Subject: How to use "Create Combinatorial Library" function?
Posted by Data_Center on Tue, 23 Feb 2016 18:32:51 GMT
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I have just started using Data Warrior and I couldn't correctly deploy "Create Combinatorial Library" function. I used a generic reaction of a carboxlic acid with an amine to form an amide bond. Then I used 11 carboxylic acids and eight amines but all the 88 products were filled with the structure of the generic product not the ones from the lists I provided. Any help. I have attached the list of the generic reaction I used along with the files of acids and amines. If anyone knows what is going, please share your thoughts and I appreciate your help.

Subject: Re: How to use "Create Combinatorial Library" function?
Posted by thomas on Sat, 27 Feb 2016 15:11:34 GMT
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Some of your atoms of the generic reactions were not mapped: methyl-C and carbonyl-O of acetic acid and methyl-C of methyl-amine. If you complete the mapping with the mapping tool by clicking any unmapped atom on the reactant side and drag it to the respective atom on the product side, then it works.

I admit that DataWarrior should provide a conclusive error message.