
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) [temp1.png](#), downloaded 962 times




2) [temp2.png](#), downloaded 886 times

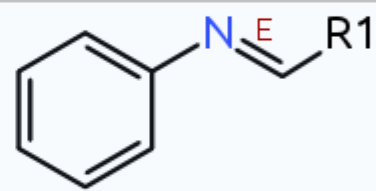
Find And Replace ✕

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