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Subject: Combinatorial library issues

Posted by [timritchie](#) on Sat, 28 Mar 2020 11:24:36 GMT

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Hello,

I've been having problems with generating combichem libraries with the new version (5.2).

Sets of reagents that worked previously now are not accepted as valid.

Also I cannot map the atoms between reagents and products even for simple transformations.

Has something changed in the new version?

Thanks and regards,

Tim Ritchie.

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Subject: Re: Combinatorial library issues

Posted by [thomas](#) on Sun, 29 Mar 2020 12:08:45 GMT

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Hi Tim,

there changed a lot in the combinatorial library creation: There are new templates and the exclude group logic was improved, but the mechanism to generate product structures stayed more or less the same. Semi-automatic atom mapping should work as before. Can you send me a small example with clear description how to reproduce a problem? Then I will make sure that is is solved.

Thanks in advance and sorry for the inconvenience, Thomas

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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

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### File Attachments

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1) [reaction.png](#), downloaded 411 times

2) [Error\\_DoesNotQualify.png](#), downloaded 433 times

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Subject: Re: Combinatorial library issues  
Posted by [thomas](#) on Sun, 26 Apr 2020 16:24:01 GMT  
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Hi Angus,

I have tried to reproduce with the current development version and with 5.2.1. In both cases I don't get an error. Strange is also the mapping, which in your picture doesn't complete. When I manually map just two or three of your manually mapped atoms, then all the others are automatically mapped.

Do you use an older version than 5.2.1? If yes, I suggest to update to 5.2.1 and then even replace with newest builds from [openmolecules.org/datwarrior/dw521win.zip](http://openmolecules.org/datwarrior/dw521win.zip) (or dw521x.zip for Linux or Mac).

Thomas

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Subject: Re: Combinatorial library issues  
Posted by [amorrisson](#) on Mon, 27 Apr 2020 11:41:39 GMT  
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Thanks Thomas, not sure how I managed it but working now. Angus

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