Subject: LLE column doesn't update with new compound data
Posted by mvamos on Wed, 12 Aug 2015 00:46:27 GMT
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The LLE calculation column didn't update for me when I added new data. I merged in new IC50 data on which the LLE calculation is based. The structures for the compounds were already present and I merged the .csv file containing the IC50 data.

If I go again through Chemistry>Add Compound Properties>LE & Tox>LLE to add a new column (now appended with a 2 at the end because it's a duplicate of the previous), the values for the new data populate correctly.

In the attached photo, you can see the original LLE column on the left, and the 2nd LLE on the right.

Perhaps this is a small bug?

File Attachments

1) Untitled.png, downloaded 2006 times

LLE from Normalized ...	LLE from Normalized ...
	4.6792
	4.4664
	2.9938
2.6512	2.6512
2.3882	2.3882
3.7737	3.7737

Subject: Re: LLE column doesn't update with new compound data
Posted by thomas on Fri, 14 Aug 2015 05:41:51 GMT
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this is the expected behaviour. The LLE calculation is a one time matter. There is no mechanism that would update LLE values when the original IC50 is updated or when new IC50 values are appended. After appending new rows you could remove the then incomplete LLE column and calculate a new one. If you do this often, you could create a macro for that. Regards, Thomas

Subject: Re: LLE column doesn't update with new compound data
Posted by Christoph on Mon, 29 May 2017 23:49:14 GMT
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Hi everyone,

I had similar issues. I added more molecules and was wondering why the SMILES-structure column doesn't automatically update and add the SMILES for my new molecule. It would be nice to have an "update" option for the columns which DataWarrior once filled in.

Only a suggestion...

Best wishes,
Christoph

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

Subject: Re: LLE column doesn't update with new compound data
Posted by Christoph on Mon, 05 Jun 2017 15:18:50 GMT
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Hi Thomas,

Thank you very much for letting us know more about the background.

Since there is a workaround on this issue I can live with the current version of course.

Because it would however be a very nice feature if all 'derived' columns could be updated automatically, maybe this idea would be something for the list of features for the next major version of the program at some time in the future.

Best wishes,
Christoph