
Subject: Enumerate Combinatorial Library - Uncaught Exception

Posted by [amorrison](#) on Tue, 11 Feb 2020 11:06:06 GMT

[View Forum Message](#) <> [Reply to Message](#)

Hi,

I'm trying to enumerate a virtual library and get the same error. I've simplified it to a generic reaction and still get the same error. I've attached images of the simplified reaction, reactants and error.

Thanks in advance,

Angus

File Attachments

- 1) [Error.PNG](#), downloaded 339 times
 - 2) [Reactants.PNG](#), downloaded 343 times
 - 3) [Reaction.PNG](#), downloaded 345 times
-

Subject: Re: Enumerate Combinatorial Library - Uncaught Exception

Posted by [thomas](#) on Tue, 11 Feb 2020 13:16:56 GMT

[View Forum Message](#) <> [Reply to Message](#)

Hi Angus,

thank you for sending this. Interestingly, I have received a very similar report just recently and have fixed it a few days ago. The dw500 links I have updated today. For cases like this I have two more suggestions:

- I would set the 'no more substituents' query feature for the single bonded oxygen in the carboxylic acid. This prevents wrong substructure matches if there are esters etc in any starting material.
- Effectively this is a one-dimensional combichem library. You may define that simpler by removing the carboxylic acid from the reactants of the generic reaction and leave these atoms unmapped on the product side. Then you also don't need to define acetic acid as second reactant in the reactant panel.

thanks again, Thomas
