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 411 times
2) reactants.png, downloaded 476 times
3) reaction.png, downloaded 487 times