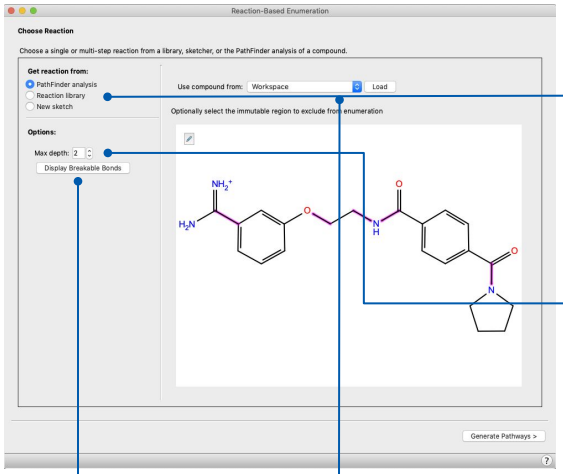
Reaction-Based Enumeration

1. Choose Reaction



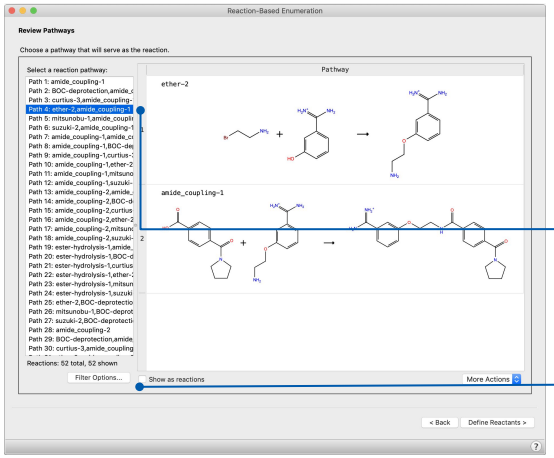
Pathfinder can be used to generate a set of synthetically reasonable pathways, but is not a retrosynthesizer. It is the recommended option for generating reaction pathways for Reaction-Based Enumeration

For a linear synthesis the depth is equal to the number of steps in a reaction

Reaction-Based Enumeration accepts only a single input structure per enumeration

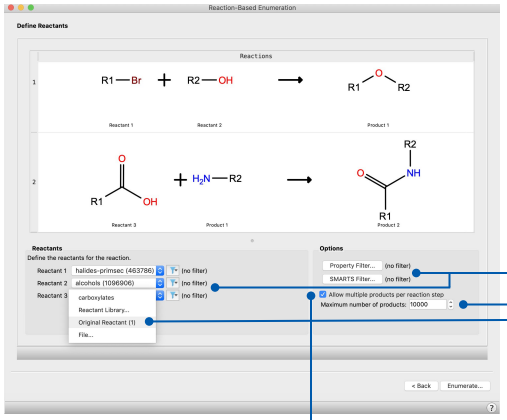
Display breakable bonds in the sketcher (highlighted in pink). Once activated, you can lasso a region of the molecule in the sketcher to set it as immutable

2. Review Pathways



Pathfinder uses a set of 130 reactions to generate potential pathways for enumeration. It is recommended that you select a pathway with reactions that would allow you to vary your desired fragment(s) of your input molecule

3. Define Reactants



Property and SMARTS filters can be used for both the reactants and products
(Note: REOS and PAINS filters are available as pre-generated product filters)

When a maximum is set, a random seed is used to generate the maximum number of products

Select whether you would like the fragment used in the enumeration to be chosen from your input structure or a curated library of eMolecules building blocks

If a reaction between a particular combination of your reactants could generate several possible products, you have the option to return all products or just the first one

If you would like to enumerate with several pathways simultaneously, consider using the **Automated Reaction-Based Enumeration** panel