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.

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

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 354 times
2) Error_DoesNotQualify.png, downloaded 373 times

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 (or dw521x.zip for Linux or Mac).

Thomas

Subject: Re: Combinatorial library issues
Posted by amorrison 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