Subject: Row wise chemical reaction
Posted by P_Fitz on Fri, 06 Dec 2019 18:54:33 GMT
View Forum Message <> Reply to Message

The enumerate chemical libraries feature of data warrior is awesome, but does not do quite what I want it to for this particular application.

I have a list of Carboxylic acids that correspond with specific Amino acids that they are combined with. Enumerate chemical libraries with these sets creates all possible combinations of the two. Is there a way to just combine specific Amino acids with specific Carboxylic acids? Basically I just want to combine reactants row-wise rather than combinatorially.

Thanks!

Patrick

Subject: Re: Row wise chemical reaction
Posted by nbehrnd on Tue, 17 Dec 2019 10:22:29 GMT
View Forum Message <> Reply to Message

Hello Patrick,

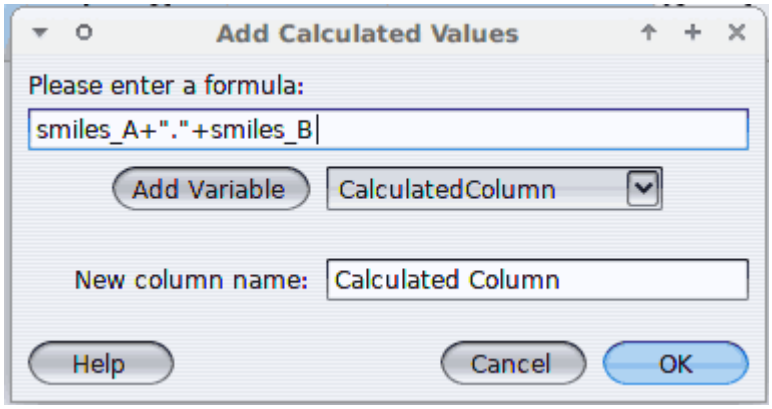
I understand your aim is to bring line wise structures deposit in independent columns into a cell in common.

If so, 1) convert the structures you already have in the .dwar file as SMILES. You find this function along chemistry -> from chemical structure -> Add SMILES code, to be applied for each column of structures. 2) To concatenate the SMILES, reach for Data -> Add Calculate Values. In the new sub-menu, you define a string addition, of the SMILES, as shown below:

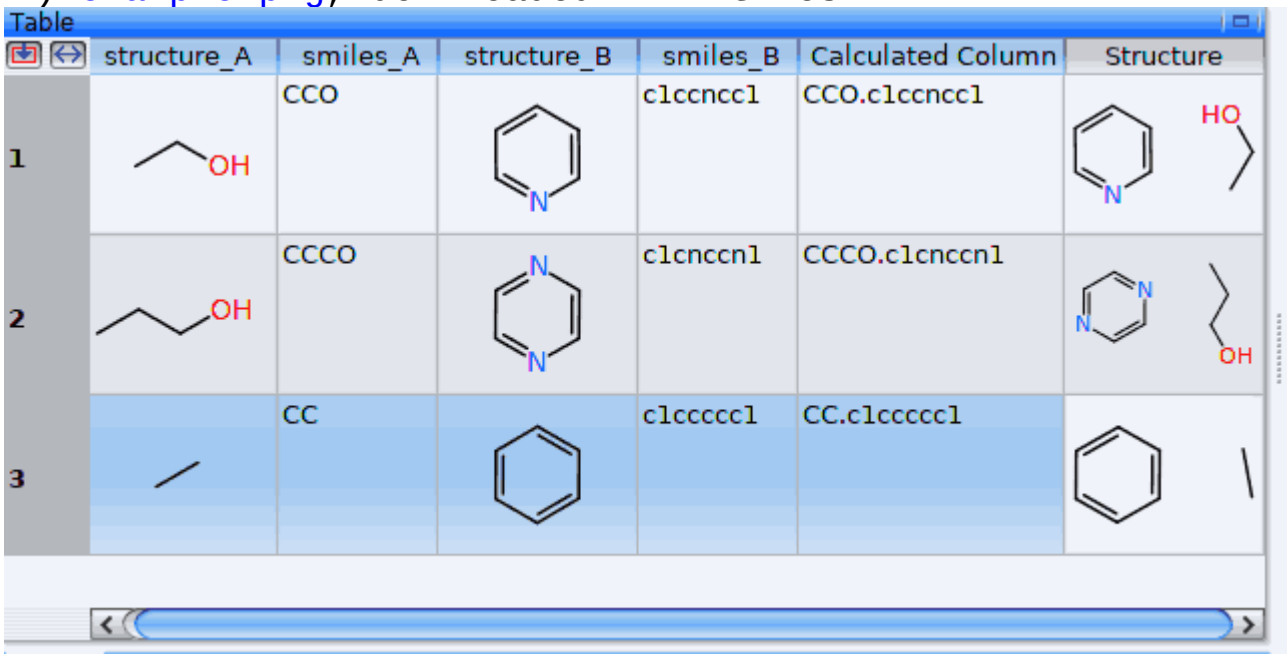
After confirmation by «ok», DataWarrior creates a new column with the result. You then 3) convert the concatenated SMILES string into a sketch with Chemistry -> Add Structures From Name. This equally creates a niew column, with both molecules represented in one cell:

Norwid

File Attachments
1) string_addition.png, downloaded 2071 times



2) example.png, downloaded 2117 times



3) MWE_joining_structures.dwar, downloaded 869 times

Subject: Re: Row wise chemical reaction
Posted by thomas on Tue, 17 Dec 2019 22:16:55 GMT
View Forum Message <> Reply to Message

If I understand correctly, you don't only want to combine two molecules, you rather want to react them, which would require one more step on top of Norwid's suggestion. Without a few nasty hacks, this is not possible right now. It would need a new functionality, where you could selected one or multiple structure columns as starting materials and define a generic reaction with an equal number of generic reactants that defines how to construct the product.

This wouldn't be too complicated, but is still too much to be included in the upcoming update. Maybe after that...

Subject: Re: Row wise chemical reaction
Posted by P_Fitz on Mon, 13 Jan 2020 22:02:35 GMT
View Forum Message <> Reply to Message

Yes that is correct, I do not just want to have them next to each other, I want to react them. Thanks for your reply and for supporting Data Warrior!

Subject: Re: Row wise chemical reaction
Posted by P_Fitz on Thu, 19 May 2022 23:57:58 GMT
View Forum Message <> Reply to Message

Just curious if this was ever implemented. Thanks for making Datawarrior freely available and supporting it!

Subject: Re: Row wise chemical reaction
Posted by thomas on Thu, 02 Jun 2022 12:56:29 GMT
View Forum Message <> Reply to Message

I just have implemented the feature and deployed it in the development version, which you can download as replacement files for the 5.5.0 version. The links appear in the fineprint of the download page after checking 'read and understood'. Now, when opening the 'Merge Columns' dialog and selecting some structure columns you can also specify a generic reaction that defines how to react the selected compound with each other. An example is in the help text accessible from the dialog. Please let me know, whether this works for you...

Subject: Re: Row wise chemical reaction
Posted by P_Fitz on Wed, 15 Jun 2022 22:24:06 GMT
View Forum Message <> Reply to Message

Hi Thomas,

Thanks so much for implementing this feature. Based on how the help screen looks (the suzuki reaction example) this is exactly how I want this feature to work. I've been trying to do the same thing with amide formation and it does not seem to be working. I went back and drew the same reaction scheme (at least I think so) for enumerating a library and that works. The numbering when I connected the bonds was slightly different there.

I'm not sure why, but after I draw the reaction, the A and B reactants seem to get switched. I think maybe the carboxylic acid is being interpreted as an fmoc amino acid and since it does not have an fmoc amino acid I'm getting an empty column as the reaction product. I've attached a screenshot of the reaction and my data columns. The output of the reaction is as I said an empty column.

As always, thanks for continuing to support Data warrior!

Patrick Fitzgerald

File Attachments

1) 20220615 functionality test.pdf, downloaded 675 times

Subject: Re: Row wise chemical reaction
Posted by P_Fitz on Wed, 15 Jun 2022 22:27:48 GMT
View Forum Message <> Reply to Message

I switched the order of my columns in the Table view and that seemed to work to do combine the molecules. This was reproducible. Switching them back stopped it from working, and then switching them again made it work.

Subject: Re: Row wise chemical reaction
Posted by nbehrnd on Mon, 20 Jun 2022 18:34:36 GMT
View Forum Message <> Reply to Message

Dear Thomas,

For the nicely working «merge by reaction» function, I would like to file for feature suggestion. May one extend the reaction editor's functionality to match the one already present when running chemistry -> enumerate combinatorial library, i.e. to add

+ define .and. save (eventually re-use) a reaction with user defined name in the .rxn format
+ access the already available templates of the combinatorial library (Stille, Wittig, etc.)

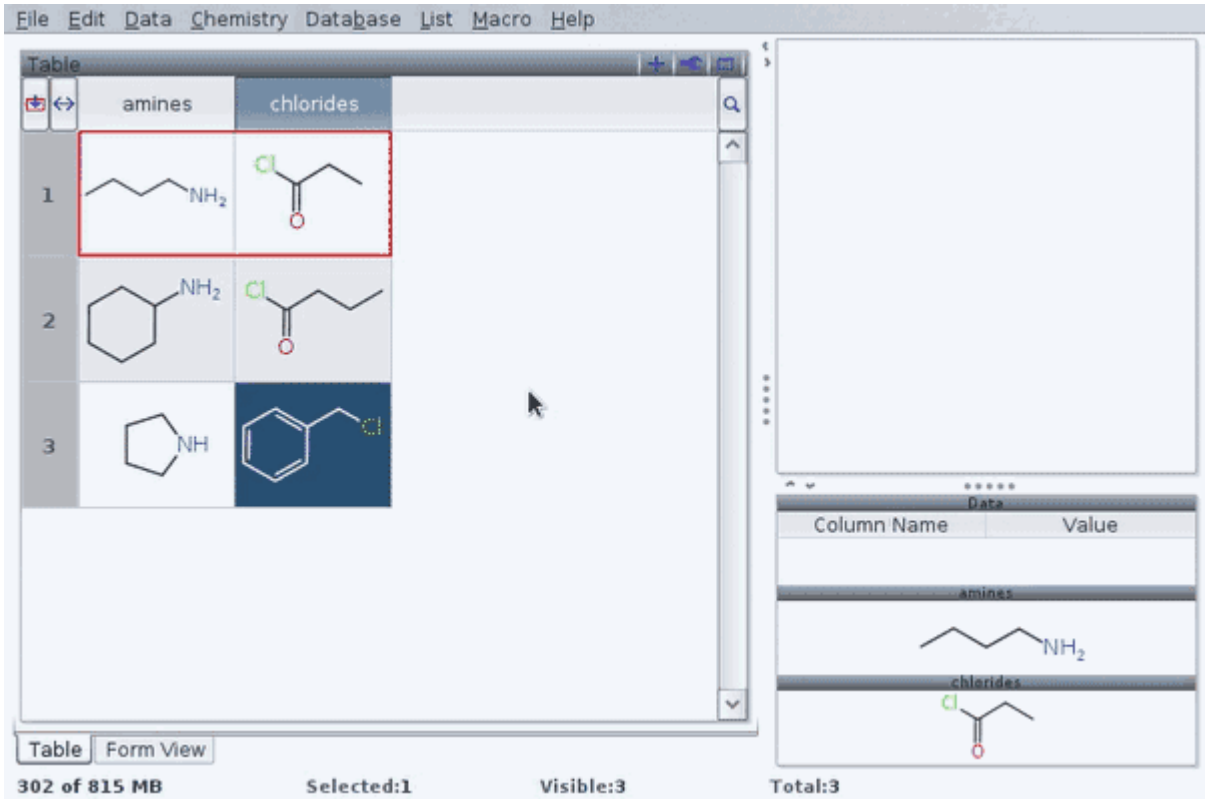
By now, the GUI of the two seem to differ:

The observations refer to DW 5.5.0 for Linux including the update by 2022-06-17.

Norwid

File Attachments

1) suggest_01.gif, downloaded 1826 times



2) reactions.dwar, downloaded 649 times

Subject: Re: Row wise chemical reaction
Posted by nbehrnd on Mon, 20 Jun 2022 18:44:58 GMT
View Forum Message <> Reply to Message

Dear Thomas,

related to the above feature suggest is a second one, this time to extend working via chemistry -> enumerate combinatorial library.

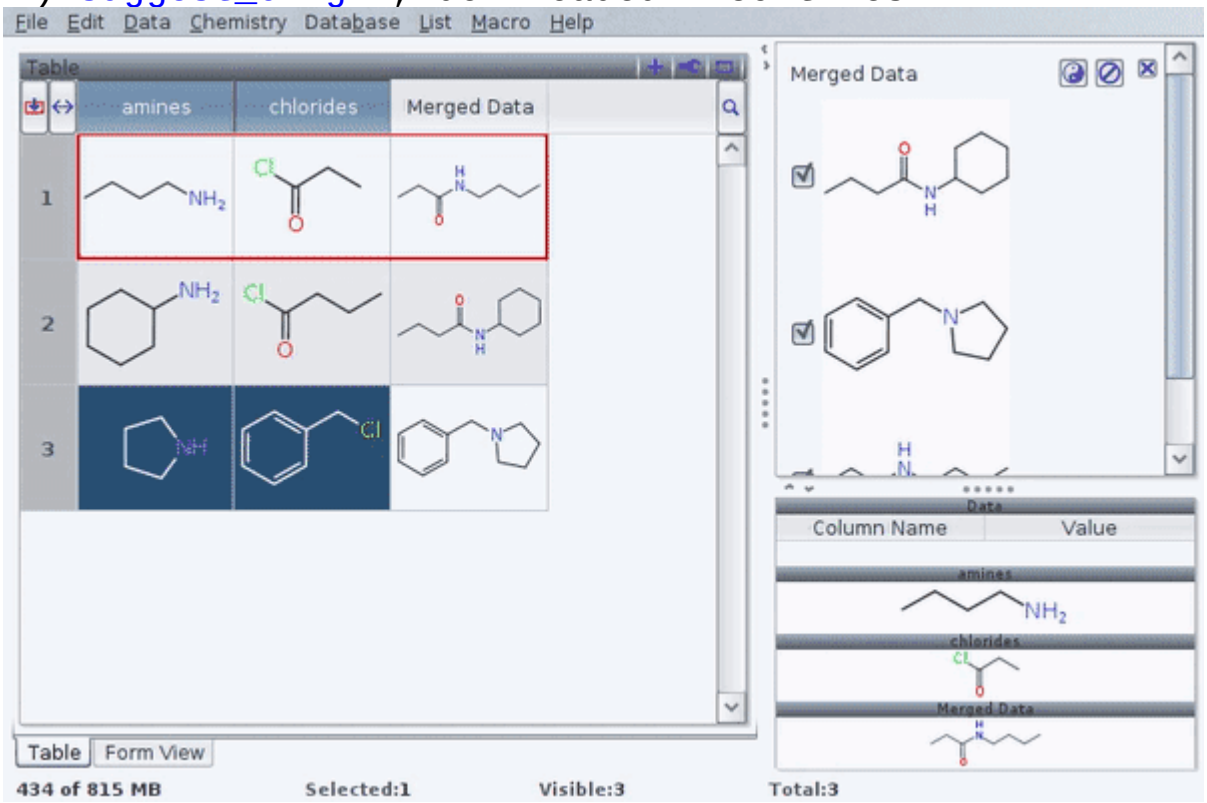
So far, reactants either are to be sketched again .or. load from a file about either one of the reactants. Would it be possible to extend the «add» function so that one may refer back to the currently open file to define the starting material by column? With the above test file reactions.dwar, this would be to point to column «amines» for one, and «chlorides» for the second line when «enumerate combinatorial library» asks for the reagents to permutate with each other.

At present «merge by reaction» constraints the set of products generated to reactions line-by-line.

Norwid

File Attachments

1) suggest_02.gif, downloaded 1759 times



Subject: Re: Row wise chemical reaction
Posted by thomas on Sat, 25 Jun 2022 13:48:52 GMT
View Forum Message <> Reply to Message

Hi Patrick,

yes, you are right. The reactants got switched, because they were encoded in lexical order by mistake, when they were stored as part of the task configuration. I have corrected this issue now in the current dev version.

Thank you for pointing me to the problem so clearly.

Thomas

Subject: Re: Row wise chemical reaction
Posted by P_Fitz on Tue, 28 Jun 2022 17:30:08 GMT
View Forum Message <> Reply to Message

I'm glad my comment made sense! Thanks for being so receptive to feedback/changes.

Subject: Re: Row wise chemical reaction
Posted by thomas on Thu, 14 Jul 2022 08:27:13 GMT
View Forum Message <> Reply to Message

Dear Norwid,

thank you for the suggestion to add starting materials from an existing column. I have implemented that two or three weeks ago, but forgot to mention it in this thread.

Thomas