Subject: Re: LLE column doesn't update with new compound data
Posted by thomas on Fri, 02 Jun 2017 20:41:14 GMT
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Hi Christoph,

DataWarrior has no mechanism to automatically update cell content that was originally derived from other cell content. If I started that, this could get easily very complex and chaotic, because editing a structure might then change computed properties, which in turn could trigger changes on derived columns. SAR tables, chemical space plots, SOMs, custering results, ..., would all require an automatic update after adding or changing some rows. To be consistent I would need to update everything and not just SMILES columns. DataWarrior would then be another program. For some time I thought about giving individual columns an 'automatic update' status, but even that would have lots of consequences. Finally, I dropped the idea. Again I suggest to create a small macro deleting the SMILES column and re-creating it.

Hope you can live without it.

Best wishes, Thomas