Subject: DW 5.0 Enumerate library reactant selection disabled Posted by P_Fitz on Thu, 05 Dec 2019 22:50:00 GMT

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I am trying to enumerate a library. The reaction I want is simple. All I want to do is convert Carboxylic acids to methyl amides. I have attached the reaction file. When I go to select the reactants however, I cannot add any because there is no popup window. Dragging a .csv with the smiles, or a .dwar file also does not allow me to select reactants.

I am using DW 5.0. I also updated some of the files when I was trying to use the diverse set funciton. I am currently working on MAC high sierra 10.13.6. I will also try to see if the issue exists on windows later today.

File Attachments

1) Untitled Reaction.rxn, downloaded 632 times

Subject: Re: DW 5.0 Enumerate library reactant selection disabled Posted by P_Fitz on Fri, 06 Dec 2019 18:33:57 GMT

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Woops I figured it out. I didn't realize that you had to right click in the box to add data files. It is less intuitive now than when there was an add files button. The suggest from enamine is sort of interesting. It would be nice if that had more filters you could apply.

Thanks for supporting Data warrior. It is awesome!