Subject: Splitting reactants column
Posted by jeusamio on Fri, 28 Jul 2023 11:33:43 GMT
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Hi,

I'm working through a file of reactions with two or three reactants and one to four products. I have found about the Extract reactants functionality but it groups them into a single cell with several structures. Since all my reactants contain at least an aldehyde and an alkene/alkyne, I was thinking if there is an option to copy the reactants and keep only the individual molecules that match a given substructure (like a CHO, for example).
Is there a way to do this?

Thank you very much.

Javier

Subject: Re: Splitting reactants column
Posted by thomas on Tue, 01 Aug 2023 10:20:29 GMT
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Hi Javier,

that seems a useful functionality, but doesn't exits yet. An implementation would not be complicated and I am thinking of two ways to achieve something close:

1: Extend 'Split Multiple Value Rows' to also work with chemical structure columns. Then, a row that contains n reactants in one cell would be duplicated n times with every row containing just one of the n reactants. With a structure filter one could focus on the relevant ones, e.g. CHO in your case.

2: Rename and extend 'Add Largest Fragment' to 'Extract Fragment'. Then the there should be at least these options: 'Largest' and 'By Substructure'.

Give me a few days...

Thomas

Subject: Re: Splitting reactants column
Posted by thomas on Thu, 10 Aug 2023 12:47:37 GMT
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Functionalities 1 and 2 suggested in my recent post have been implemented and deployed in the current dev update.

Subject: Re: Splitting reactants column
Posted by jeusamio on Mon, 04 Sep 2023 15:17:08 GMT
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Hi Thomas,

Thank you so much for your dedication. I will try and wait until the next stable version is released to try the new feature, but if I'm too impatient I might just clone the dev version :) .

Thanks!

Javier

Subject: Re: Splitting reactants column
Posted by thomas on Sun, 10 Sep 2023 12:47:56 GMT
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You don't need to clone the github repositoy for that feature. Dev version means that you can download a zip-archive with replacement files. Updating to the current dev version is just a matter of replacing a few files: On openmolecules.org/datawarrior/download.html click 'read and understood...'. Some small print appears that contains two links for the dev update files...