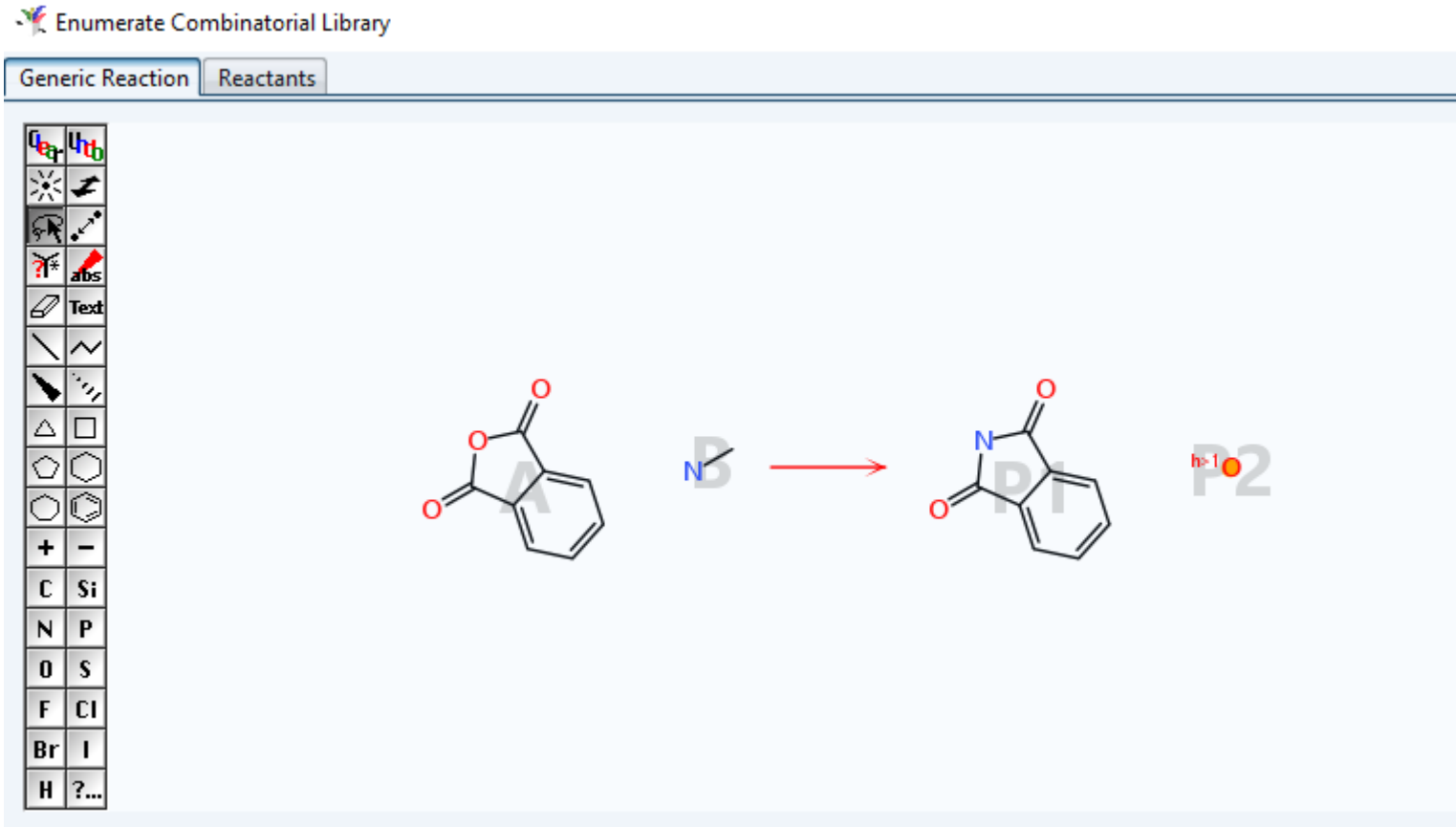
Subject: Combinatorial Library Enumeration
Posted by ndandu on Mon, 21 Jun 2021 15:49:18 GMT
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I have installed the latest version of Datawarrior on my Windows machine. I am having difficulty in performing queries on the generic reactions. I am unable to do mapping of the reactants to products (it doesn't show the numbers) and also having a tough time finding options on how to put queries on the "define generic reactions" window. Please let me know if there are any shortcut keys that are helpful?

File Attachments

1) genericReaction.png, downloaded 954 times



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 595 times