

Subject: Re: Row wise chemical reaction
Posted by [nbehrnd](#) on Mon, 20 Jun 2022 18:44:58 GMT
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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 1467 times

The screenshot displays a software interface with a table and a merged data window. The table has three columns: 'amines', 'chlorides', and 'Merged Data'. It contains three rows of chemical structures. The first row shows a primary amine reacting with an acid chloride to form a secondary amide. The second row shows a cyclic amine reacting with an acid chloride to form a cyclic amide. The third row shows a cyclic amine reacting with a benzyl chloride to form a tertiary amine. The 'Merged Data' window on the right lists the resulting products with checkboxes. Below the table, a 'Data' window shows the column names and their corresponding chemical structures.

	amines	chlorides	Merged Data
1	<chem>CCCCN</chem>	<chem>CCC(=O)Cl</chem>	<chem>CCCCNC(=O)CC</chem>
2	<chem>C1CCCCC1N</chem>	<chem>CCC(=O)Cl</chem>	<chem>CCC(=O)N1CCCCC1</chem>
3	<chem>C1CCNC1</chem>	<chem>c1ccc(cc1)CCl</chem>	<chem>c1ccc(cc1)CN1CCNC1</chem>

Column Name	Value
amines	<chem>CCCCN</chem>
chlorides	<chem>CCC(=O)Cl</chem>
Merged Data	<chem>CCCCNC(=O)CC</chem>