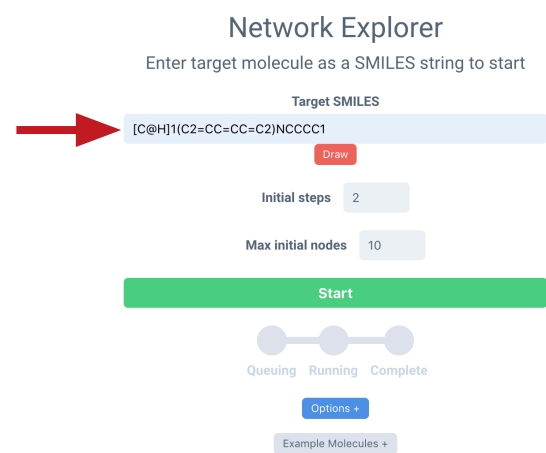## 1. Enter target molecule

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.

Network Explorer

Enter target molecule as a SMILES string to start

Target SMILES

[C@H]1(C2=CC=CC=C2)NCCCC1

Draw

Initial steps 2

Max initial nodes 10

Start

Queuing   Running   Complete
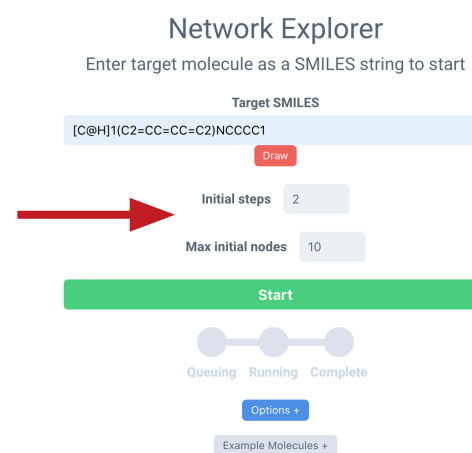
Options +

Example Molecules +

2. Set the size of the initial network

Change the number of steps, and the maximum number of nodes to set the size of the initial network.

The initial steps defines the steps away from the target molecule.

The max initial nodes defines the maximum number of nodes allowed initially. If more nodes than the maximum are identified, nodes will be automatically removed based on the relative molecule complexity (which assumes moving towards less complex starting materials is desirable)

Other options are available in the options tab.

Network Explorer

Enter target molecule as a SMILES string to start

Target SMILES

[C@H]1(C2=CC=CC=C2)NCCCC1

Draw

Initial steps 2

Max initial nodes 10

Start

Queuing   Running   Complete

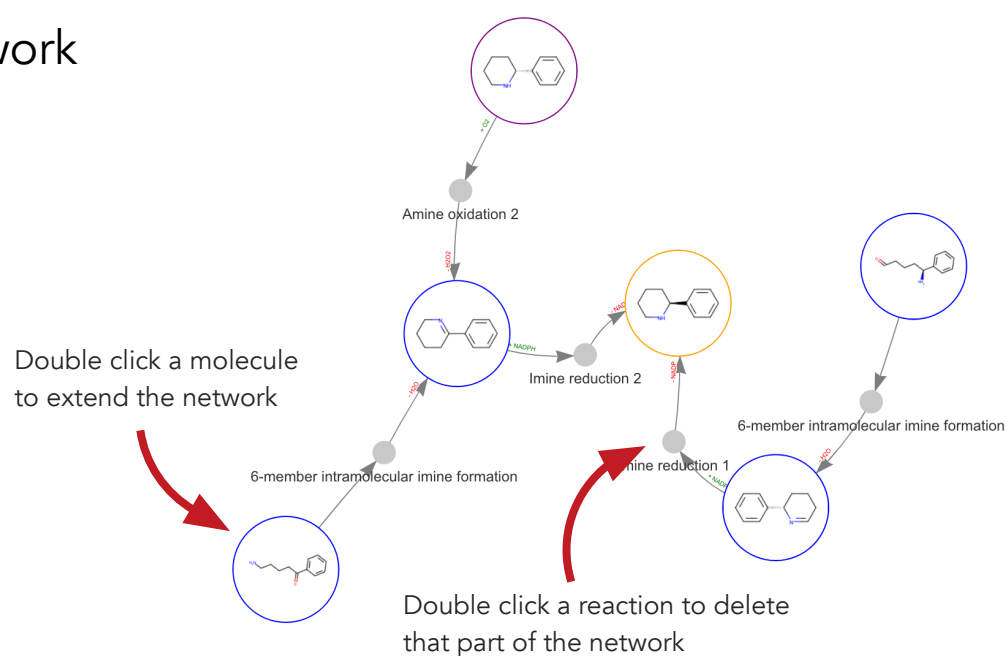Options +

Example Molecules +

3. Extend or delete parts of the network

To extend the network, double click on a molecule to add all possible reactions that generate that product.

To delete part of the network, double click a reaction you wish to remove.

Continue adding and removing nodes to explore the possible routes to your molecule.

Zoom in and out using the mouse scroll, and navigate the network by left clicking in white space and dragging. Hovering over a node offers additional information.

Help   Colour legend   Node info   Options   Add custom reaction   TA

Amine oxidation 2

Imine reduction 2

6-member intramolecular imine formation

Imine reduction 1

6-member intramolecular imine formation

Double click a molecule to extend the network

Double click a reaction to delete that part of the network

4. Additional options

A number of buttons are available at the top of the page offering additional options.

Help and Colour legend provide further assistance.

Node info offers information on the currently selected node. (Single click a node to select it).

Options allows some visualisation settings to be changed.

Add custom reaction allows a user-defined transformation to be added to the network. First select the product of your custom reaction on the network, this will fill the 'Product' field. Next click 'add custom reaction' and enter or draw the substrate(s) of your reaction. Click add reaction to add it to the network. User-defined chemical reactions can be added in this way.

Help   Colour legend   Node info   Options   Add custom reaction   TA

Amine oxidation 2

Imine reduction 2

Secondary alcohol oxidation

Secondary amine deamination 6-member intramolecular imine formation

Decarboxylation (Amine)

Secondary alcohol oxidation

Secondary amine deamination

Nitrile reduction

Aldehyde deamination