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 2008 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 |