Subject: Re: Reaction enumeration with aromaticity
Posted by mattiafelice.palermo on Wed, 02 Jun 2021 21:22:20 GMT
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Hi Thomas,

thank you so much for your prompt fix and for the in-depth explanation. I apologize for the late reply, today in Italy it's national holiday!

I have updated to the development version and tried the equivalent reaction you have shown in the picture (double bond+aromatic flag), and it works as expected :)

Unfortunately, trying to do the same with the delocalized bond version still outputs an empty product. Perhaps I'm doing something wrong? I am attaching the rxn file in case it can be of use. Let me know if I can provide any additional information to reproduce the error.

Anyways, even though for me it is more intuitive to work with the delocalized representation, of course the double bond + aromatic flag will definitely do!

Thank you very much for your help and for the wonderful free software!!

Mattia

File Attachments

1) QUI_ox-red_002.rxn, downloaded 702 times