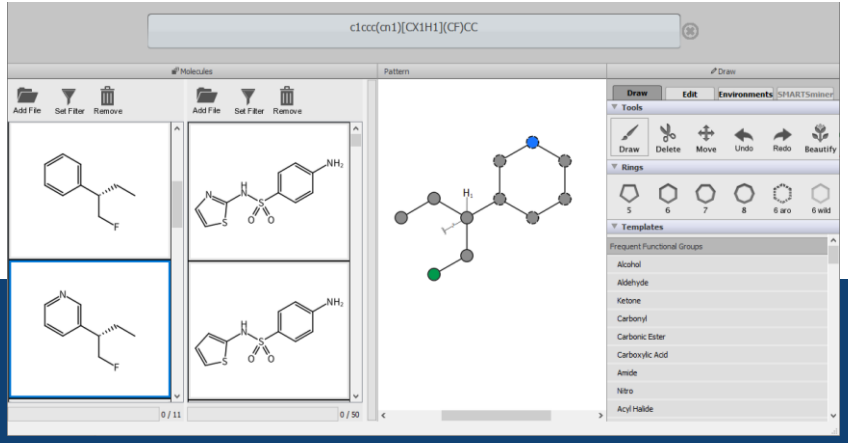
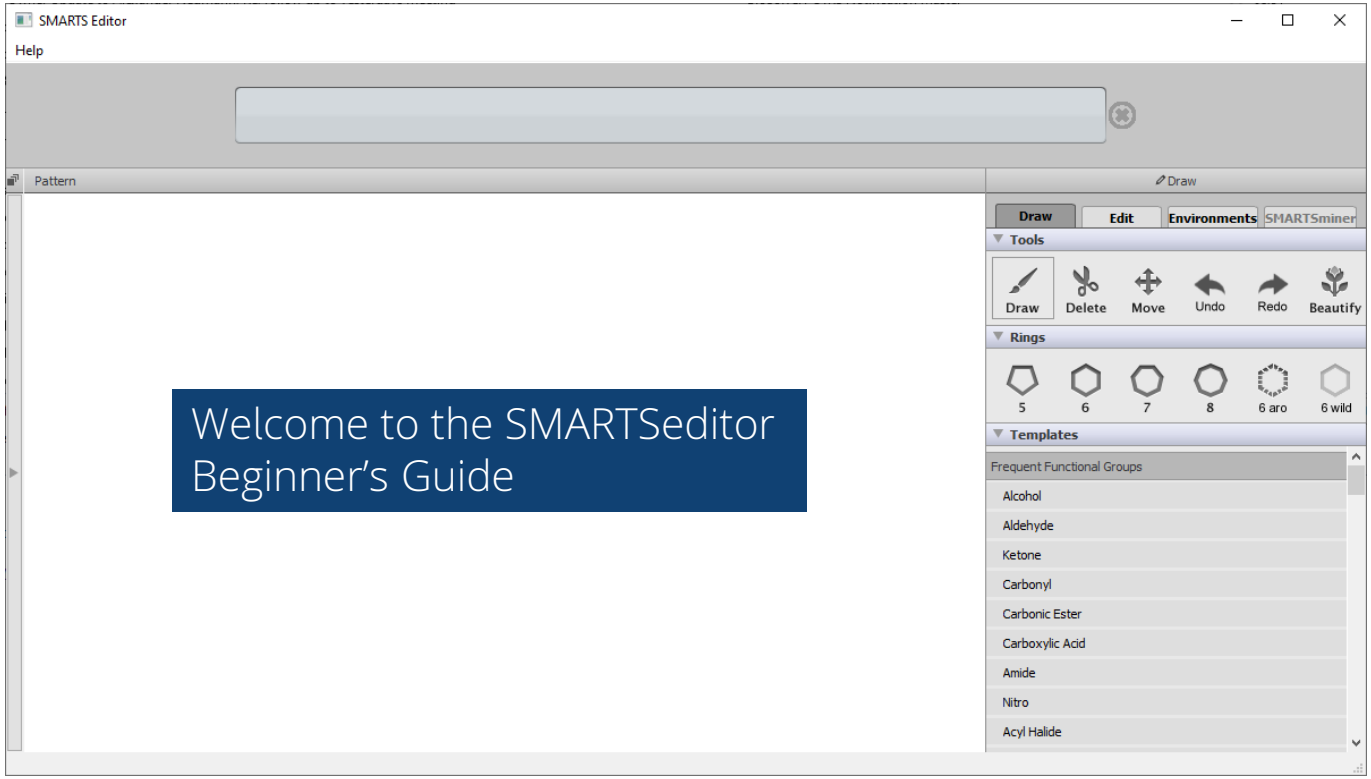
BioSolveIT
expect actives!



SMARTSeditor Beginner's Guide

1. Basics


SMARTS Editor
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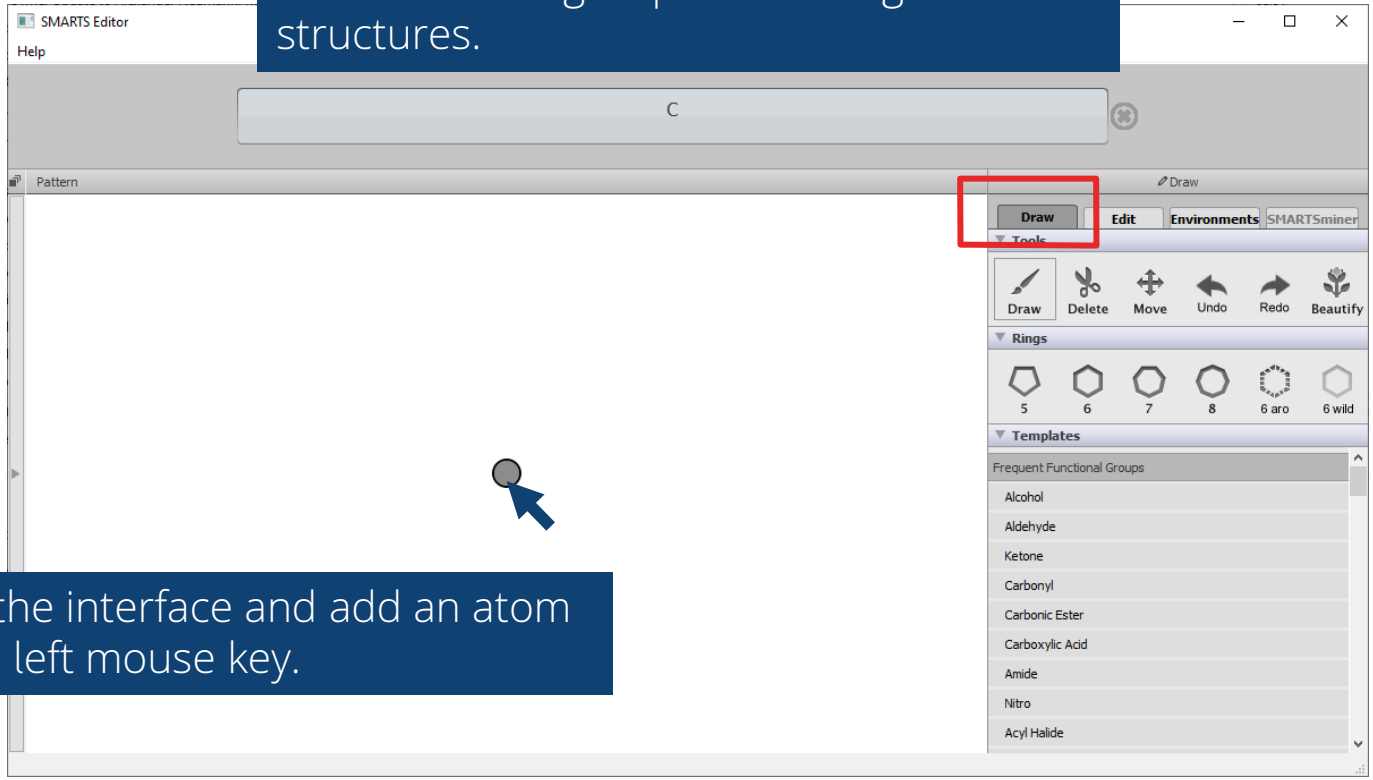
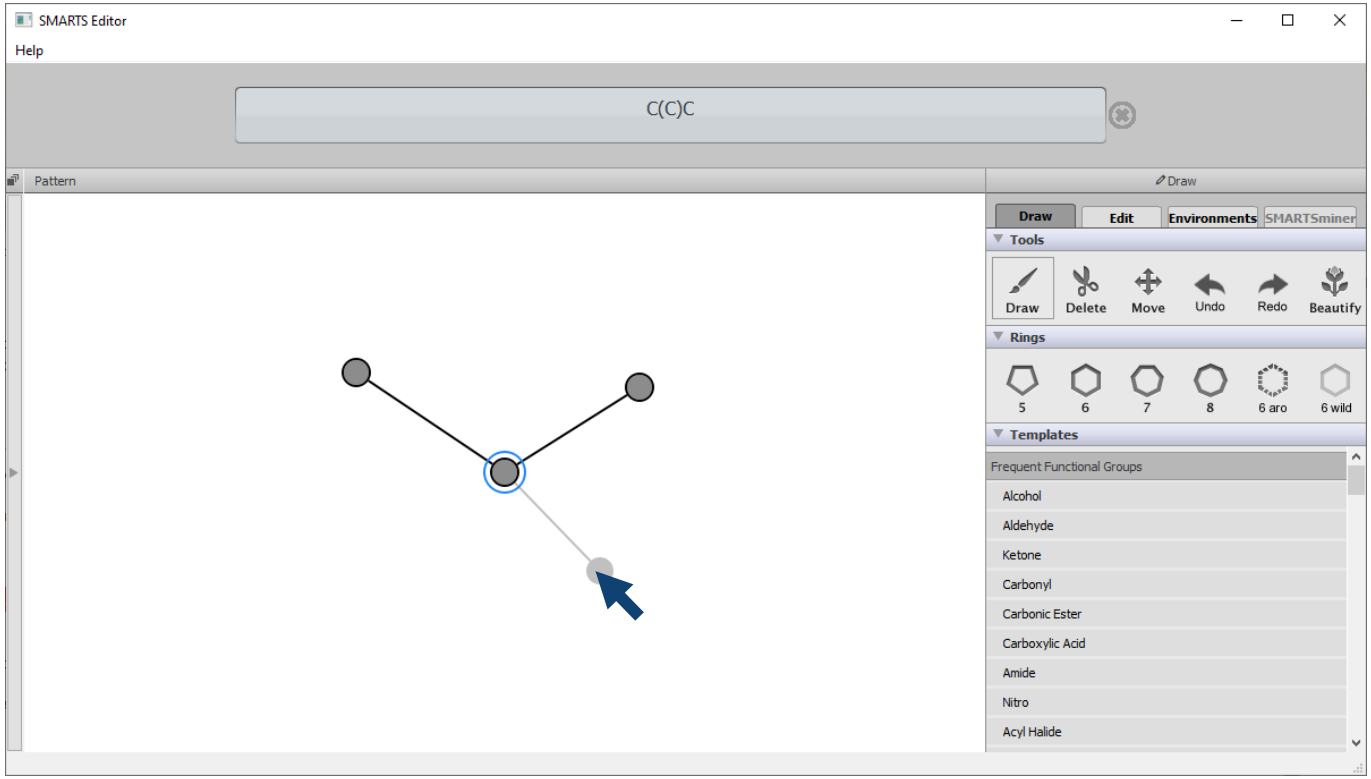
Carbonic Ester
Carboxylic Acid
Amide
Nitro
Acyl Halide
Welcome to the SMARTSeditor Beginner's Guide

While in the ‘Draw Mode’ you can create structures from scratch or add decoration and functional groups to existing structures.

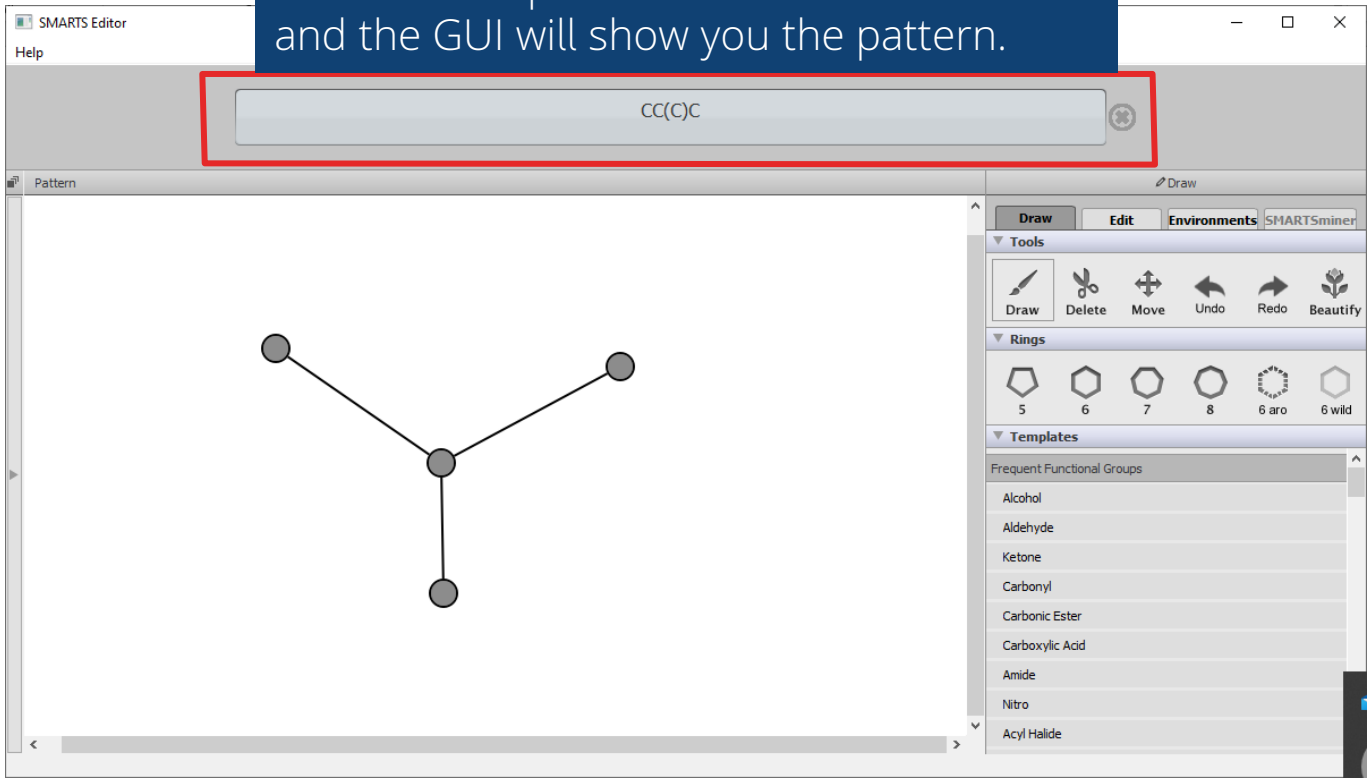


Hover over the interface and add an atom by using the left mouse key.

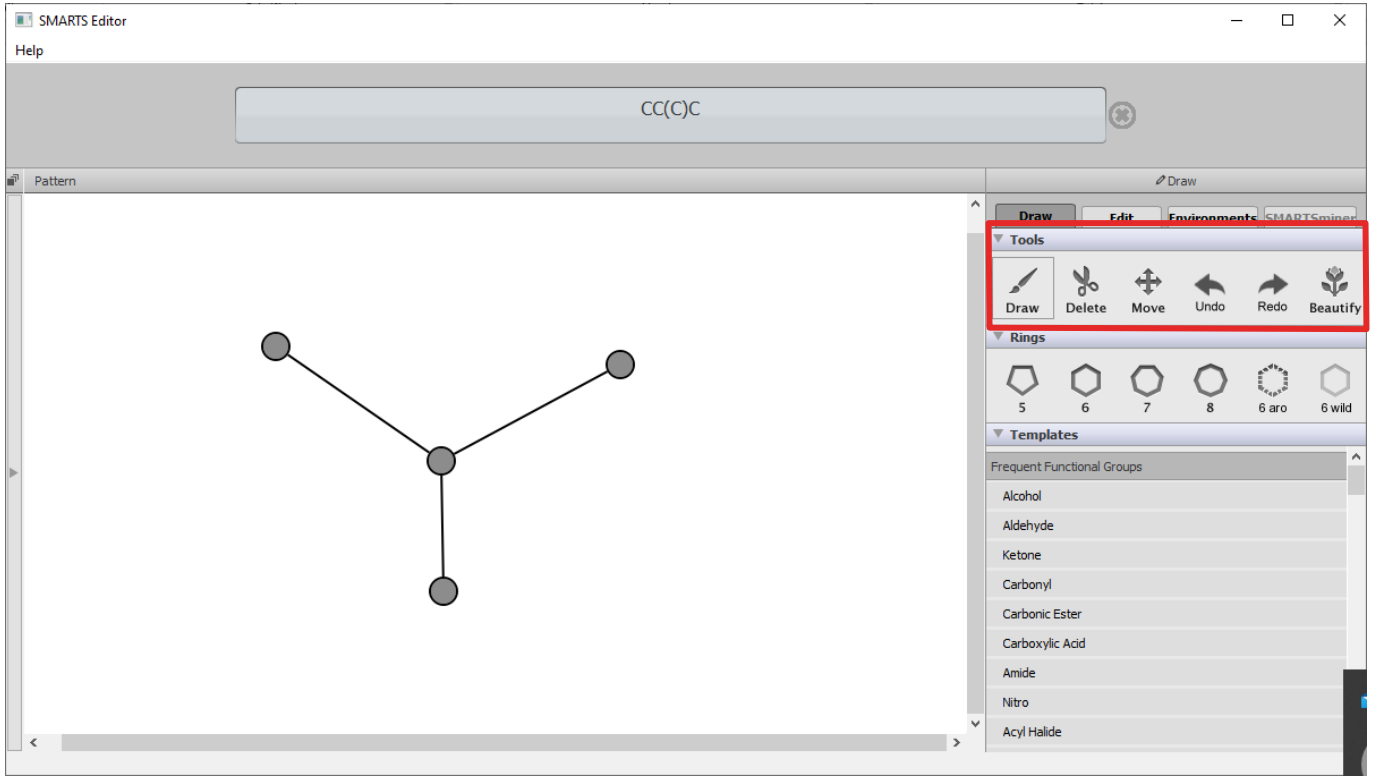
You can left click from an atom and drag to create a new atom.



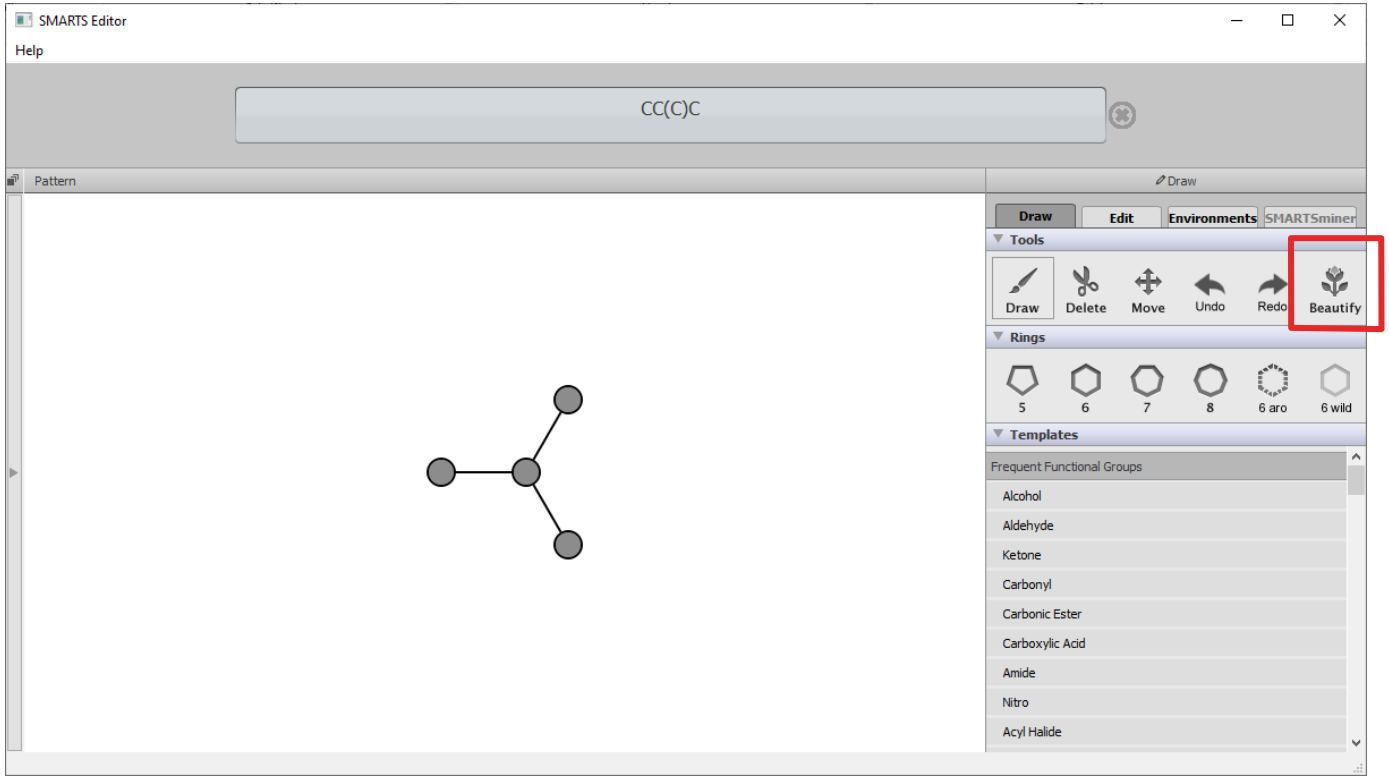
The SMARTS string displays the structure you are working with.
You can also paste SMARTS definition here and the GUI will show you the pattern.



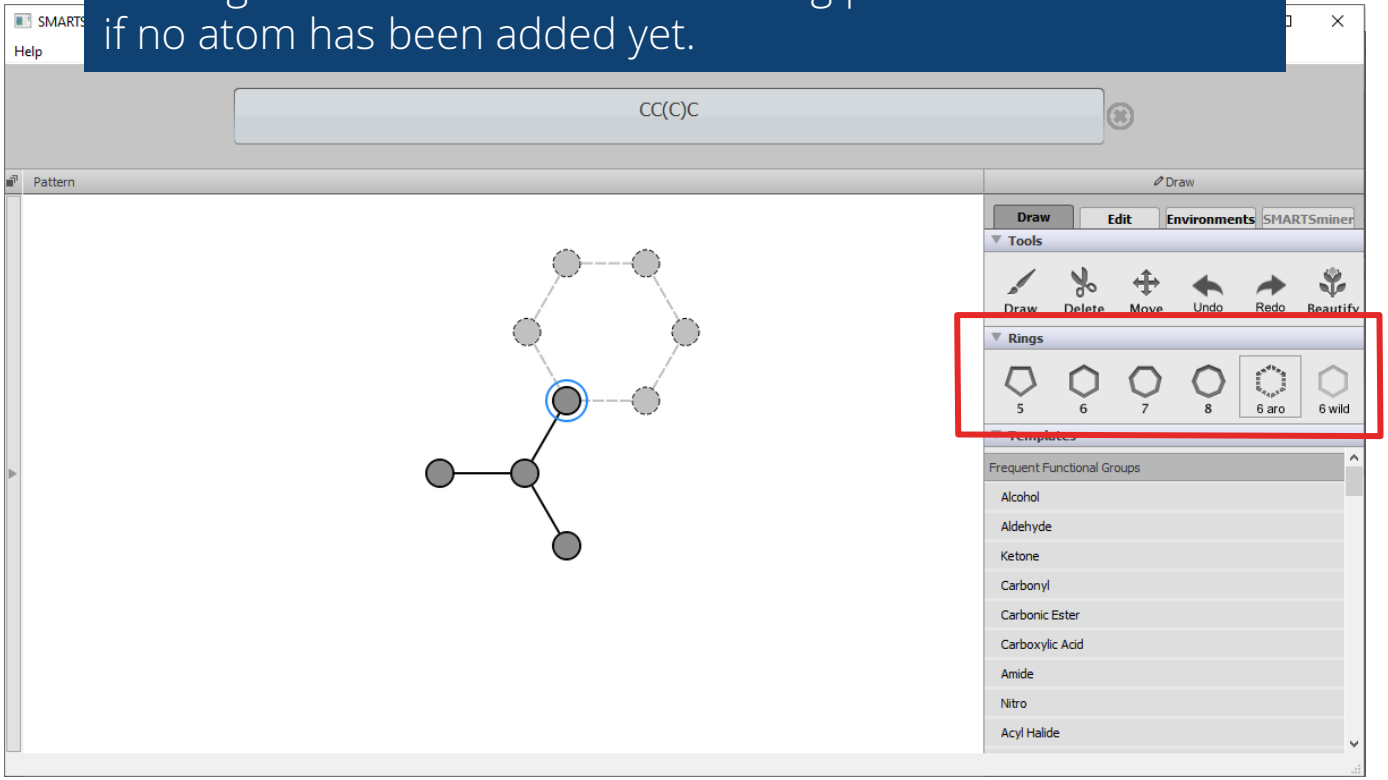
To edit your structure (e.g. remove atoms) use the tools in the box.



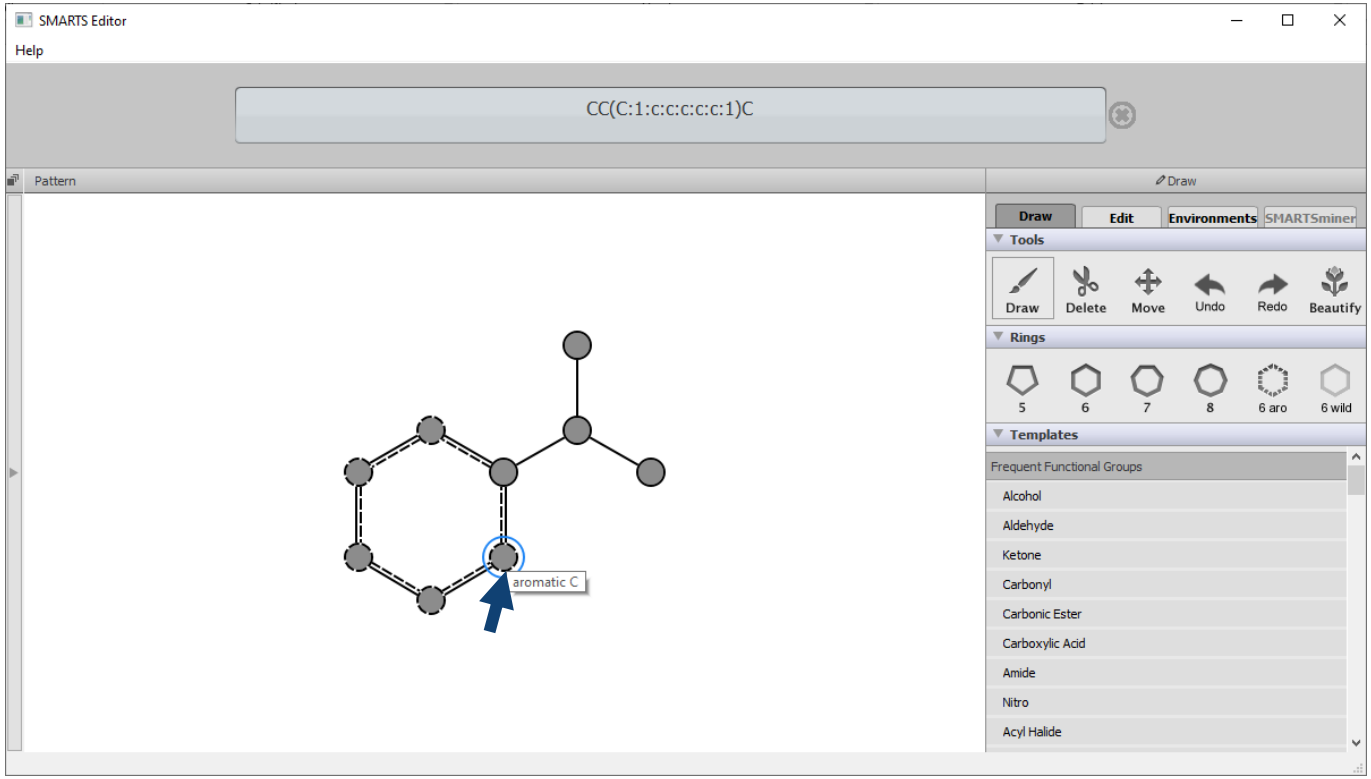
You can clean up the structure with the ‘Beautify’ function.



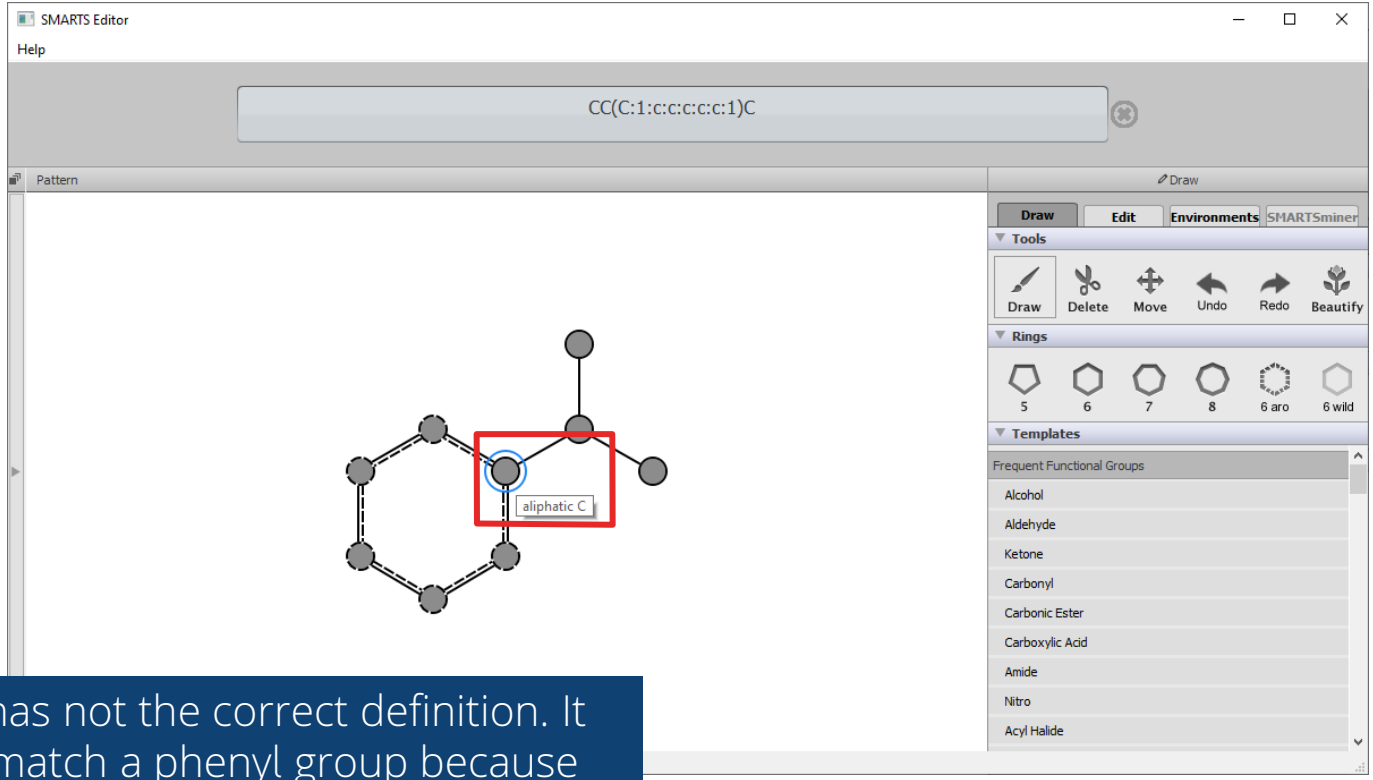
You can add rings or functional groups to a structure by selecting one of those in the right boxes and place them on existing atoms or use them as starting points for decoration if no atom has been added yet.



Hovering over an atom gives you details on its properties.

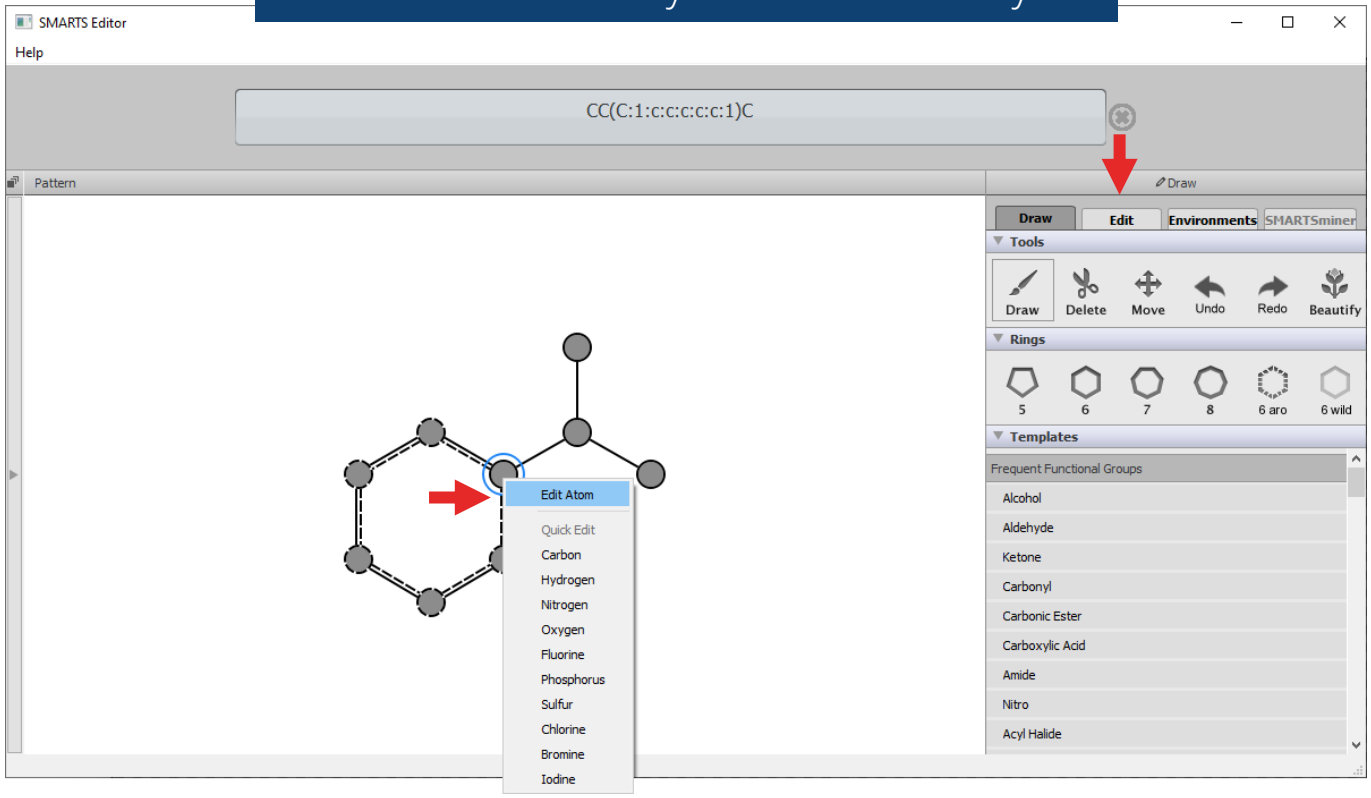


2. Defining Atom Properties

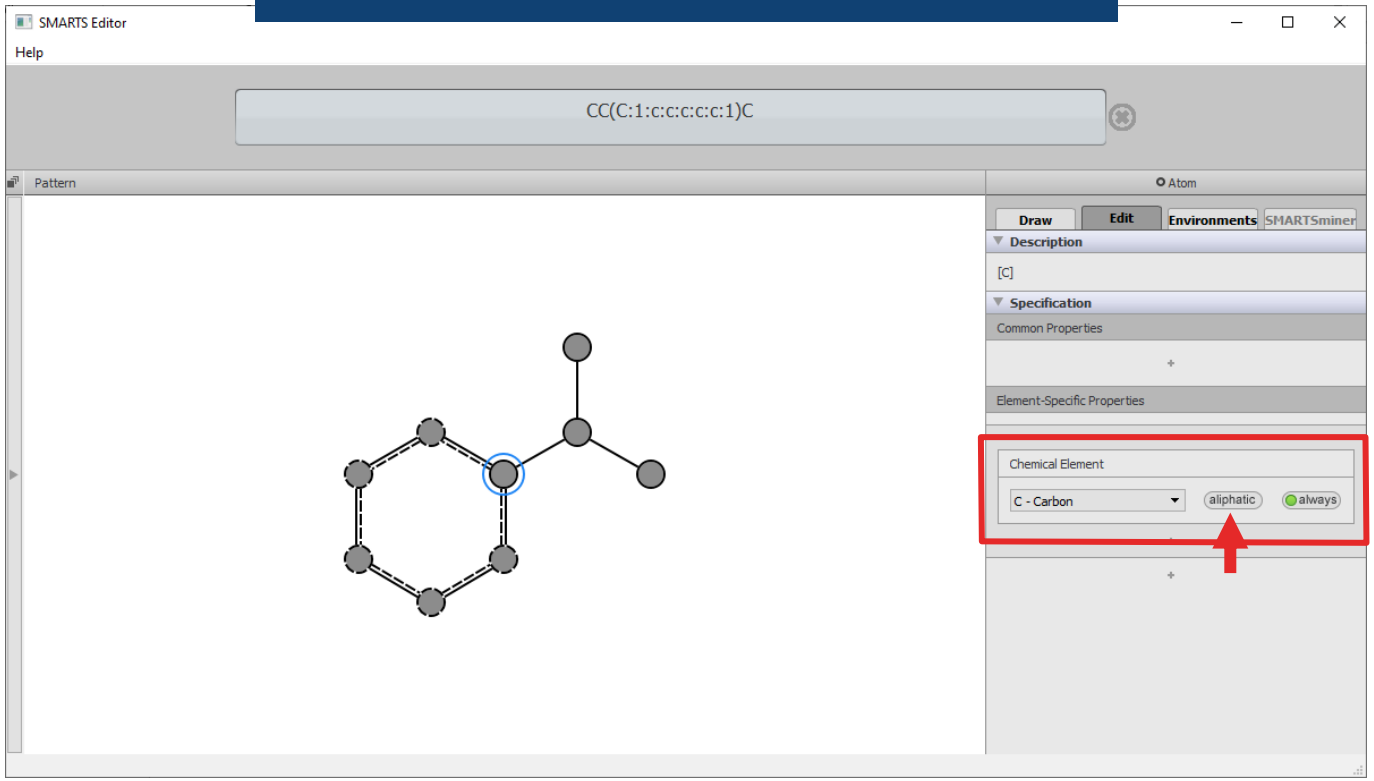


This atom has not the correct definition. It would not match a phenyl group because the atom is not aromatic. Let's change that.

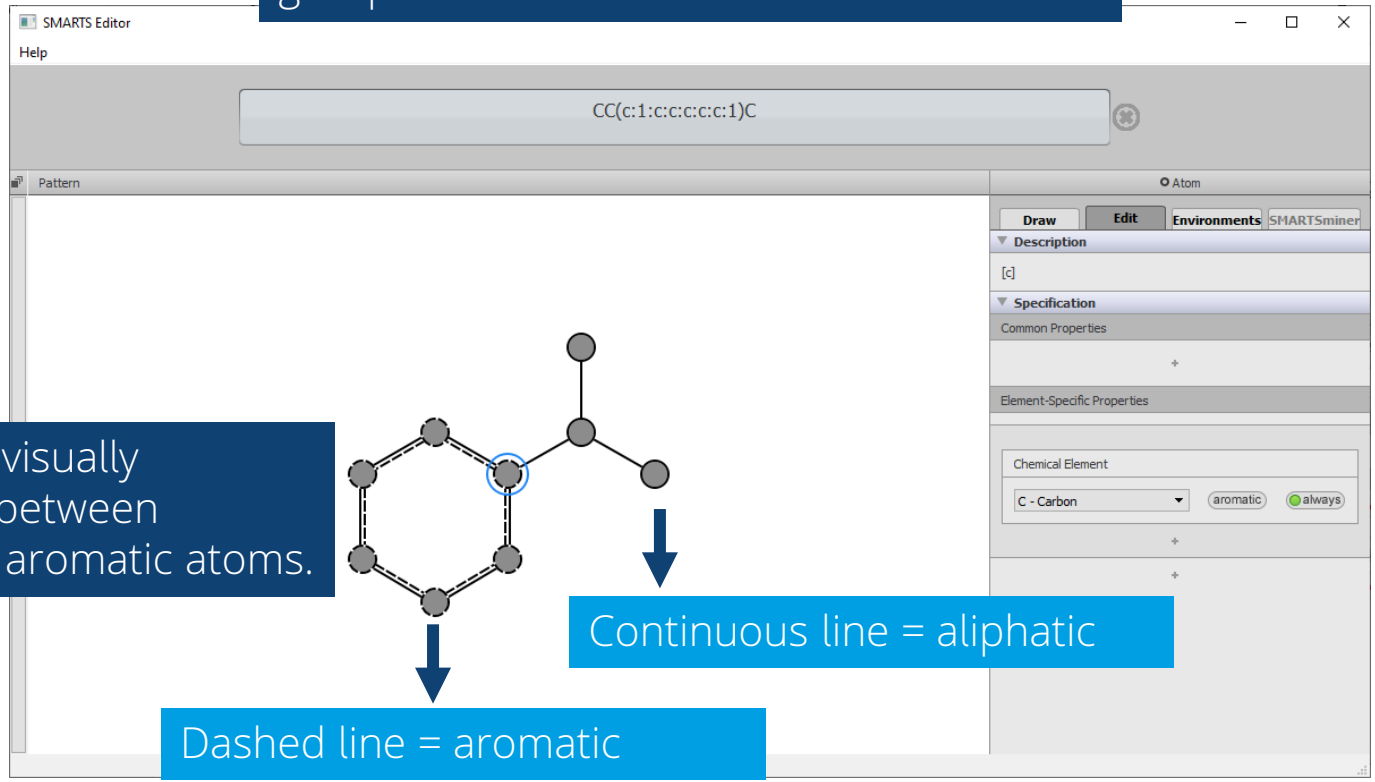
Right click on the atom and select ‘Edit Atom’. You can also go to the ‘Edit Mode’ and select the atom you want to modify.



Change the property of the atom from ‘aliphatic’ to ‘aromatic’ by clicking on the button.

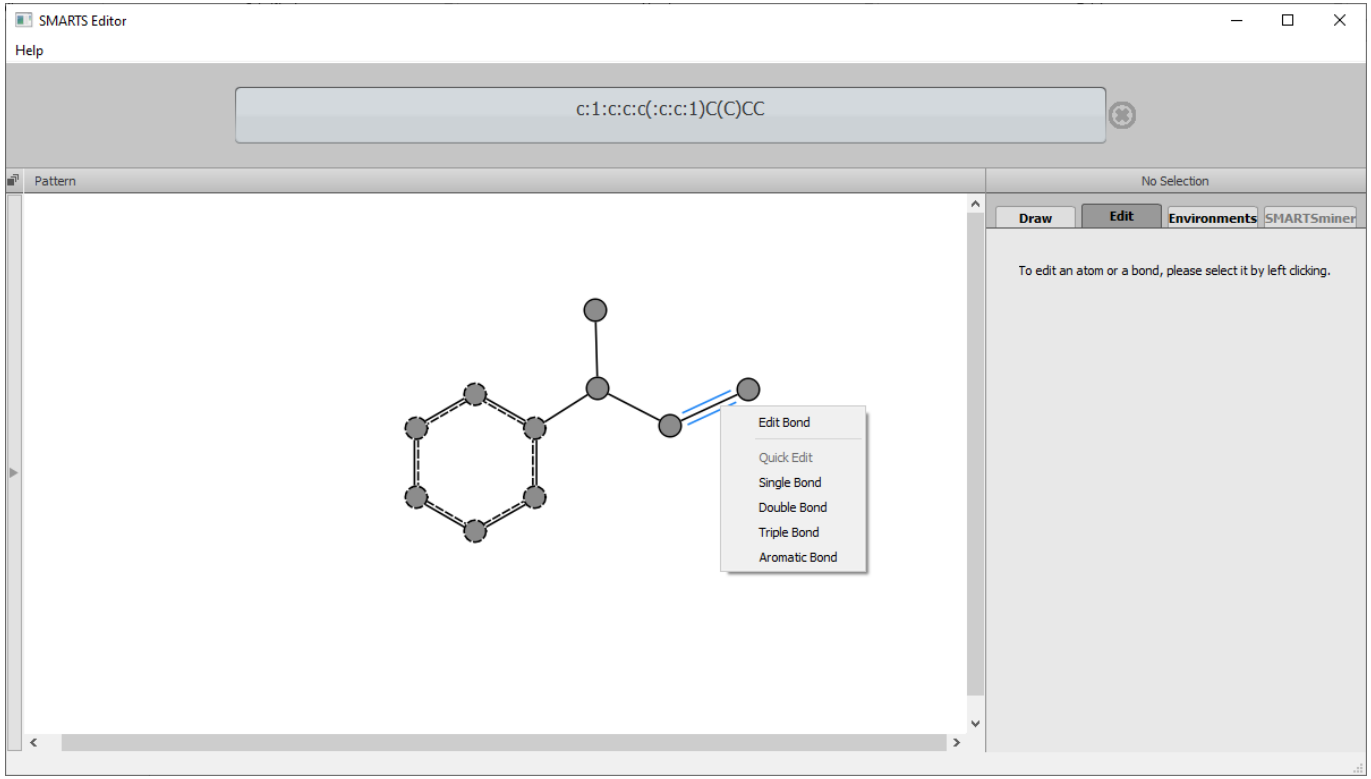


You changed the property of the atom. Now the definition would match a phenyl group.

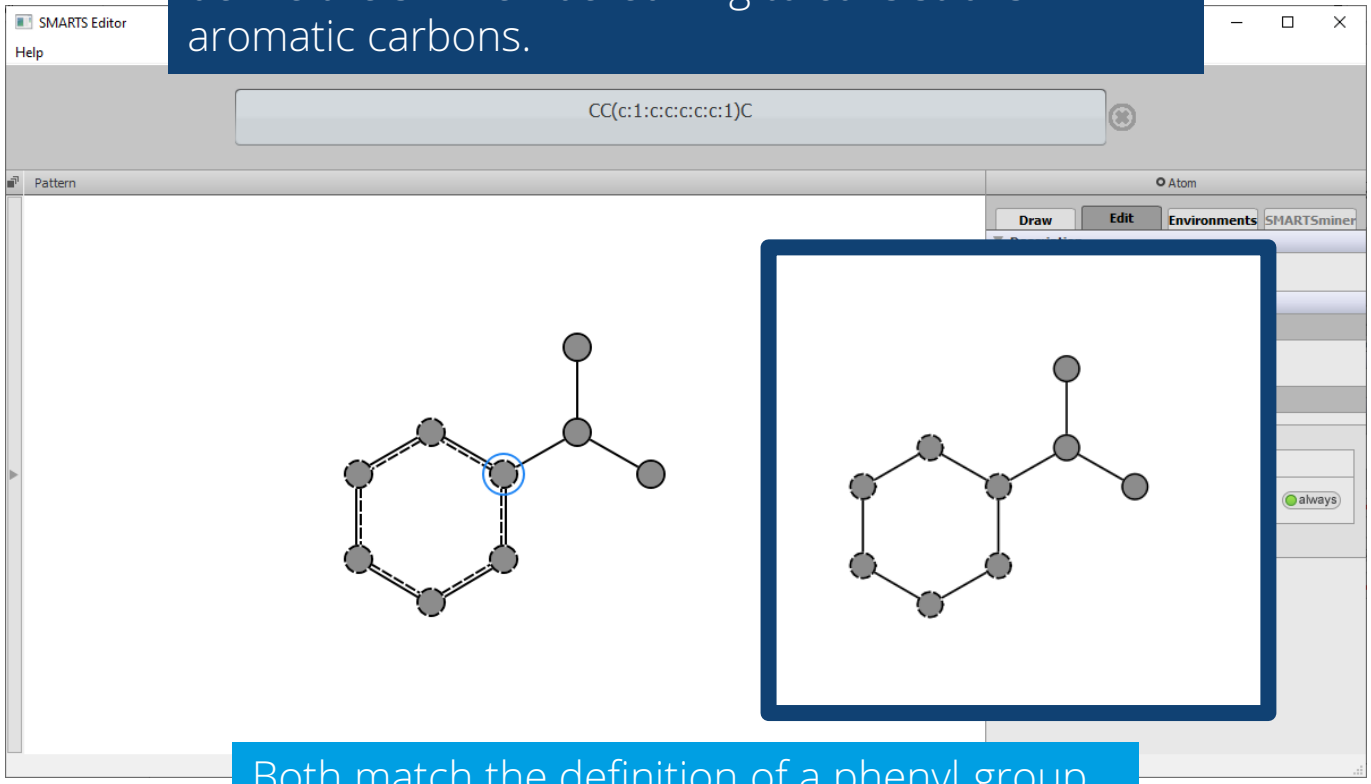


You can also visually differentiate between alipathic and aromatic atoms.

Likewise you can also edit and define the properties of a bond.

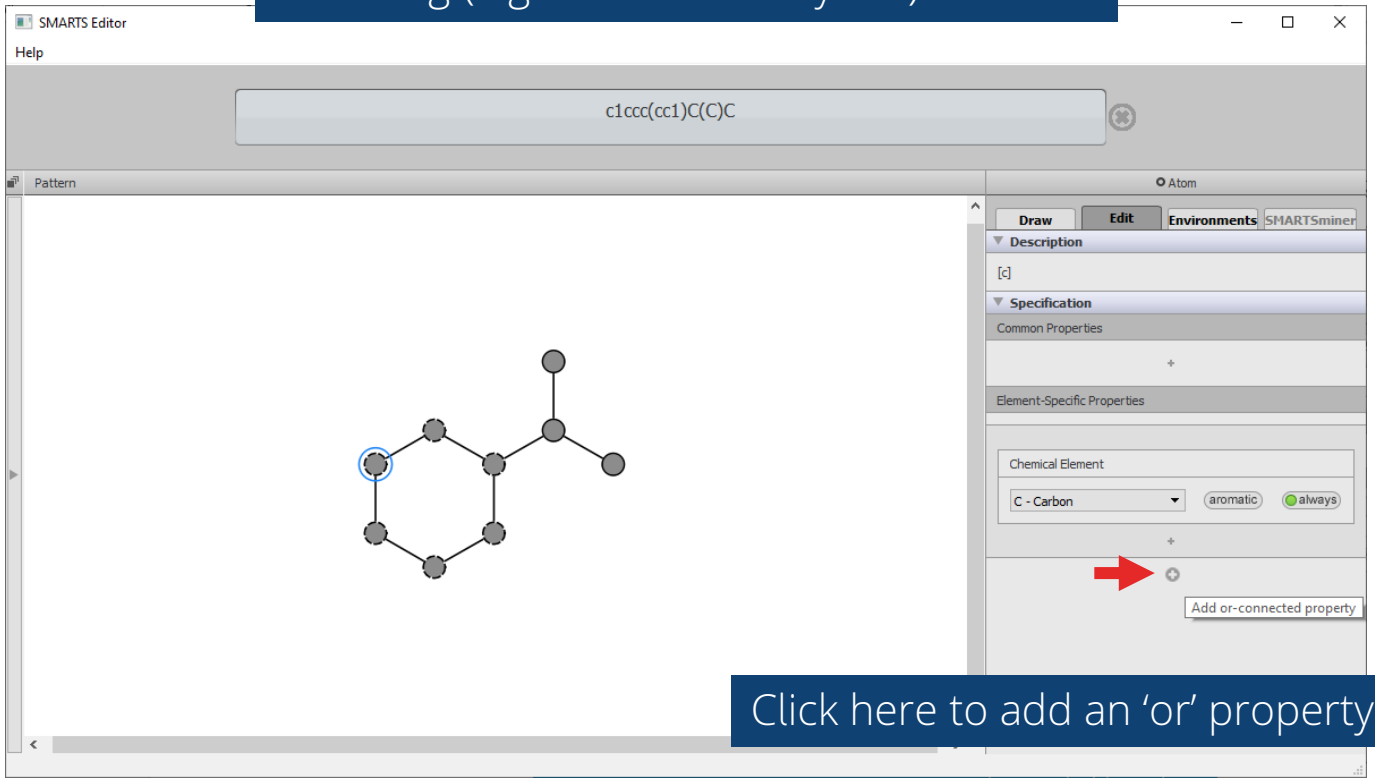


The definition of the aromatic bonds is not always necessary. To match a phenyl group it is enough to define the six membered ring to consist of six aromatic carbons.



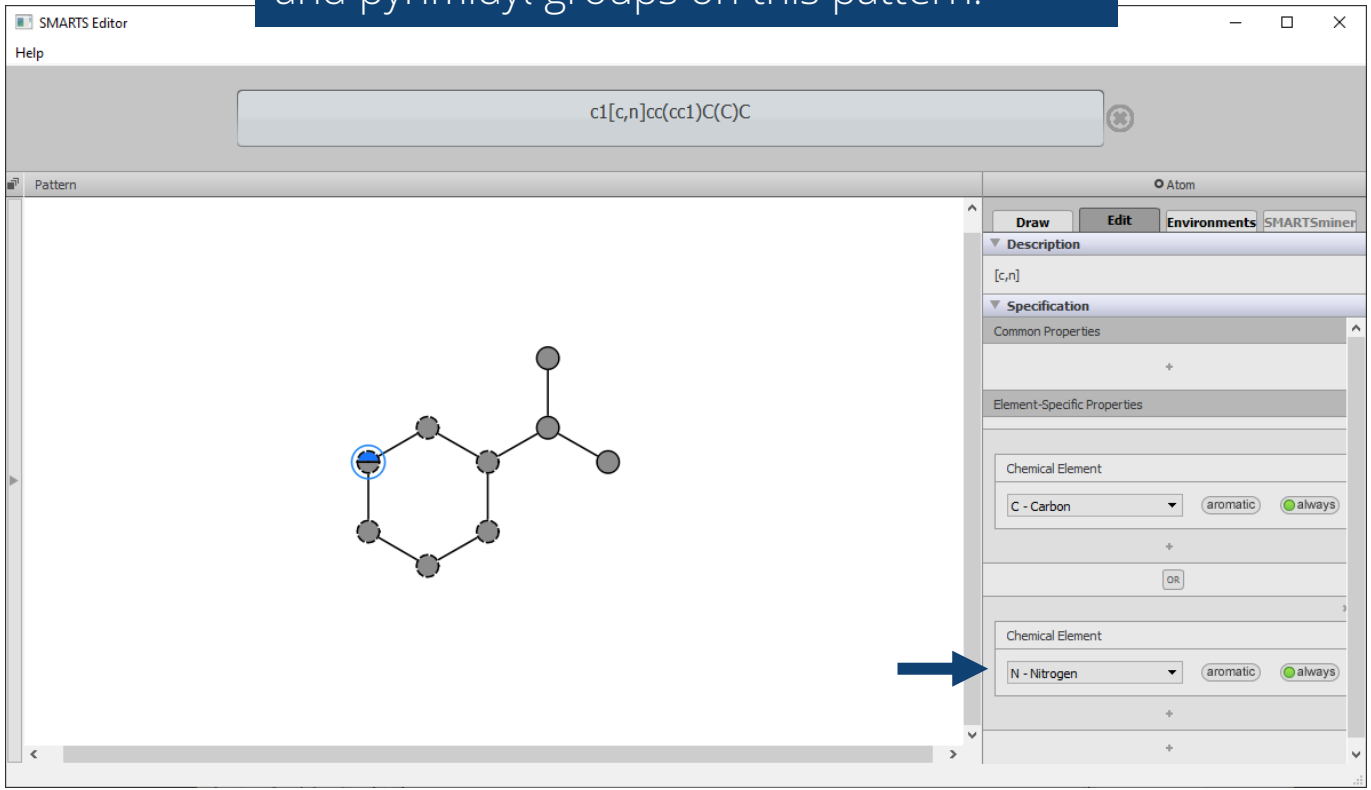
Both match the definition of a phenyl group.

Next we want to expand the definition of the six-membered ring to allow a broader matching (e.g. other heterocycles).

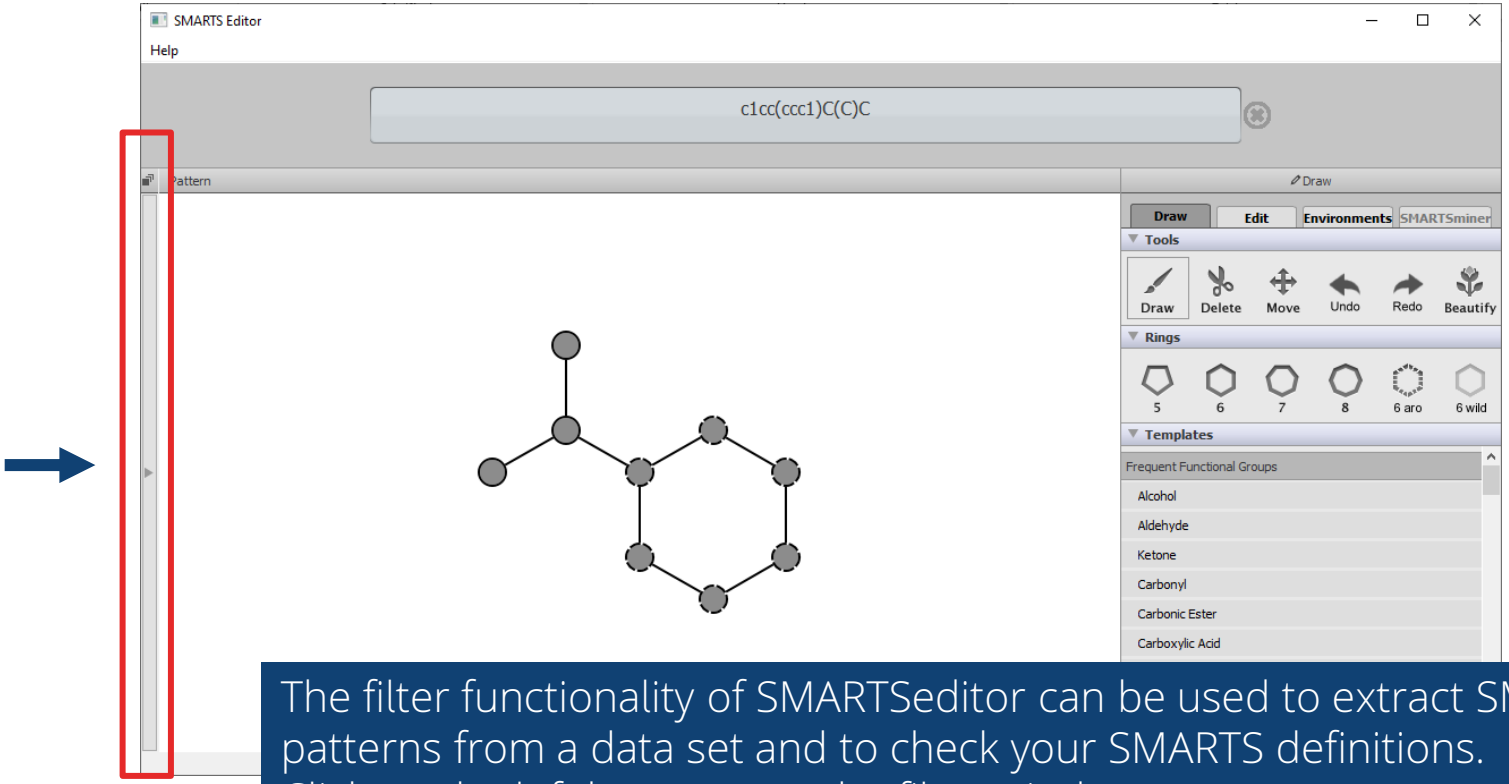


Click here to add an ‘or’ property.

Adding the ‘or’ definition of an aromatic nitrogen, we allow the matching of phenyl and pyrimidyl groups on this pattern.

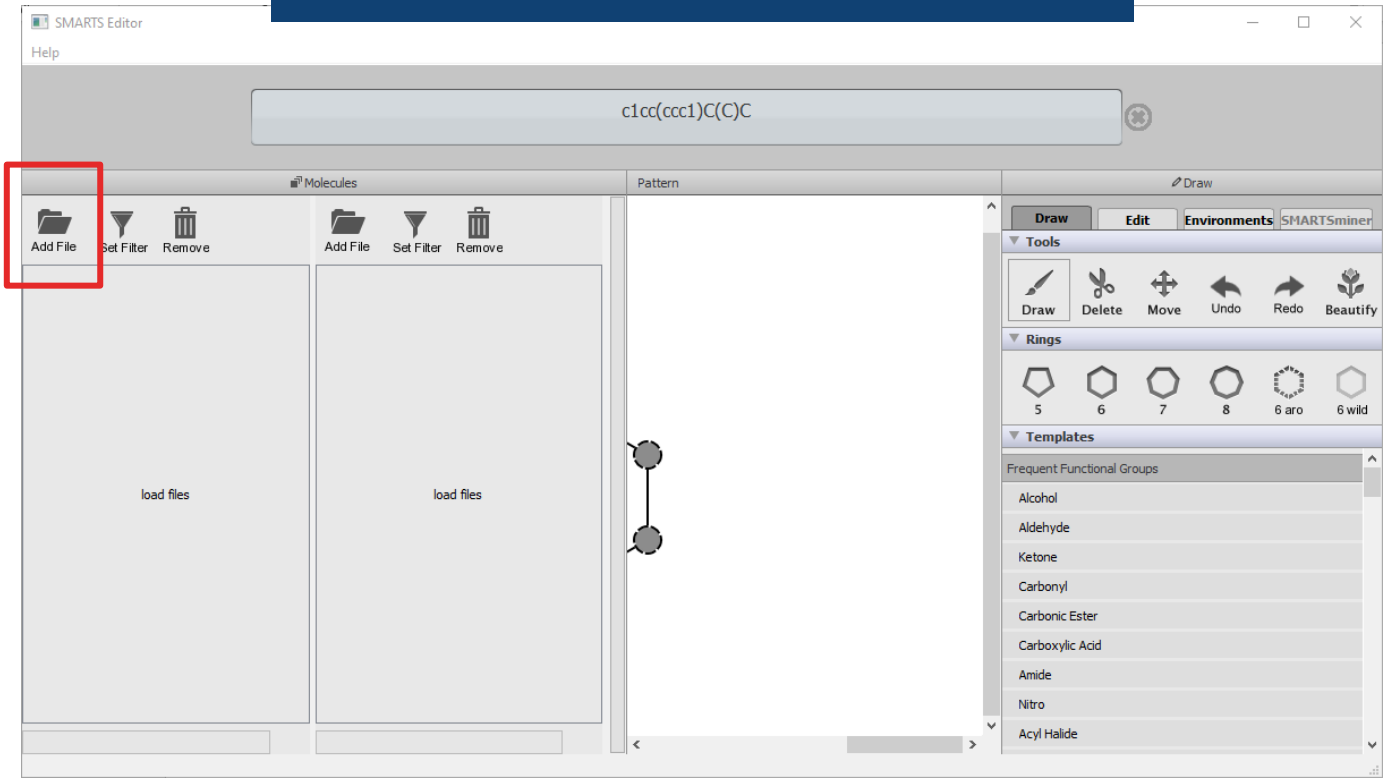


3. Filters

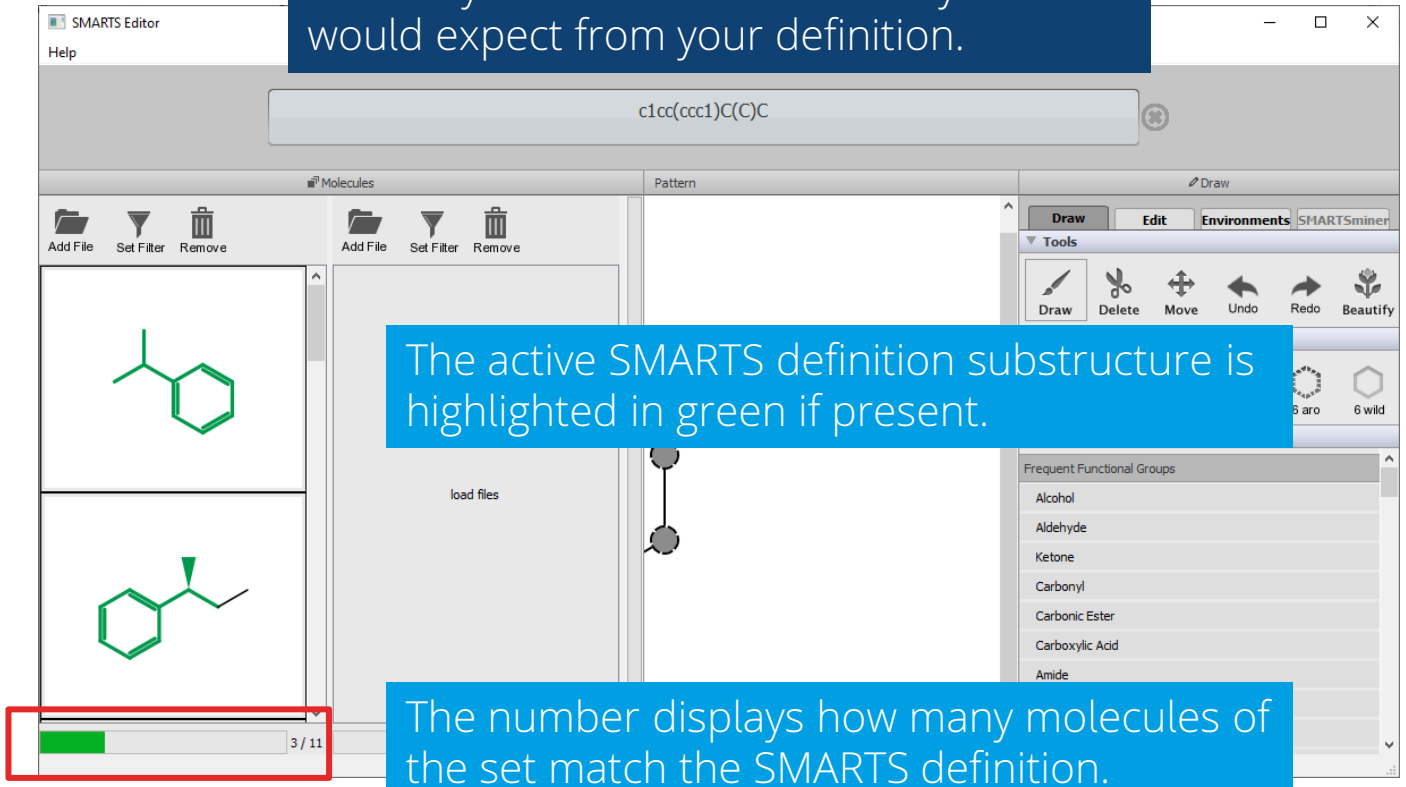


The filter functionality of SMARTSeditor can be used to extract SMARTS patterns from a data set and to check your SMARTS definitions.
Click on the left bar to open the filter window.

You can add data sets of molecules (e.g. sdf, pdb, SMILES) by clicking on the 'Add File' button.



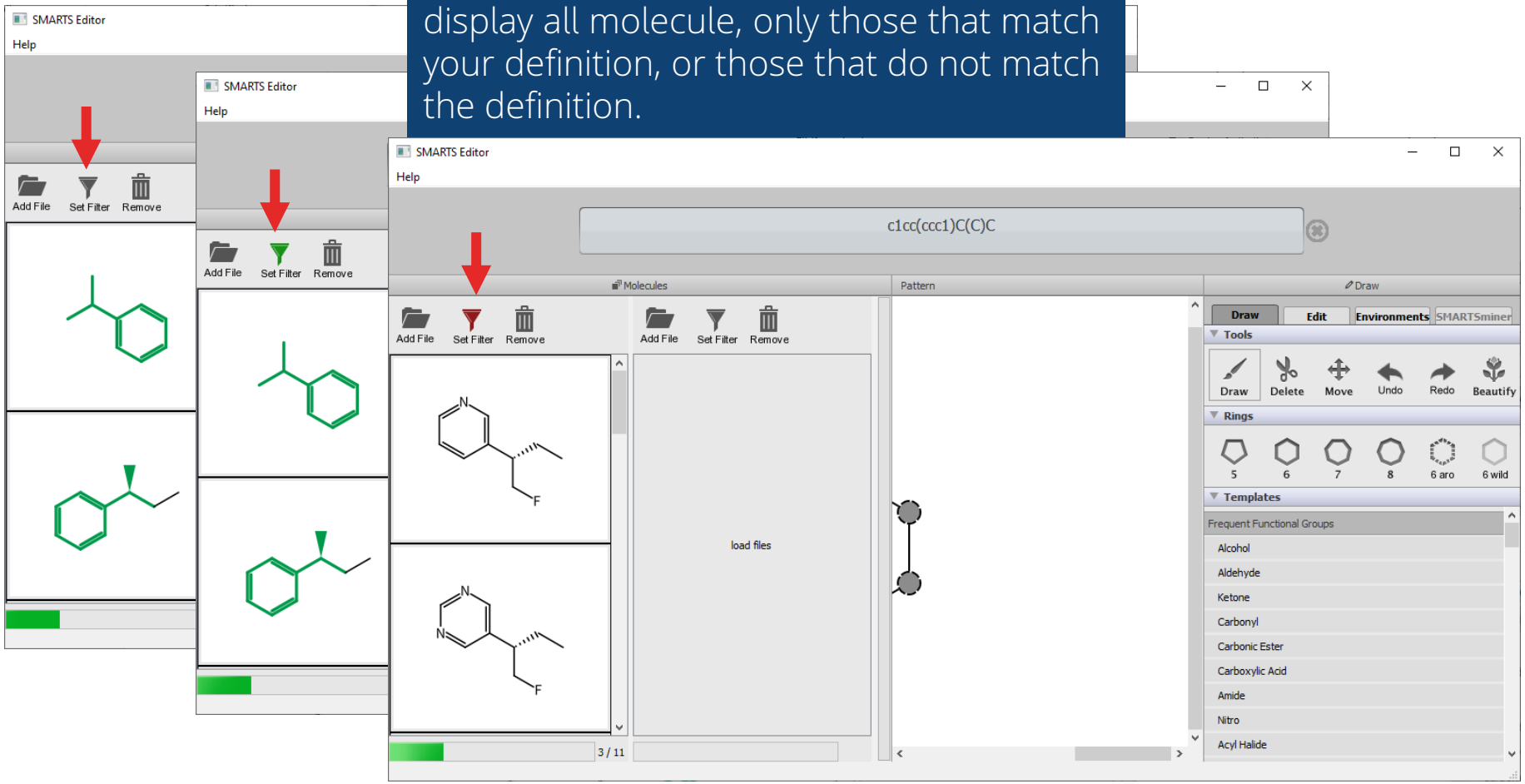
Molecules that match the active SMARTS pattern are recognized and can be used to check if you receive the matches you would expect from your definition.



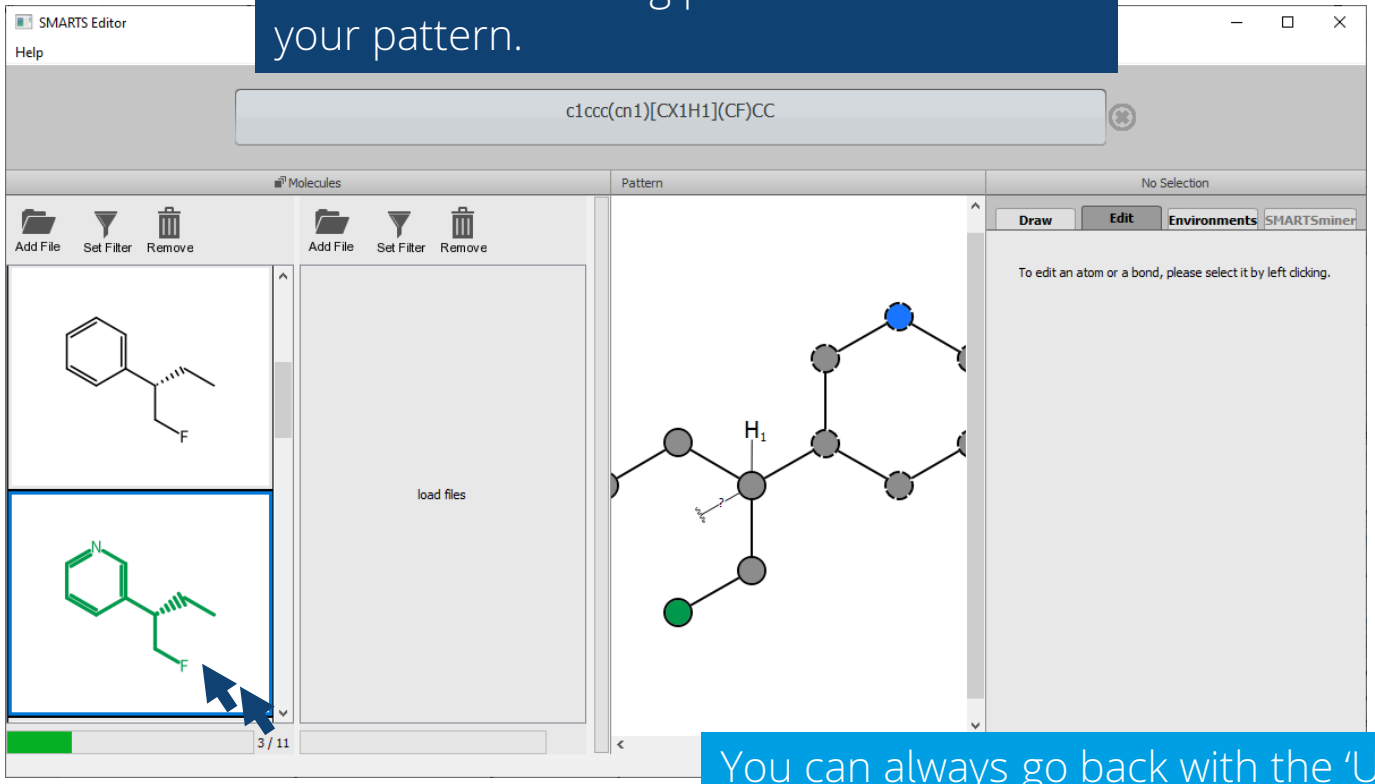
The active SMARTS definition substructure is highlighted in green if present.

The number displays how many molecules of the set match the SMARTS definition.

You can toggle the ‘Set Filter’ button to display all molecule, only those that match your definition, or those that do not match the definition.

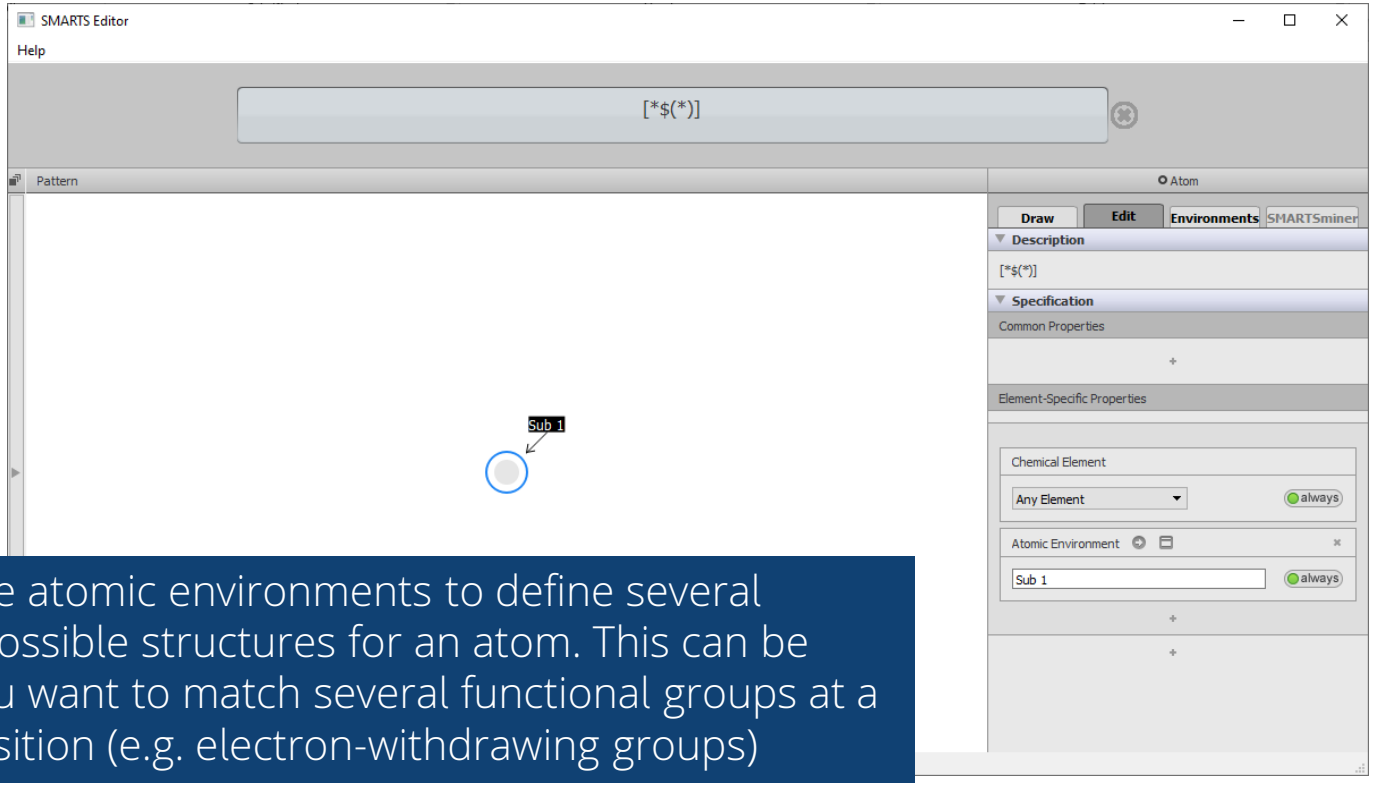


Double clicking on a molecule loads its SMARTS definition into the GUI. You can use those as starting point to fine-tune your pattern.



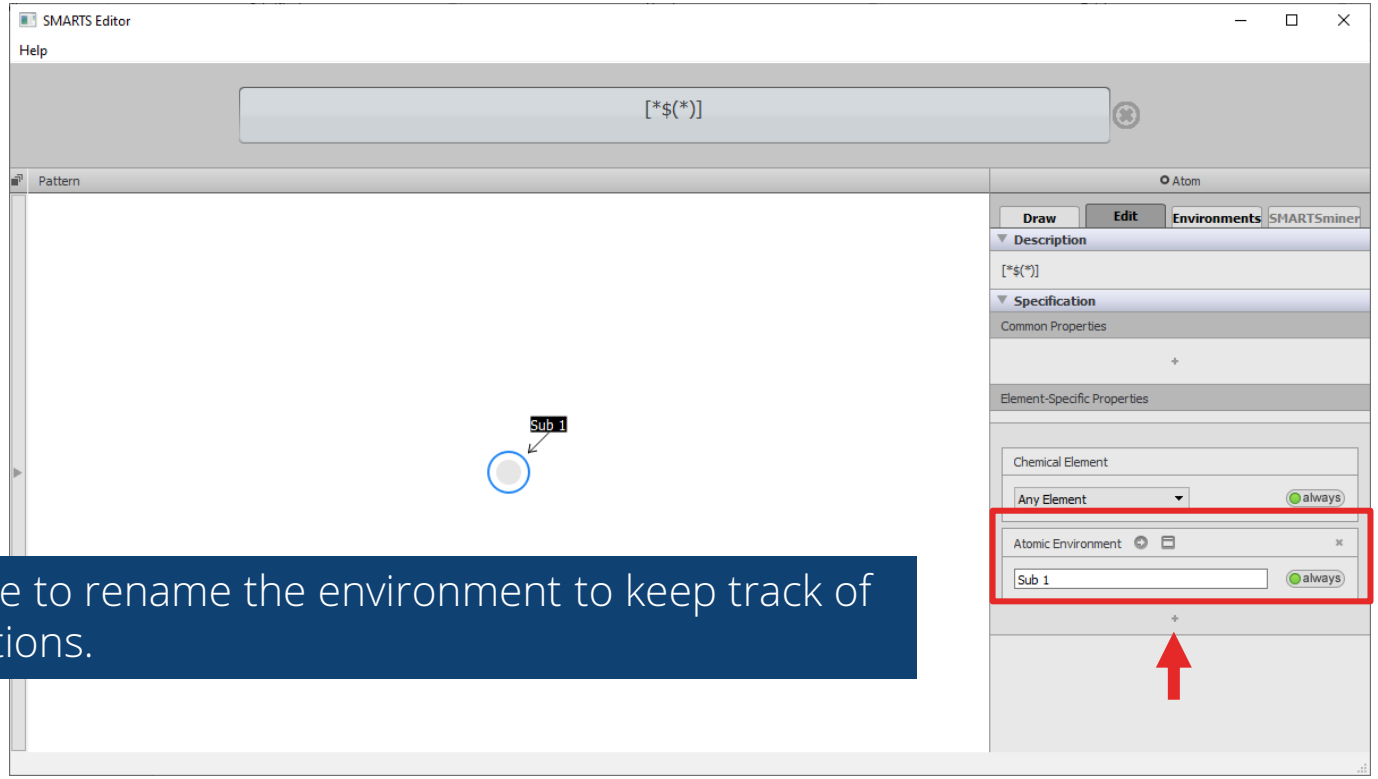
You can always go back with the 'Undo' button in the Draw section.

3. Atomic environment



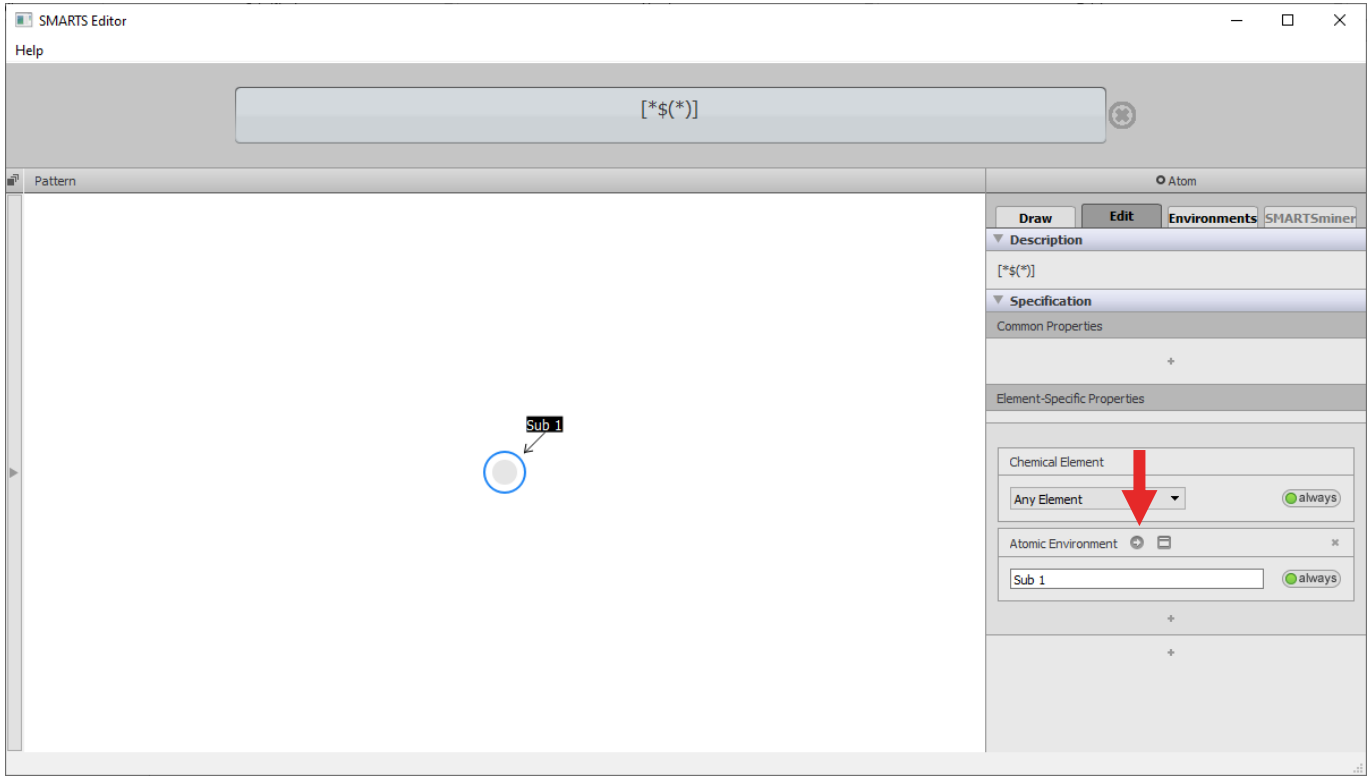
You can use atomic environments to define several recursive possible structures for an atom. This can be useful if you want to match several functional groups at a needed position (e.g. electron-withdrawing groups)

Add ‘Atomic environment’ to your element-specific properties.

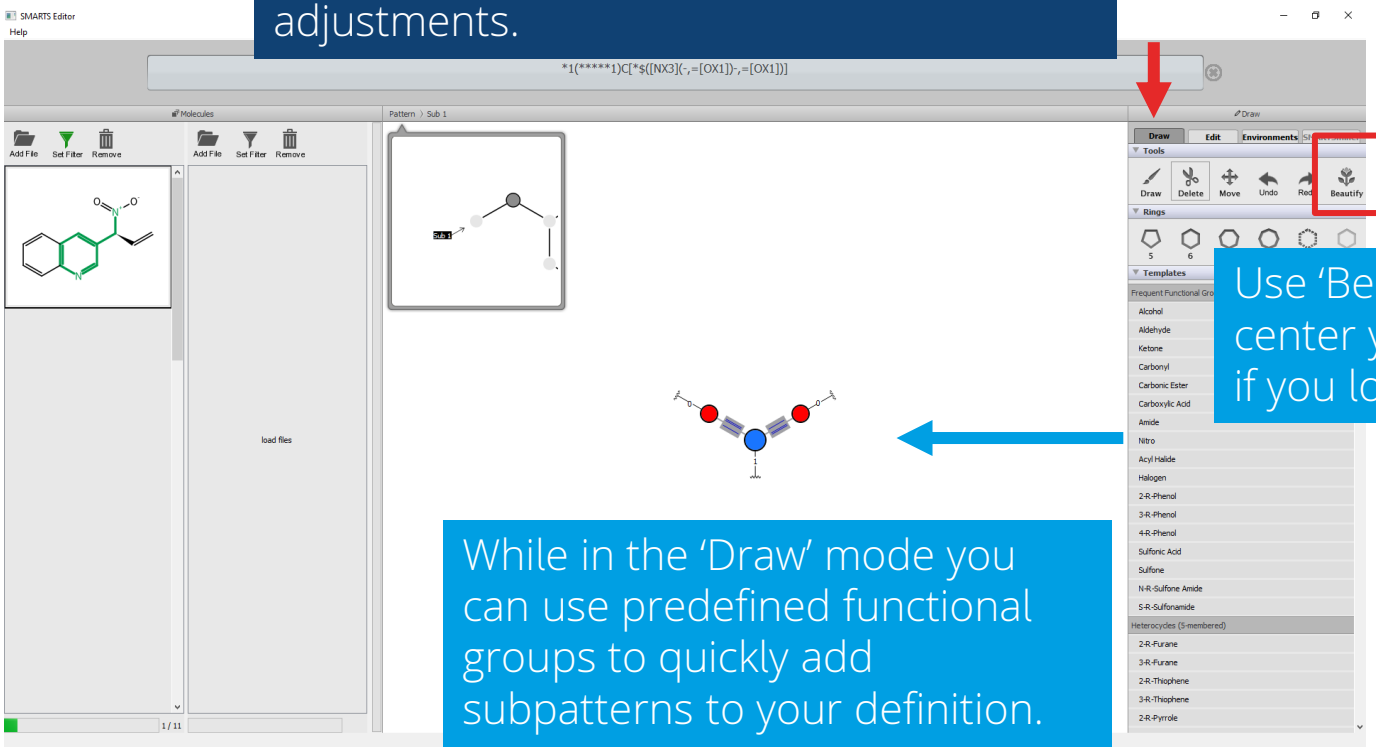


It is possible to rename the environment to keep track of your definitions.

Click on the arrow to edit the atomic environment.



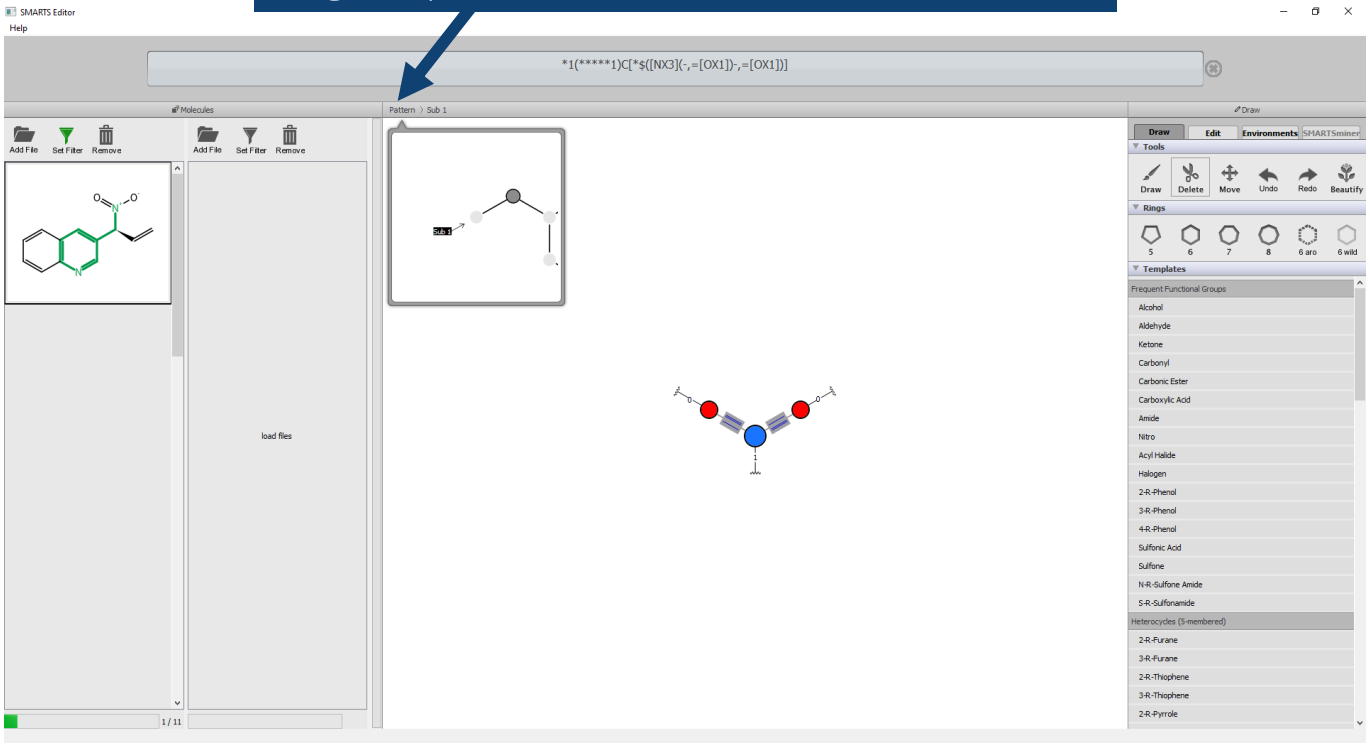
Define the subpattern you want to match. Once you are done, you can go back to your main pattern to make further adjustments.



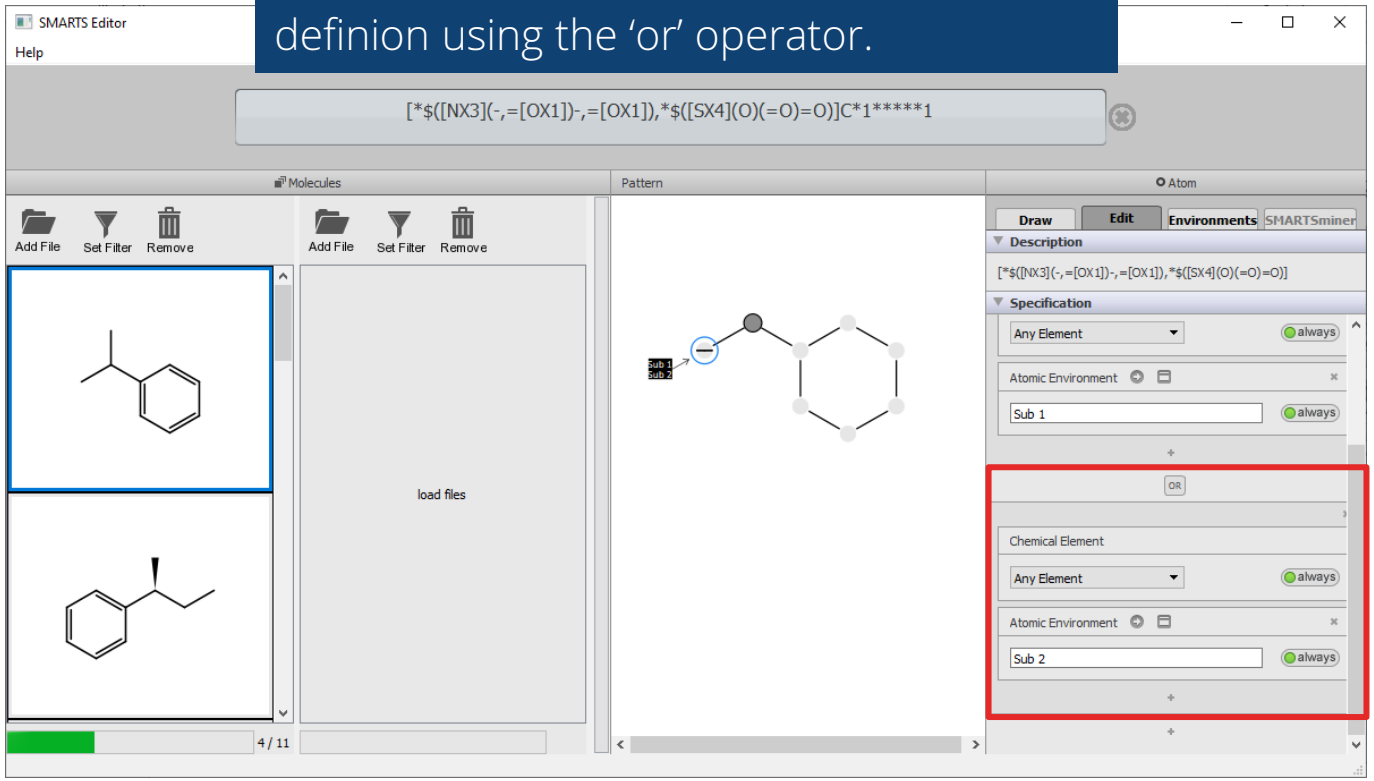
Use 'Beautify' to center your pattern if you lose track.

While in the 'Draw' mode you can use predefined functional groups to quickly add subpatterns to your definition.

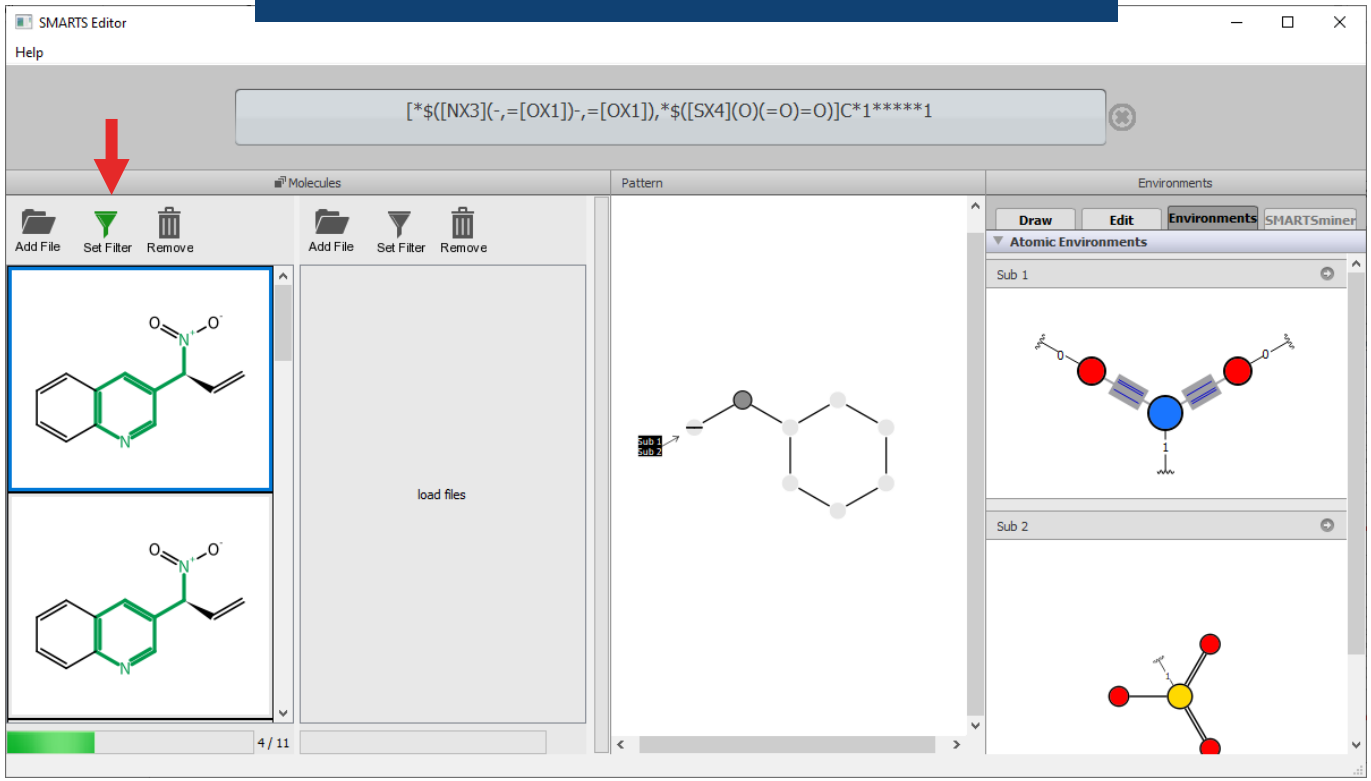
Once done, click here to return to your original pattern.



To add a second subpattern go to the ‘Edit’ mode and select the subpattern atom. Add a second atomic environment definion using the ‘or’ operator.



You can always use the filter to check if your definitions result in the desired matches.



Enjoy the SMARTSeditor!