

1. Enter target molecule

Either directly as a SMILES string, or by drawing the molecule.

This is the molecule you wish to synthesise. SMILES strings can also be copied from software such as chemdraw.

A number of example molecules are also available.

2. Set the scoring parameters

Max steps determines the maximum length of the pathway.

Pathways are generated and then scored on a number of criteria. Pathways are ranked according to a weighted score which incorporates each of these normalised criteria. To favour one criteria over another adjust the weights.

Additional options such as the maximum number of nodes to be considered in the network generation are available under options

3. Explore pathway suggestions

Pathways are displayed in order of ranking. Scroll through the pathway suggestions by clicking the green arrows, or changing the pathway number.

In some cases where pathways are identical except for the order of the reactions, these have been grouped together and are shown as pathway variants, which can also be clicked through using the red arrows.

Pathway Explorer
Enter target molecule as a SMILES string to start

Target SMILES
eg CCCC=O Draw

Max steps

Weight Complexity Change

Weight Number of Enzymes

Weight Starting Material

Weight Known Enzyme Steps

Weight Cofactor Stoichiometry

Start

Queuing Network Pathways Scoring Complete

Options +

Pathway num: <-- --> Pathway variant: <-- 1 of 1 -->

Reaction network diagram showing steps: Carboxylic acid reduction, 6-member intramolecular imine formation, Aldehyde amination, and Imine reduction 2.