Subject: Re: Use of calculated column functions
Posted by nbehrnd on Thu, 12 Mar 2020 21:03:52 GMT
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Your observation is true because I understood your question as aiming for a (Boolean) on/off or True / False categorical two-level criterion. Please clarify if this was misunderstood by mine.

So far, I did not mind that instead categorical "1" and "0" strings the calculated column reads like floating numbers "1.0", and "0.0" instead and seems to be limited to two levels. To label molecules of molecular weight greater than 100, the computation would be adjusted to (TotalMolweight > 100) == 1. If searching for molecules with a molecular weight either below 80 .OR. greater 100, a plausible instruction were (TotalMolweight > 100 || TotalMolweight < 80) == 1; and the toluene molecule as an example for the range of 80 < MW < 100 is identified by (TotalMolweight > 80 && TotalMolweight < 100) == 1.

I see that attributing a string as a result of such a computation may be useful, or to extend the Boolean two-level perspective for, e.g. annotating members of a compound list as basic / neuter / acidic. Even more so as such an attribution by Add Calculated Values may consider multiple criteria from multiple columns at once. For both however, I do not know if DW contains such a functionality.