Subject: Combinatorial Library
Posted by becky26 on Thu, 11 Apr 2024 12:13:44 GMT
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Hi,

New to data warrior and I'm trying to enumerate a combinatorial library for a multicomponent reaction I am working on. I have tried defining a reaction in the step wise way, but I always end up producing thousands of the product I defined. I am aiming to input commercially available building blocks for my reaction to assess possible scope but struggling with defining the reaction.

I only have success generating more than 1 product when I use the templates, but the templates are not applicable to my reaction.

I've followed the manual but must be missing something.

Any help would be much appreciated.

Subject: Re: Combinatorial Library
Posted by thomas on Thu, 11 Apr 2024 13:02:55 GMT
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Can you give me a little example of what you do that doesn't work?

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

Thanks for replying.

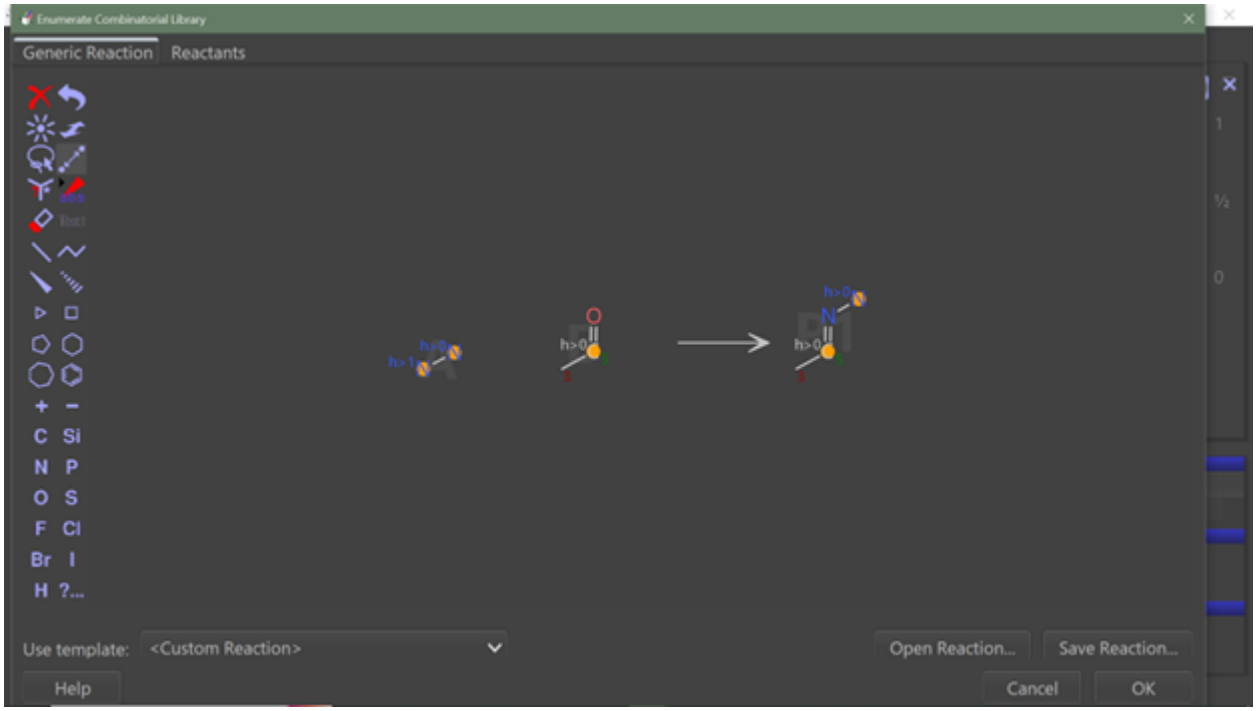
I am defining the first step in my reaction my modifying the amide template, I'm trying to have the general reaction for a hydrazone, I check that all the atoms map. Then I import a file of the aldehyde and hydrazine commercial building blocks into the reagent page and they all display correctly. The 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

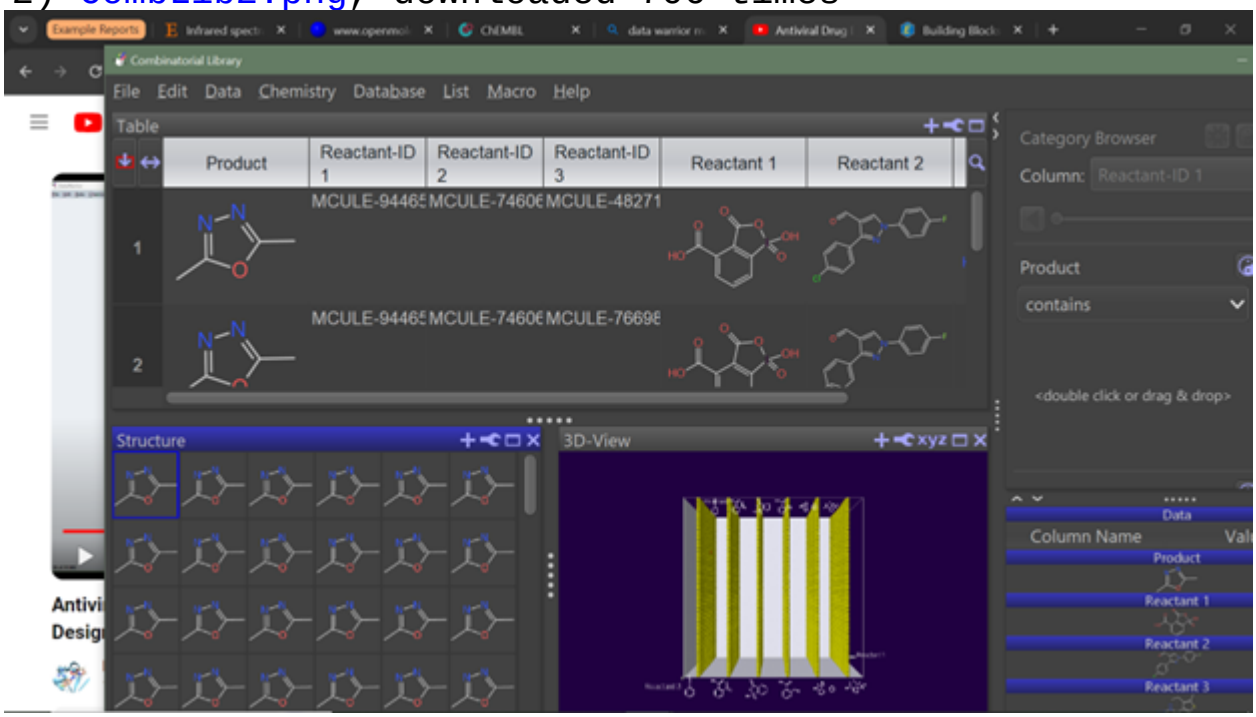
Thanks

File Attachments

1) CombLib1.png, downloaded 705 times



2) CombLib2.png, downloaded 706 times



Subject: Re: Combinatorial Library
Posted by nbehrnd on Tue, 16 Apr 2024 20:18:47 GMT
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Hi becky26,

based on the screen photos shared by you, I set up a small combinatorial library with 10 by 10 reagents proposed by DW (version 06.01.03 in Linux Debian). There was no particular problem observed, many different products were generated (though no oxadiazole), see the .zip archive attached below. There however is a small discrepancy between the reaction scheme you report with CombLib1.png (a two component reaction) vs the reagent array you eventually used (CombLib2.png) indicating three components to yield the product.

Norwid

File Attachments

1) 2024-04-16_dw_combinatorial.zip, downloaded 594 times

Subject: Re: Combinatorial Library
Posted by thomas on Wed, 24 Apr 2024 12:04:30 GMT
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the resolution of you first image is a little low, but it seems that the atoms of your first reactant are not mapped to product atoms. In that case DataWarrior assumes the atoms in the product are not coming from the reactant and will not consider that reactant.
