Subject: Add reaction from structure

Posted by yrin0878 on Fri, 28 Apr 2023 01:18:52 GMT

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Hi I'm beginner of datawarrior.

It is a good software to analyze chemical data.

But I have a problem.

I have over 100 building blocks, and I want to add a same reaction to all that building blocks. But when I'm trying to add a reaction, I have to make a reaction column then, draw the reaction to each structures.

This takes too long time:(

Can I apply one reaction to that all structures? Tell me the way to deal with this problem.

Thank you

File Attachments

1) datawarrior_Q.png, downloaded 369 times