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 "sidegrop" 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 781 times
- 2) reactants.png, downloaded 841 times
- 3) reaction.png, downloaded 889 times