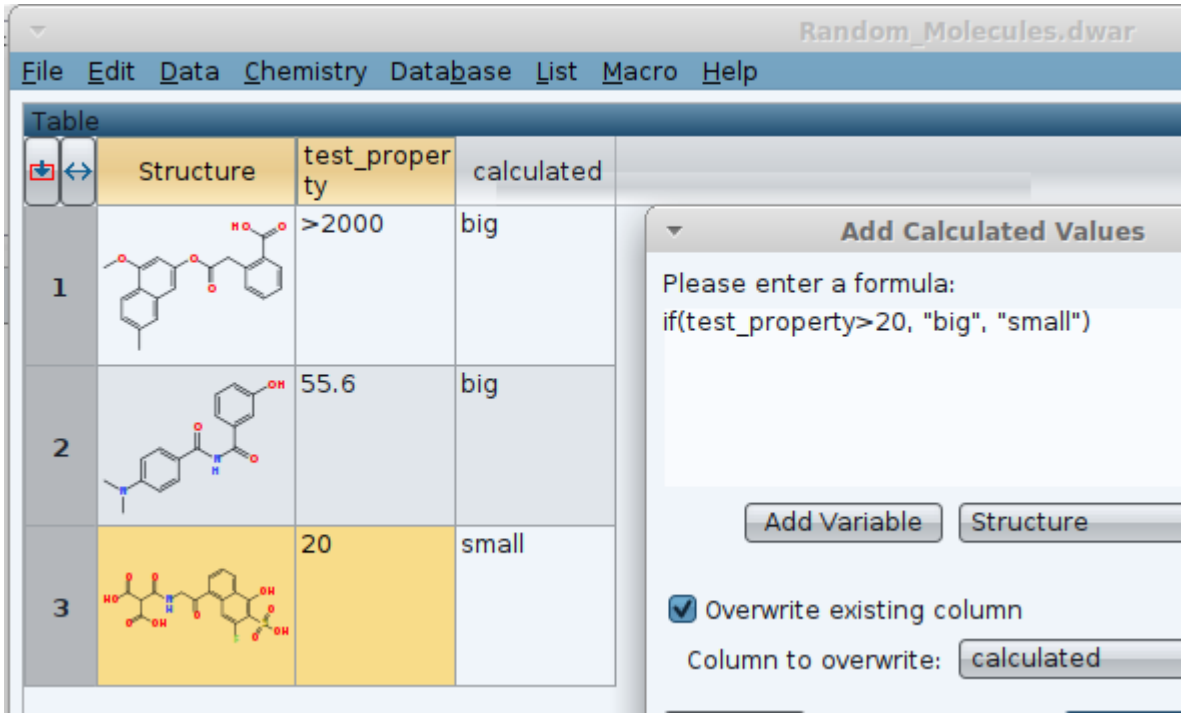
However: I assumed a right-click on the third column and subsequent "Re-Calculate All Columns" would be more helpful for a global update of the array of maybe multiple columns of calculated values. Hélàs no, it replaced the original entries in the second column by the results of my formula, and yielded the "NaN" indicator in the third column (dw_screenphoto_03.png). This observation is less intuitive to me.

Regards,

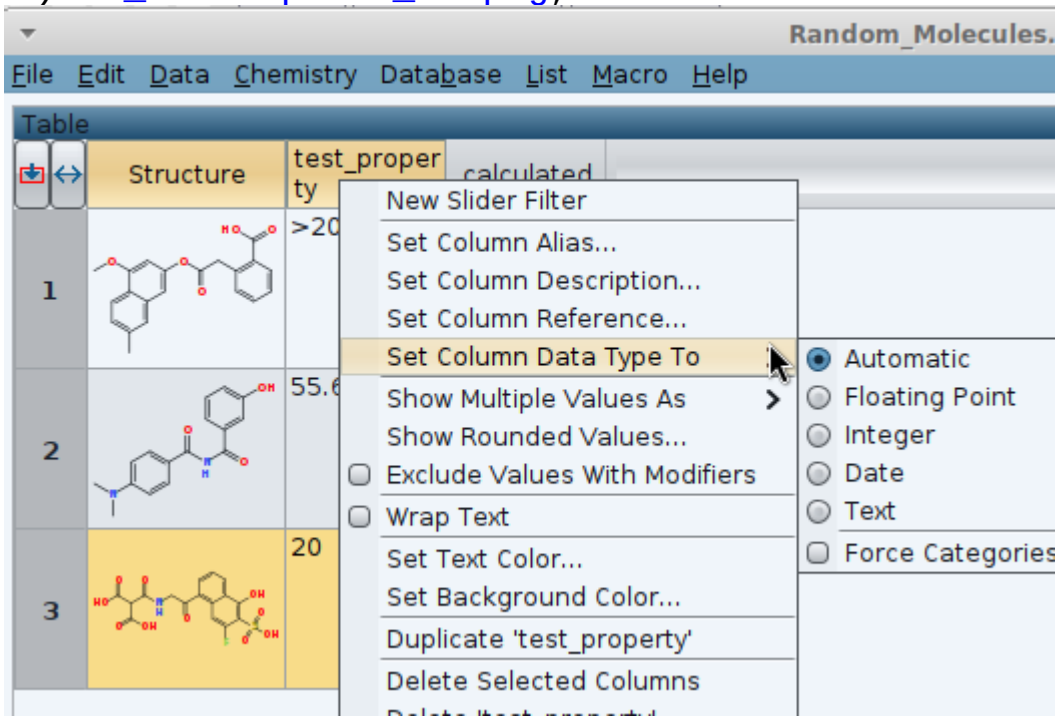
Norwid

File Attachments

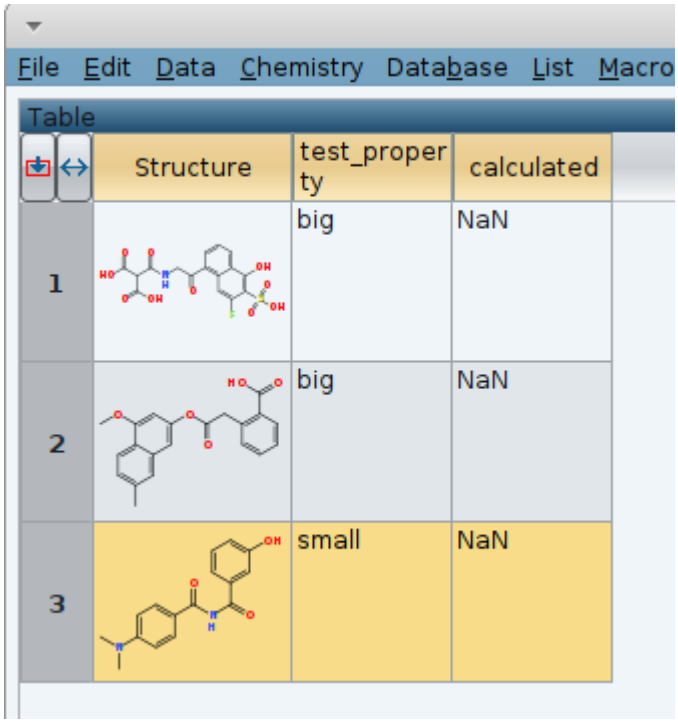
1) Random_Molecules.dwar, downloaded 609 times
2) dw_screenphoto_01.png, downloaded 880 times



3) dw_screenphoto_02.png, downloaded 794 times



4) dw_screenphoto_03.png, downloaded 867 times


File Edit Data Chemistry Database List Macro
Table
Structure
test_property
calculated
1
big
NaN
2
big
NaN
3
small
NaN