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