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Subject: Row wise chemical reaction

Posted by [P\\_Fitz](#) on Fri, 06 Dec 2019 18:54:33 GMT

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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

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