Subject: Re: Combinatorial Library Enumeration
Posted by nbehrnd on Tue, 22 Jun 2021 20:21:44 GMT
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Dear ndandu,

the generation of the reaction map requires one complete reaction. Thus, in the explicit reaction of the anhydride with methylamine, the amide must include the methyl group, too. Subsequently, map remaining atoms of the anhydride in the product, followed by those inherited by the amine. The short .mp4 attached below might illustrate this further.

Norwid

File Attachments

1) map_reaction.mp4, downloaded 596 times