
Subject: Reaction enumeration with aromaticity

Posted by [mattiafelice.palermo](#) on Tue, 01 Jun 2021 16:19:01 GMT

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Hello everyone,

I'm trying to create a reaction where a quinone-containing molecule (non aromatic) is reduced to hydroquinone (aromatic).

The input reaction I wrote is:

In the input reaction, the carbon bonds of the product rings and "sidegroup" are automatically converted to delocalized by Datawarrior.

These are the reactants:

When I try to run the reaction, Datawarrior outputs a list of empty products:

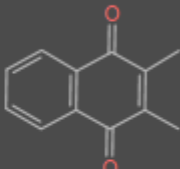
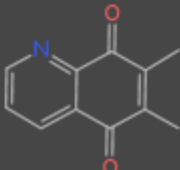
I am probably doing some very basic mistake, but I cannot figure out what I'm doing wrong... Can anybody point out what should I do to obtain the list of products?

Thank you very much for your help and let me know if you need any additional information!

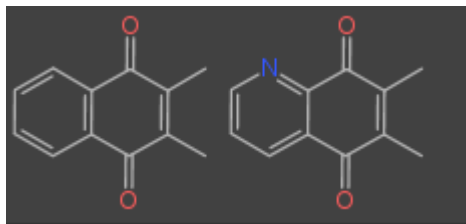
Mattia

File Attachments

1) [products.png](#), downloaded 1085 times

Table			
	Product	Reactant-ID	Reactant 1
1		2	
2		3	

2) [reactants.png](#), downloaded 1145 times



3) [reaction.png](#), downloaded 1167 times

