Subject: Re: Row wise chemical reaction
Posted by P_Fitz on Wed, 15 Jun 2022 22:24:06 GMT
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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 406 times