Subject: Re: Combinatorial library issues
Posted by amorrison on Fri, 24 Apr 2020 08:45:33 GMT
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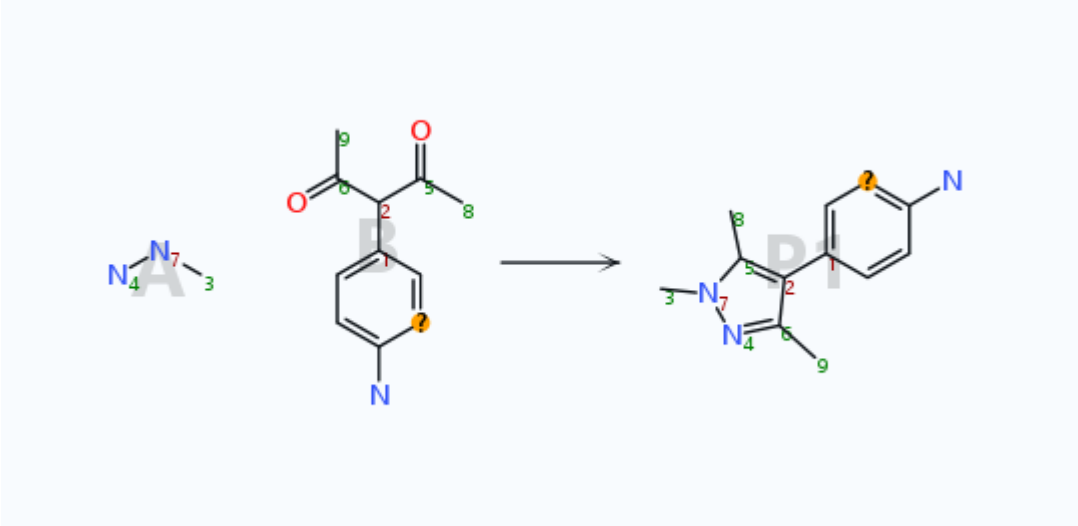
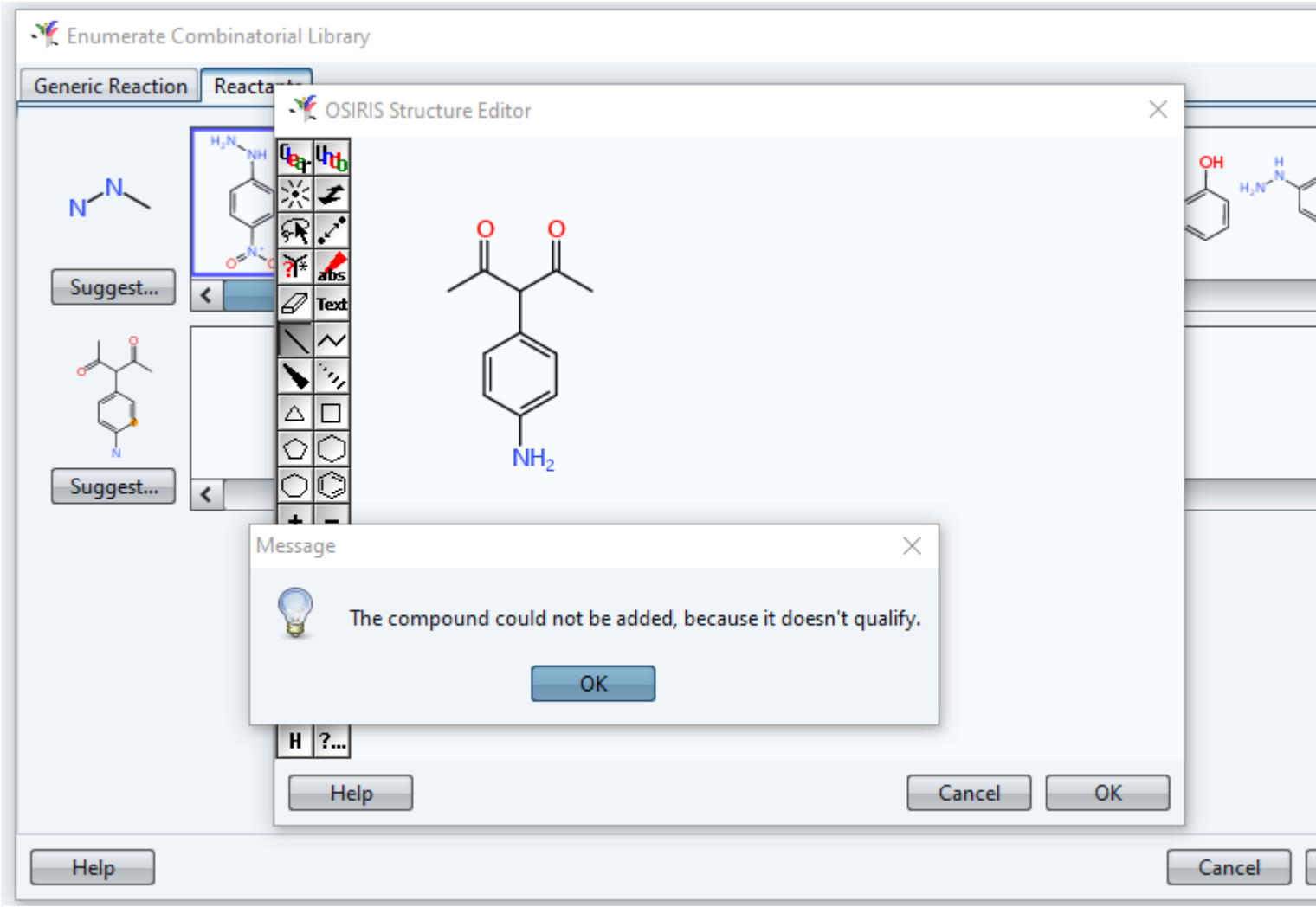
Hi Thomas,
I too have been having some issues with combinatorial enumeration. I've attached a couple of screenshots of a fairly simple pyrazole formation where I would like to include anilines and aminopyridines. I think the reaction and mapping looks right, but it wont accept the aniline example.
Any help would be appreciated.
Thanks,
Angus

File Attachments

1) reaction.png, downloaded 1110 times



2) Error_DoesNotQualify.png, downloaded 1031 times


Enumerate Combinatorial Library
Generic Reaction
Reactants
Suggest...
Suggest...
OSIRIS Structure Editor
Text
abs
NH2
Message
The compound could not be added, because it doesn't qualify.
OK
H
?...
Help
Cancel
OK
Help
Cancel