
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.
