Subject: Re: Combinatorial Library
Posted by becky26 on Fri, 12 Apr 2024 10:18:32 GMT
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Hi,

Thanks for replying.

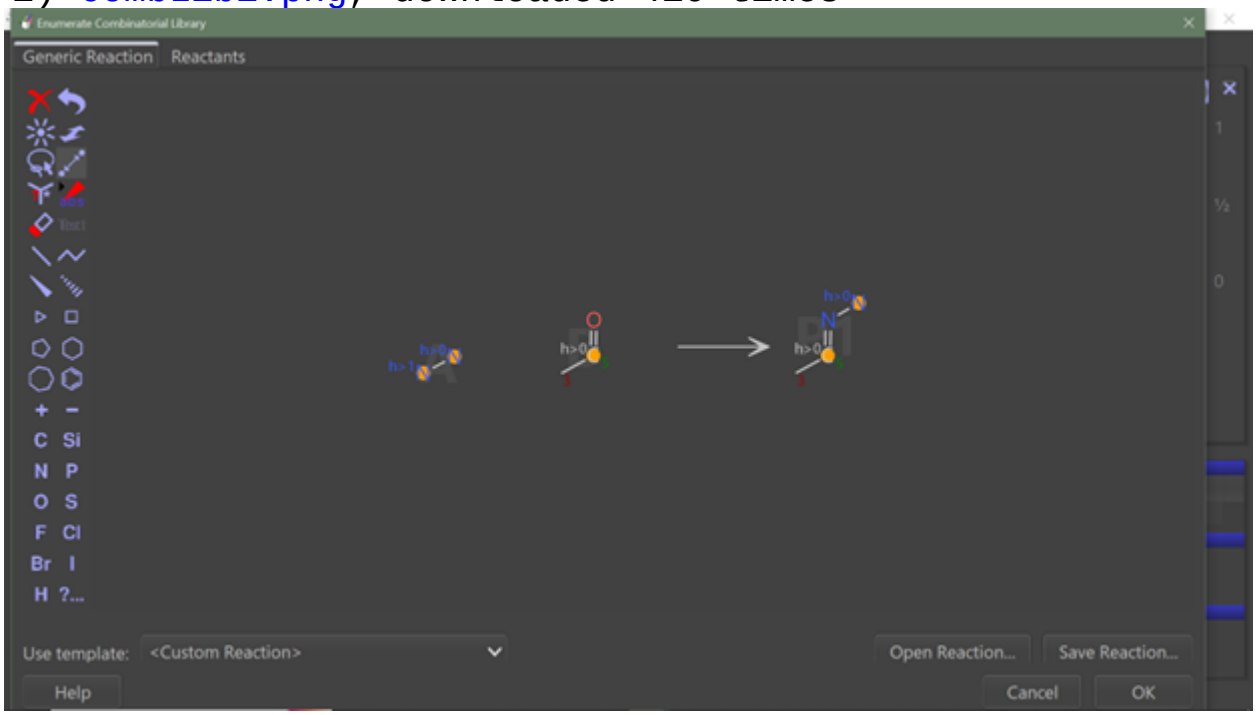
I am defining the first step in my reaction my modifying the amide template, I'm trying to have the general reaction for a hydrazone, I check that all the atoms map. Then I import a file of the aldehyde and hydrazine commercial building blocks into the reagent page and they all display correctly. The enumeration runs, but all reactions no matter the reagents they use generate the same basic scaffold that was defined in the initial reaction page.

I've attached some pictures

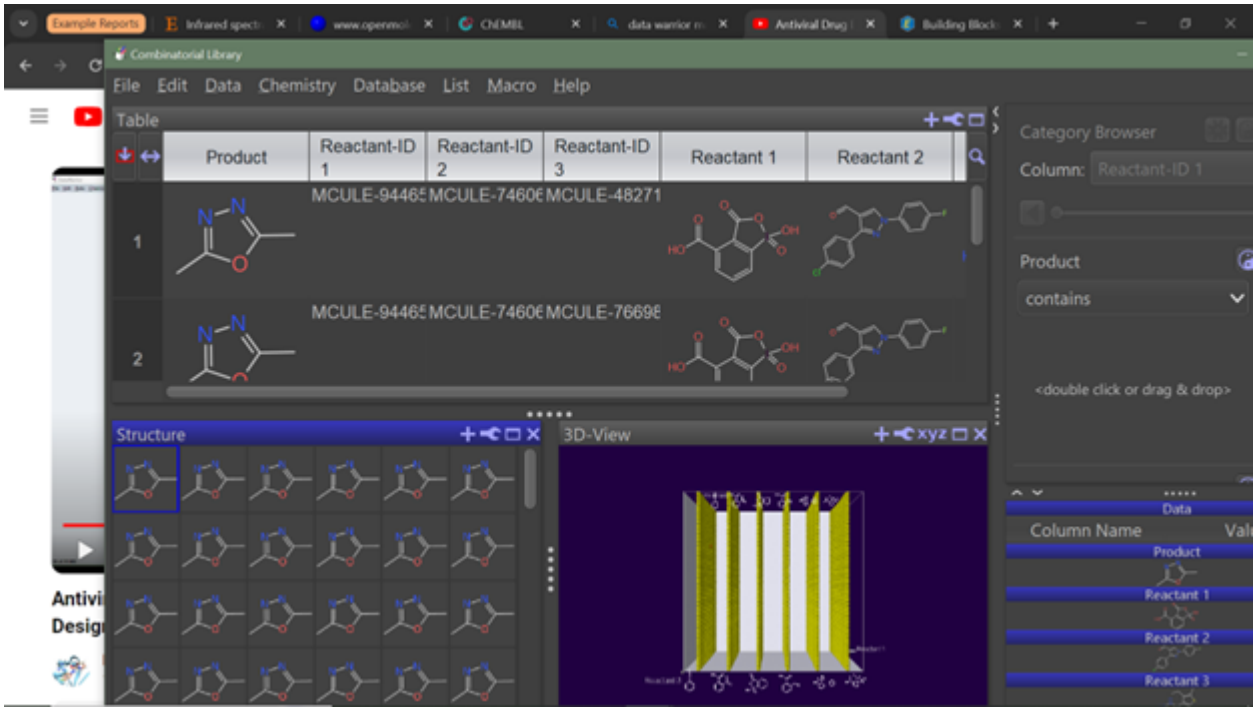
Thanks

File Attachments

1) CombLib1.png, downloaded 410 times



2) CombLib2.png, downloaded 445 times


Combinatorial Library
File Edit Data Chemistry Database List Macro Help
Table
Product
Reactant-ID 1
Reactant-ID 2
Reactant-ID 3
Reactant 1
Reactant 2
Category Browser
Column: Reactant-ID 1
Product
contains
<double click or drag & drop>
Structure
3D-View
Data
Column Name
Product
Reactant 1
Reactant 2
Reactant 3