Subject: How to create a combinatorial library?
Posted by sebawei on Wed, 30 Sep 2015 08:34:38 GMT
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Hi

I'm starting to use DataWarrior and I have a problem with the "Create a combinatorial library" tool. I tested it a few times with different reactions and molecules and I always were not able to generate any products. After the calculation I get four windows: a "Table" window, a "Product" windows, a "2D View" Window and a "3D Window". The Product window is showing me a lot of empty boxes and in the Table window I can find a column which is called "Product", but it is empty too.
What am I doing wrong?

Thanks for your help

Sebastian

Subject: Re: How to create a combinatorial library?
Posted by thomas on Sat, 10 Oct 2015 14:17:04 GMT
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Hi Sebastian,

the most likely reason is that one (or more) of your generic products (which are substructure definitions) is not found in the list of starting materials that you assign to it. If you post the reaction.rxn file and sdf- or dwar-files of the reactants, or if you post screenshots of the reaction and of the reactants, then I will be in a better position to help you.

Kind regards and sorry for the late reply,

Thomas