
Subject: Add reaction from structure

Posted by [yrim0878](#) 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 238 times

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 it says "<to add compounds..." make a right mouse click, select

"Add From File...", select your 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

File Attachments

1) [templ.png](#), downloaded 465 times

2) [temp2.png](#), downloaded 441 times

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.
