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