Posted by yrin0878 on Fri, 28 Apr 2023 01:18:52 GMT

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Hi I'm beginner of datawarrior.
It is a good software to analyze chemical data.
But I have a problem.

I have over 100 building blocks, and I want to add a same reaction to all that building blocks.
But when I'm trying to add a reaction, I have to make a reaction column then, draw the reaction to each structures.
This takes too long time :(

Can I apply one reaction to that all structures?
Tell me the way to deal with this problem.

Thank you

File Attachments
1) datawarrior_Q.png, downloaded 440 times

File Edit Data Chemistry Database List Macro Help

Table

#	BB ID	Structure of SMILES	SMILES	Amine protecting group	이름
1	AA0001		CC(C)(C)OC(=O)NCCC(C1=CC=CC=C1)C(=O)O	Boc	α-[2-[[(1,1-Dimethylethoxy)carbonyl]amino]ethyl]benzeneacetic
2	AA0002		CC(C)(C)OC(=O)NCC(C1=CC=CC=C1)C(=O)O	Boc	α-[[[(1,1-Dimethylethoxy)carbonyl]amino]methyl]benzeneacetic acid
3	AA0003		CC(C)(C)OC(=O)NCC(C)(C)C(=O)O	Boc	4-[[(1,1-Dimethylethoxy)carbonyl]amino]-2,2-dimethylbutanoic acid
4	AA0004		O=C(O)CC1CN(C(=O)OCC2C=3C=CC=CC3C=4C=CC=CC42)CC1	Fmoc	1-[(9H-Fluoren-9-ylmethoxy)carbonyl]-3-pyrrolidineacetic acid
5	AA0005		C(OC(NCC[C@@H](C(O)=O)O)=O)C1C=2C(C=3C1=CC=CC3)=CC=CC2	Fmoc	(2S)-4-[[(9H-Fluoren-9-ylmethoxy)carbonyl]amino]-2-hydroxybutan
6	AA0006		OC(C(C1CCOCC1)NC(OCC2C(C=CC=C3)=C3C4=C2C=CC=C4)=O)=O	Fmoc	2-(((((9H-Fluoren-9-yl)methoxy)carbonyl)amino)-2-(tetrahydro-2H-py
7	AA0007		주문 중	Fmoc	2-(1-[[(9H-fluoren-9-yl)methoxy]carbonyl}piperidin-4-yl)acetic acid
8	AA0008		CC(C)(C)OC(=O)NCC(C)(C)C(=O)O	Boc	3-((tert-butoxycarbonyl)amino)-2,2-dimethylpropanoic acid
9	AA0009		O=C(NCC(C)C(O)=O)OCC1C2=C(C3=C1C=CC3)C=CC2	Fmoc	3-(((((9H-fluoren-9-yl)methoxy)carbonyl)amino)-2-methylpropanoic

456 of 563 MB   Selected:1

Q 검색하려면 여기에 입력하세요

Subject: Re: Add reaction from structure
Posted by thomas on Sat, 29 Apr 2023 12:24:20 GMT
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I assume you are just interested in the product structures. Then, you can do one of two things:

- Choose "Chemistry->Enumerate Combinatorial Library", then draw the reaction using one substructure
  on the reactant side that matches to all your reactants. Draw the modified product and make sure,
  all atoms that exist in both, reactant and product, are properly mapped (see image).
  Go to the 'Reactants' panel. Where ist says "<to add compounds..." make a right mouse click, select
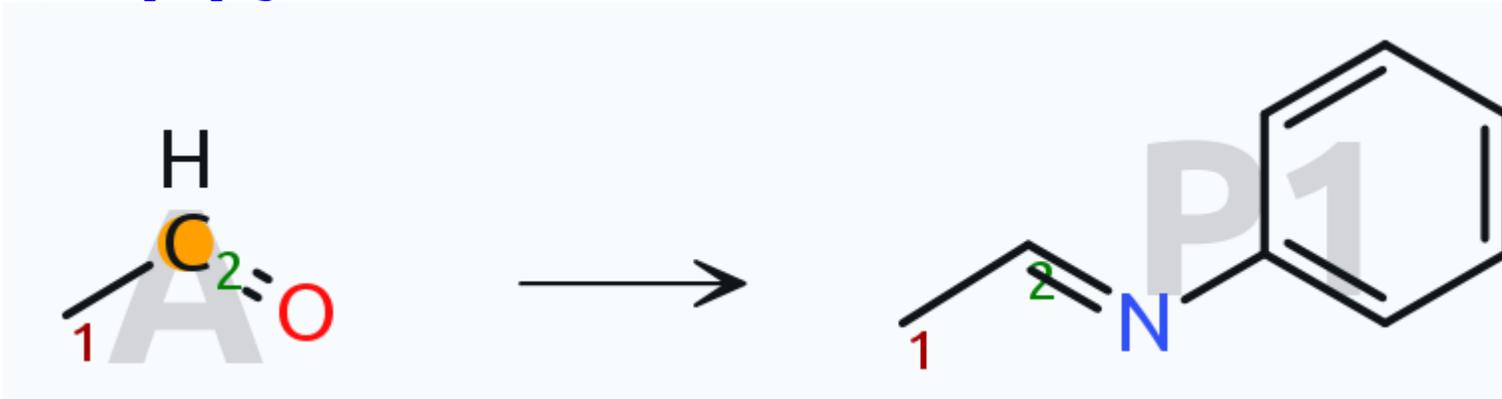 "Add From File...", select you reactant file, click 'Open' and then 'OK'. This creates a new Window
  with the product structures.

- Faster, but a little less flexible would be using 'Edit->Find And Replace' as in the image below

<u>File Attachments</u>
1) temp1.png, downloaded 747 times

2) temp2.png, downloaded 696 times

Find And Replace

Column: **Structure** ▾

Find this: ▾
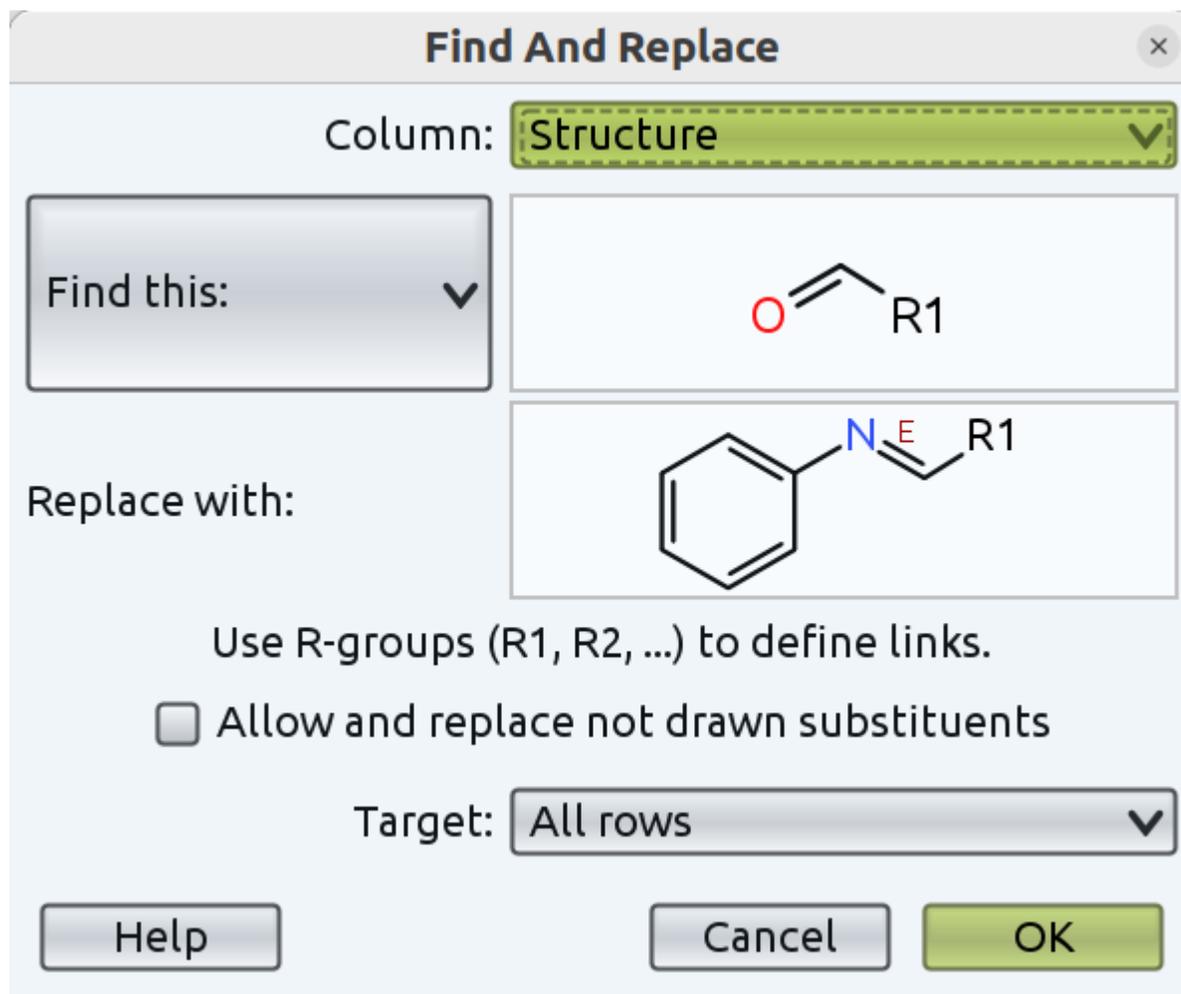

Replace with:

Use R-groups (R1, R2, ...) to define links.

☐ Allow and replace not drawn substituents

Target: **All rows** ▾

| Help | | Cancel | OK |

Subject: Re: Add reaction from structure
Posted by yrin0878 on Wed, 10 May 2023 06:58:45 GMT
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Thank you.

But I have one more question about the combinatorial library.

I want to make a library using "peptide coupling".

Reactants are -NR2 and -COOH.

Do I need to make a three libraries for -NR2, -NHR and -NH2 ?

Is there any way to enumerate combinatorial lib. only once?

Subject: Re: Add reaction from structure
Posted by thomas on Mon, 22 May 2023 19:24:23 GMT
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I assume that -NR2 results in -C(=O)-N(+)R2- and the the other two lead to an amid loosing one hydrogen?
In that case the generic reaction of these two cases is different. Therefore, you need to define a two
different generic reactions, ideally use atom query features to define amine reactants specifically in each case.
Then you can use the same reactant library for both cases, because the generic reactant only uses the matching ones.
Afterwards you can merge both files.

If you need to repeat the procedure many times with different amine or acid sets, then you may define a macro that runs
both enumerations, one after the other, saving the results of each and merging them afterwards.