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