

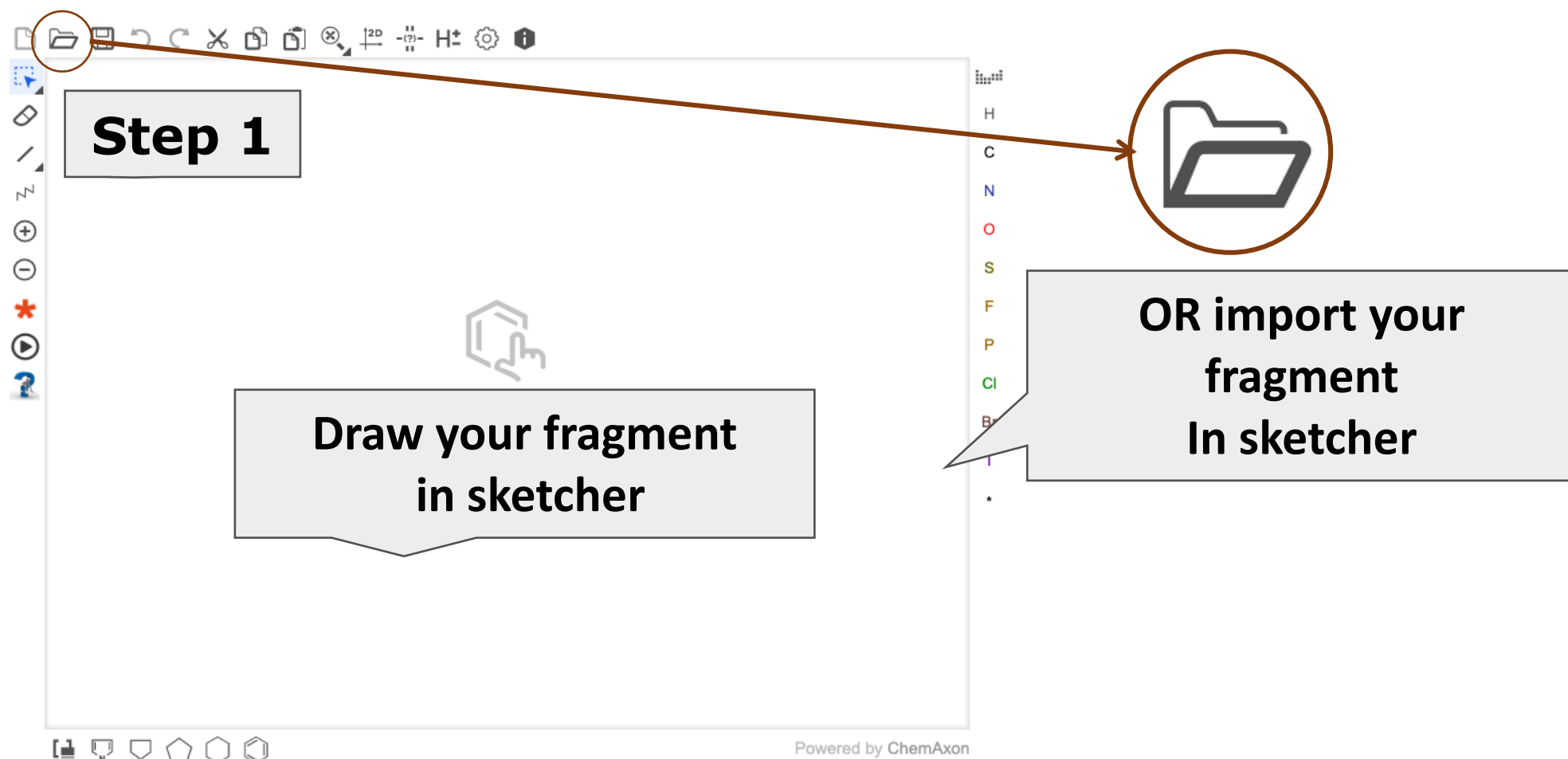
Growing

Draw Fragment

Step 1

Draw your fragment in sketcher

OR import your fragment In sketcher



Validate

Step 2

Structure

Launch Demo Reset

Name (optional)

imatinib-frag

Smiles

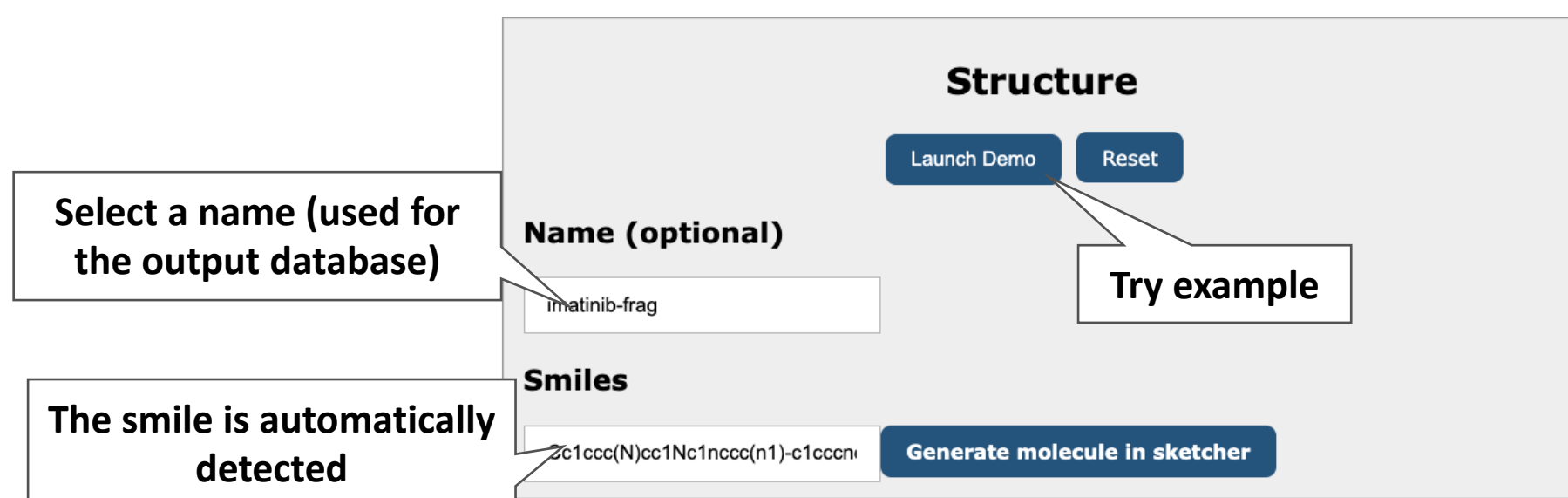
Cc1ccc(N)cc1Nc1nccc(n1)-c1cccn1

Generate molecule in sketcher

Try example

Select a name (used for the output database)

The smile is automatically detected



Chemical Functions are detected and shown in the sketcher

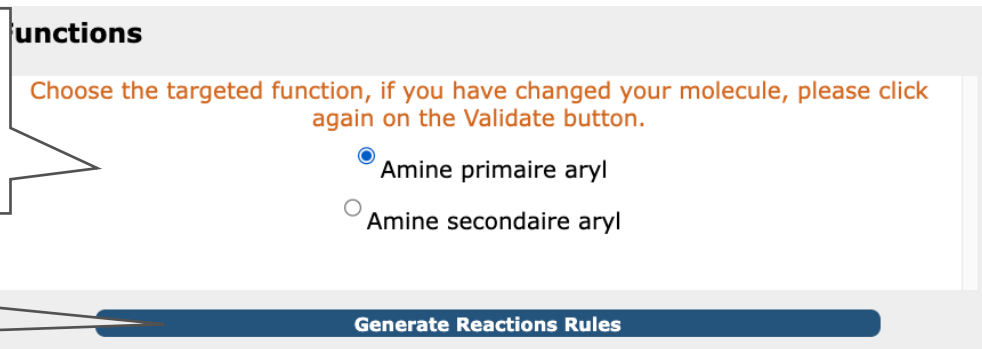
Functions

Choose the targeted function, if you have changed your molecule, please click again on the Validate button.

☒ Amine primaire aryl

☐ Amine secondaire aryl

Generate Reactions Rules



Step 3

Select Chemical Rules Then Validate

- ☐ Rule:1 Pictet-Sengler
- ☐ Rule:2 Benzimidazole carboxylic-acid/ester
- ☐ Rule:3 Benzimidazole aldehyde
- ☐ Rule:21 Pyrrole Paal-Knorr
- ☐ Rule:30 Reductive Amination
- ☐ Rule:47 Amide Schotten-Baumann add-step acyl-chloryde
- ☐ Rule:48 Sulfonamide
- ☐ Rule:51 Amination Buchwald-Hartwig

Validate Rules

