

SMARTSeditor Beginner's Guide

1. Basics

SMARTS Editor

Help

Pattern

Draw

Draw Edit Environments SMARTSminer

Tools

Draw Delete Move Undo Redo Beautify

Rings

5 6 7 8 6 aro 6 wild

Templates

Frequent Functional Groups

- Alcohol
- Aldehyde
- Ketone
- Carbonyl
- 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.

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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 screenshot displays the SMARTS Editor application window. At the top, the title bar reads "SMARTS Editor" and "Help". Below the title bar is a text input field containing the SMILES string "C(C)C". The main workspace, labeled "Pattern", shows a skeletal structure of a central carbon atom bonded to two other carbon atoms. A blue circle highlights the central carbon atom, and a blue arrow points to a new carbon atom being dragged away from it, illustrating the "left click and drag" action. On the right side, there is a "Draw" toolbar with several sections: "Tools" (Draw, Delete, Move, Undo, Redo, Beautify), "Rings" (5, 6, 7, 8, 6 aro, 6 wild), and "Templates" (Frequent Functional Groups: Alcohol, Aldehyde, Ketone, Carbonyl, Carbonic Ester, Carboxylic Acid, Amide, Nitro, Acyl Halide).



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.

The screenshot displays the SMARTS Editor interface. At the top, a text input field contains the SMARTS string CC(C)C, which is highlighted with a red rectangular box. Below this, the main workspace shows a skeletal structure of a branched alkane (isobutane). The right-hand side of the interface features a toolbar with various drawing and editing tools, including Draw, Delete, Move, Undo, Redo, and Beautify. Below the toolbar, there are sections for Rings (with icons for 5, 6, 7, 8, 6 aro, and 6 wild) and Templates (listing Frequent Functional Groups such as Alcohol, Aldehyde, Ketone, Carbonyl, Carbonic Ester, Carboxylic Acid, Amide, Nitro, and Acyl Halide).



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

The image shows a screenshot of the SMARTS Editor software. At the top, a text box contains the SMILES string CC(C)C. Below this, a central workspace displays a skeletal structure of isobutane, consisting of a central carbon atom bonded to three other carbon atoms. To the right of the workspace is a vertical toolbar with several sections: **Tools** (containing Draw, Delete, Move, Undo, Redo, and Beautify icons), **Rings** (containing icons for 5, 6, 7, 8, 6 aro, and 6 wild membered rings), and **Templates** (containing a list of frequent functional groups such as Alcohol, Aldehyde, Ketone, Carbonyl, Carbonic Ester, Carboxylic Acid, Amide, Nitro, and Acyl Halide). A red rectangular box highlights the Tools section of the toolbar.



You can clean up the structure with the 'Beautify' function.

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Frequent Functional Groups

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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.

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Hovering over an atom gives you details on its properties.

The screenshot displays the SMARTS Editor application window. At the top, the title bar reads "SMARTS Editor" and "Help". Below the title bar, a text input field contains the SMILES string CC(C:1:c:c:c:c:1)C. The main workspace, labeled "Pattern", shows a chemical structure of a benzene ring with a methyl group and a hydrogen atom attached to one of the ring carbons. A blue circle highlights one of the ring carbons, and a tooltip box labeled "aromatic C" points to it with a blue arrow. On the right side of the interface, there is a "Draw" toolbar with several sections: "Tools" (Draw, Delete, Move, Undo, Redo, Beautify), "Rings" (5, 6, 7, 8, 6 aro, 6 wild), and "Templates" (Frequent Functional Groups: Alcohol, Aldehyde, Ketone, Carbonyl, Carbonic Ester, Carboxylic Acid, Amide, Nitro, Acyl Halide).



2. Defining Atom Properties

SMARTS Editor

Help

CC(C:1:c:c:c:c:1)C

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Draw Edit Environments SMARTSminer

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Draw Delete Move Undo Redo Beautify

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5 6 7 8 6 aro 6 wild

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aliphatic C

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.

The screenshot displays the SMARTS Editor application window. At the top, the title bar reads "SMARTS Editor" and "Help". Below the title bar is a text input field containing the SMILES string CC(C:1:c:c:c:c:1)C. A red arrow points to a small circular icon with a plus sign next to the text field. Below the text field is a toolbar with tabs for "Draw", "Edit", "Environments", and "SMARTSminer". The "Edit" tab is active. The main workspace shows a chemical structure of a benzene ring with a methyl group attached to one of the carbons. A red arrow points to one of the carbon atoms in the ring, which has a context menu open. The context menu includes the following options: "Edit Atom", "Quick Edit", "Carbon", "Hydrogen", "Nitrogen", "Oxygen", "Fluorine", "Phosphorus", "Sulfur", "Chlorine", "Bromine", and "Iodine". To the right of the main workspace is a sidebar with sections for "Tools", "Rings", and "Templates". The "Tools" section includes icons for Draw, Delete, Move, Undo, Redo, and Beautify. The "Rings" section includes icons for 5, 6, 7, 8, 6 aro, and 6 wild. The "Templates" section is titled "Frequent Functional Groups" and lists: Alcohol, Aldehyde, Ketone, Carbonyl, Carbonic Ester, Carboxylic Acid, Amide, Nitro, and Acyl Halide.



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

The screenshot displays the SMARTS Editor software. At the top, a text box contains the SMILES string CC(C:1:c:c:c:c:1)C. Below this, a chemical structure is shown in the center, consisting of a benzene ring with a methyl group attached to one of its carbons. The carbon atom in the ring that is bonded to the methyl group is highlighted with a blue circle. To the right of the structure is a panel titled "Atom" with tabs for "Draw", "Edit", "Environments", and "SMARTSminer". The "Environments" tab is active, showing a "Description" section with "[C]", a "Specification" section with "Common Properties" and "Element-Specific Properties", and a "Chemical Element" section. In the "Chemical Element" section, a dropdown menu is set to "C - Carbon". Below the dropdown are two radio buttons: "aliphatic" (which is currently selected) and "aromatic" (which is unselected). A red rectangular box highlights the "aliphatic" and "aromatic" radio buttons, and a red arrow points to the "aromatic" button, indicating the target for the user's action.



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

The screenshot shows the SMARTS Editor interface. At the top, a text box contains the SMILES string CC(c1:c:c:c:c:1)C. Below this, a chemical structure is displayed, consisting of a benzene ring (represented with dashed lines) and an aliphatic chain (represented with continuous lines). A blue circle highlights one of the carbon atoms in the benzene ring. Two blue arrows point from the structure to text boxes: one points to the benzene ring with the text "Dashed line = aromatic", and the other points to the aliphatic chain with the text "Continuous line = aliphatic". On the right side of the interface, a panel titled "Atom" shows the "Specification" section with "aromatic" selected and "always" checked.

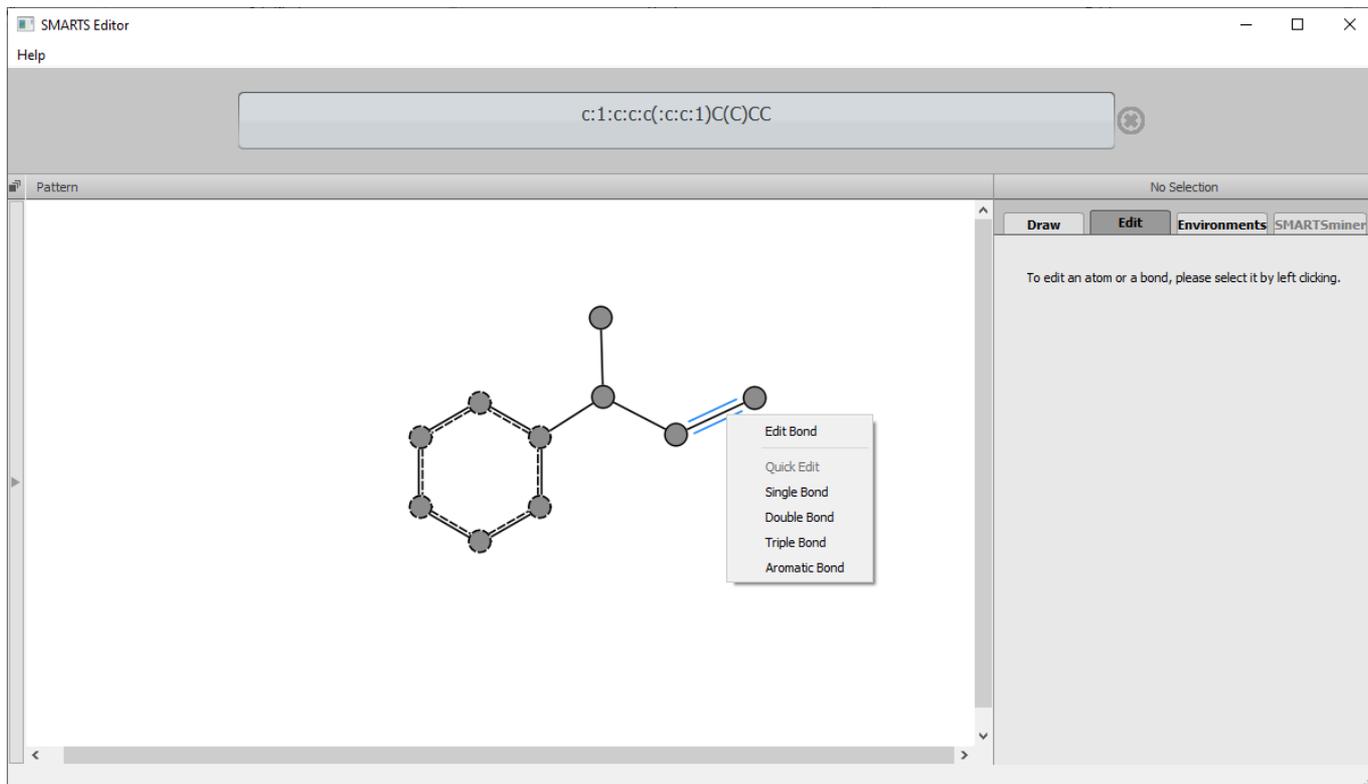
You can also visually
differentiate between
aliphatic and aromatic atoms.

Dashed line = aromatic

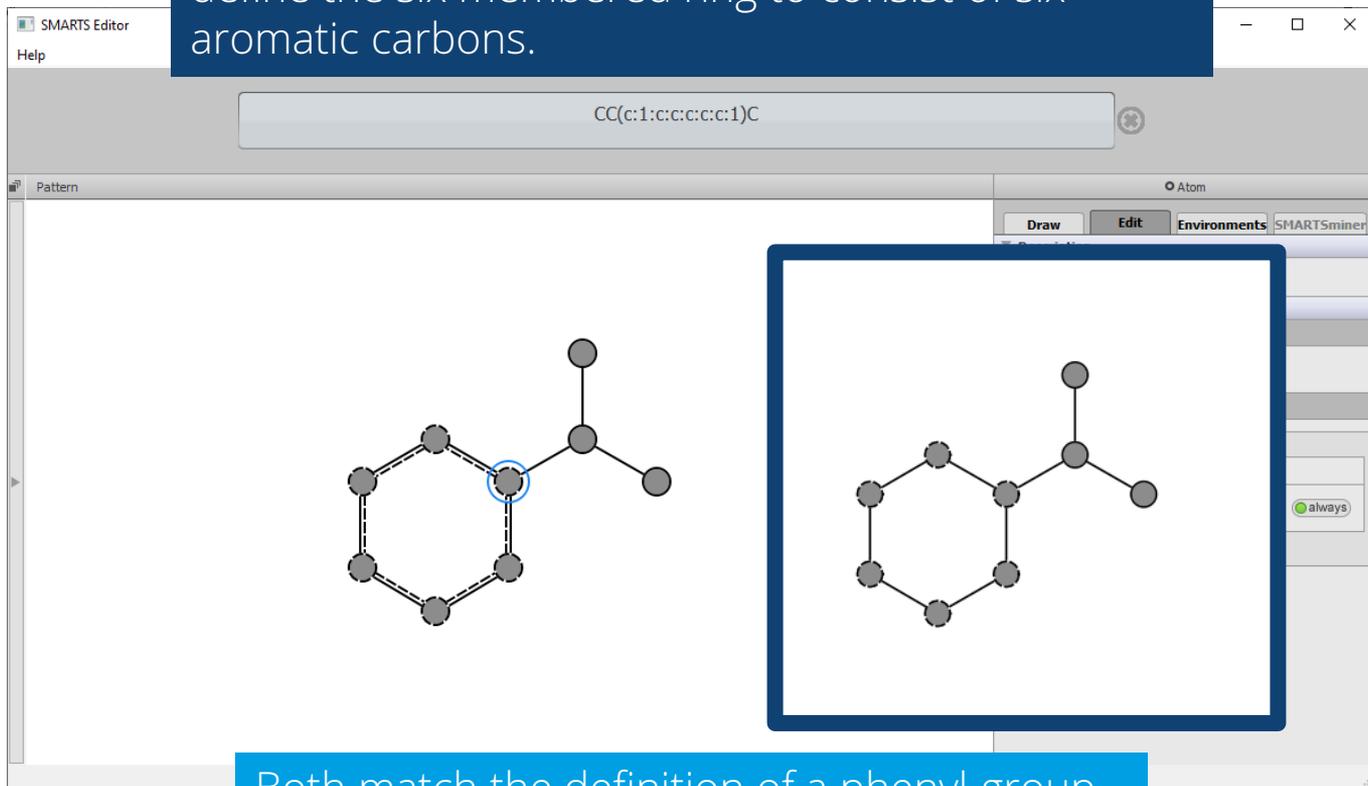
Continuous line = aliphatic



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).

The image shows a screenshot of the SMARTS Editor software. At the top, a text box contains the SMILES string c1ccc(cc1)C(C)C. Below this, the main window displays a ball-and-stick model of the molecule, which is 1-phenylethane. One of the carbon atoms in the benzene ring is highlighted with a blue circle. On the right side of the interface, there is a panel with tabs for 'Draw', 'Edit', 'Environments', and 'SMARTSminer'. The 'Edit' tab is active, showing a 'Description' section with '[c]', a 'Specification' section with 'Common Properties', and an 'Element-Specific Properties' section. In the 'Element-Specific Properties' section, there is a dropdown menu set to 'C - Carbon' and two radio buttons: 'aromatic' and 'always'. Below these, there is a '+' sign and a red arrow pointing to a button labeled 'Add or-connected property'.

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.

The screenshot displays the SMARTS Editor window. At the top, the SMILES pattern c1[c,n]cc(cc1)C(C)C is entered in a text field. Below this, the chemical structure is visualized, with a blue circle highlighting a specific atom in the ring. The right-hand panel, titled 'Atom', shows the configuration for this atom. The 'Chemical Element' dropdown is set to 'N - Nitrogen', and the 'aromatic' and 'always' checkboxes are checked. A blue arrow points from the highlighted atom in the structure to the 'N - Nitrogen' dropdown in the configuration panel.



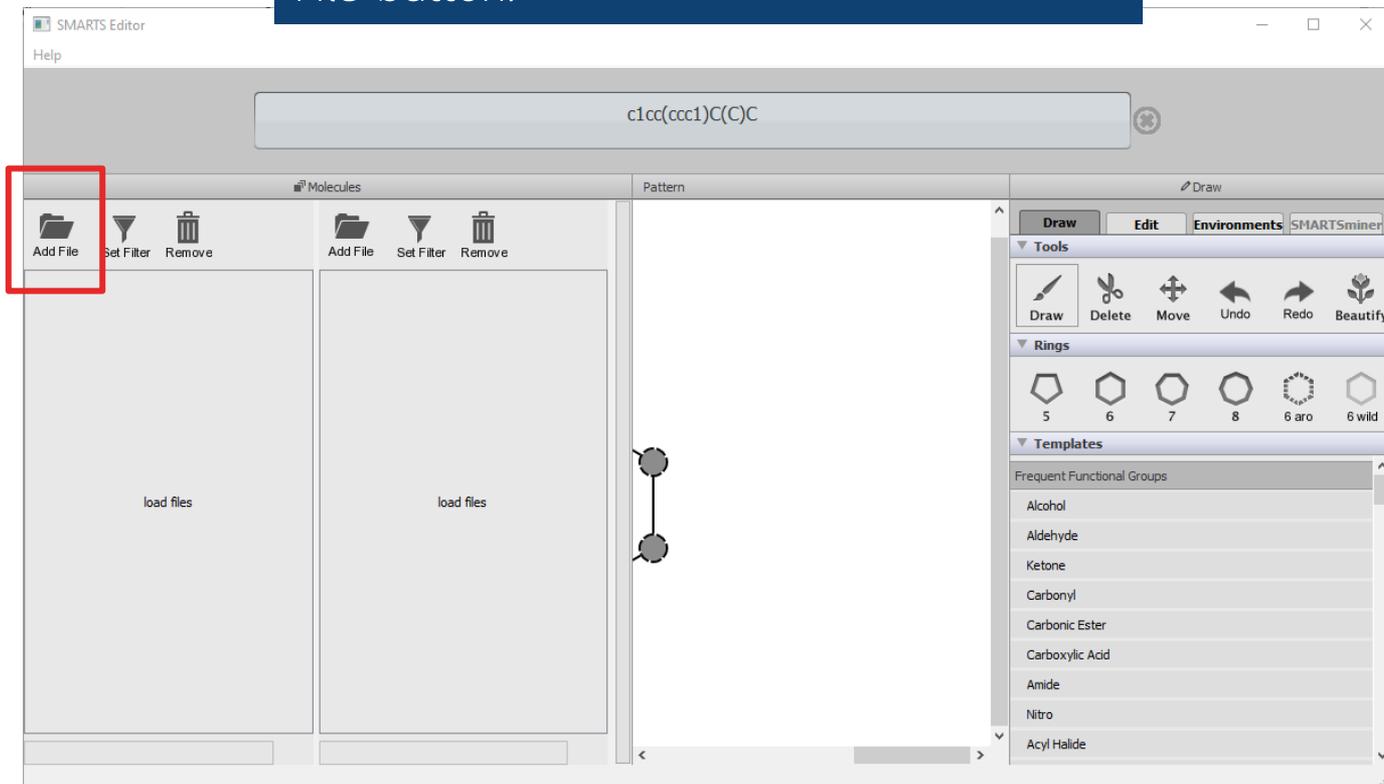
3. Filters

The screenshot shows the SMARTS Editor interface. At the top, a text box contains the SMILES string c1cc(ccc1)C(C)C. Below this is a large central area displaying a ball-and-stick model of a propylbenzene molecule. To the right of the main area is a toolbar with sections for Tools (Draw, Delete, Move, Undo, Redo, Beautify), Rings (5, 6, 7, 8, 6 aro, 6 wild), and Templates (Frequent Functional Groups: Alcohol, Aldehyde, Ketone, Carbonyl, Carbonic Ester, Carboxylic Acid). On the left side of the main area, there is a vertical bar with a red rectangular highlight around it. A blue arrow points from the left towards this bar.

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.

The image displays three overlapping instances of the SMARTS Editor software interface. Each instance has a 'Set Filter' button (represented by a funnel icon) in its top toolbar, with a red arrow pointing to it. The main window shows the SMILES string c1cc(ccc1)C(C)C in the top input field. Below the toolbar, there are sections for 'Molecules' and 'Pattern'. The 'Molecules' section contains a list of chemical structures, with the first one highlighted. The 'Pattern' section shows a single bond structure. On the right side, there is a 'Draw' panel with various tools and templates, including 'Frequent Functional Groups' like Alcohol, Aldehyde, Ketone, etc. The status bar at the bottom of the main window shows '3 / 11'.



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

SMARTS Editor

Help

c1ccc(cn1)[CX1H1](CF)CC

Molecules

Pattern

No Selection

Draw Edit Environments SMARTSmiler

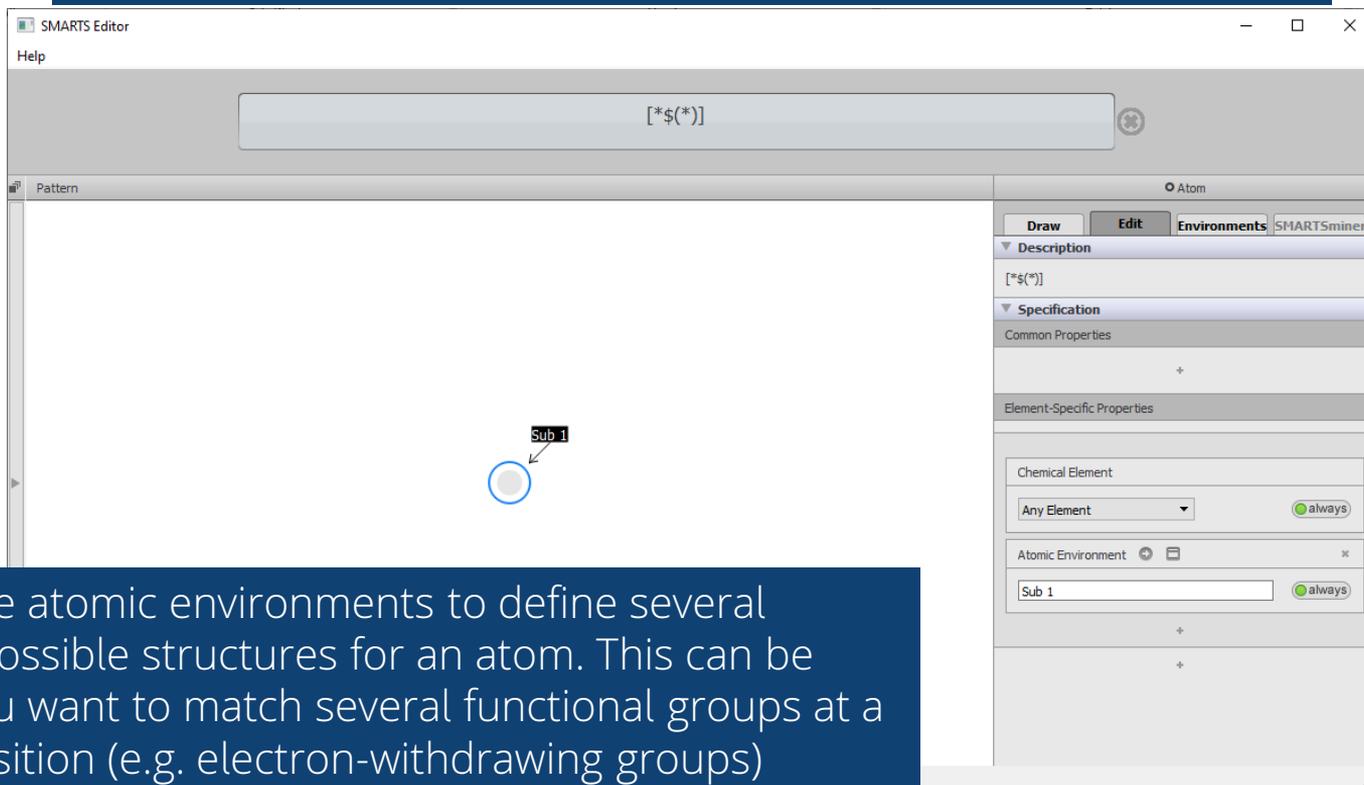
To edit an atom or a bond, please select it by left clicking.

3 / 11

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



3. Atomic environment



The screenshot shows the SMARTS Editor interface. At the top, a text box contains the pattern [*\$(*)]. Below this, the main workspace shows a single atom represented by a blue circle with a grey center, labeled "Sub 1" with an arrow pointing to it. On the right side, the "Environments" tab is active, displaying a configuration table for the atom's environments.

| Chemical Element | |
|--------------------|---|
| Any Element | <input checked="" type="radio"/> always |
| Atomic Environment | |
| Sub 1 | <input checked="" type="radio"/> always |

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.

The screenshot shows the SMARTS Editor interface. At the top, a text box contains the pattern [*\$(*)]. Below this is a workspace labeled 'Pattern' containing a blue circle representing an atom, with a label 'Sub 1' and an arrow pointing to it. On the right side, there is a 'Properties' panel for the selected atom. The panel has tabs for 'Draw', 'Edit', 'Environments', and 'SMARTSminer'. The 'Environments' tab is active, showing a list of environments. The first environment is 'Any Element' with a green 'always' indicator. The second environment, 'Atomic Environment', is highlighted with a red box and contains the text 'Sub 1' and a green 'always' indicator. A red arrow points to a plus sign below the list, indicating where to add a new environment.

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



Click on the arrow to edit the atomic environment.

The screenshot displays the SMARTS Editor application window. At the top, a text box contains the SMILES pattern [*\$(*)]. Below this, the main workspace shows a single atom represented by a grey circle with a blue outline, labeled 'Sub 1'. A red arrow points from the 'Atomic Environment' field in the right-hand panel to the 'Sub 1' label. The right-hand panel is titled 'Atom' and includes tabs for 'Draw', 'Edit', 'Environments', and 'SMARTSminer'. The 'Edit' tab is active, showing sections for 'Description' (containing [*\$(*)]), 'Specification', 'Common Properties', and 'Element-Specific Properties'. The 'Element-Specific Properties' section includes a 'Chemical Element' dropdown menu set to 'Any Element' and an 'Atomic Environment' field set to 'Sub 1'. Both fields have an 'always' status indicator.



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

*1(*****1)C[*s]([NX3](-,=[OX1]),=[OX1])

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.

SMARTS Editor
Help

*1{*****1}C[*s{[NX3](-,[OX1]),=[OX1]}

Molecules

Pattern > Sub 1

Draw

Tools

Draw Delete Move Undo Redo Beautify

Rings

5 6 7 8 6 aro 6 wld

Templates

Frequent Functional Groups

- Alcohol
- Aldehyde
- Ketone
- Carbonyl
- Carbonyl Ester
- Carboxylic Acid
- Amide
- Nitro
- Acyl Halide
- Halogen
- 2-R-Phenol
- 3-R-Phenol
- 4-R-Phenol
- Sulfonic Acid
- Sulfone
- N-R-Sulfone Amide
- S-R-Sulfonamide

Heterocycles (5-membered)

- 2-R-Furane
- 3-R-Furane
- 2-R-Thiophene
- 3-R-Thiophene
- 2-R-Pyrrole

1 / 11



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

The screenshot displays the SMARTS Editor interface. At the top, a text box contains the SMARTS string: [*\${[NX3](-,[OX1]-,[OX1]),*\${[SX4](O)(=O)=O)}C*1*****1. Below this, the interface is divided into three main sections: 'Molecules', 'Pattern', and 'Atom'.

- Molecules:** Contains two chemical structures. The top one is a benzene ring with a methyl group. The bottom one is a benzene ring with a propyl group.
- Pattern:** Shows a graph representation of the selected atom from the SMARTS string. A blue circle highlights a specific atom, labeled 'Sub 1' and 'Sub 2'.
- Atom:** Contains configuration options for the selected atom. The 'Edit' tab is active. The 'Description' field shows the current SMARTS string. The 'Specification' section includes:
 - 'Any Element' dropdown set to 'Any Element' with an 'always' toggle.
 - 'Atomic Environment' dropdown set to 'Sub 1' with an 'always' toggle.
 - An 'OR' button, highlighted with a red box, used to add a second subpattern.
 - 'Chemical Element' dropdown set to 'Any Element' with an 'always' toggle.
 - 'Atomic Environment' dropdown set to 'Sub 2' with an 'always' toggle.



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

The screenshot displays the SMARTS Editor interface. At the top, a text box contains the SMARTS pattern: [*\$([NX3](-,[OX1])-,=[OX1]),*\$([SX4](O)(=O)=O)]C*1*****1. A red arrow points to the 'Set Filter' button in the 'Molecules' panel. Below the filter, two chemical structures are shown in a list, both of which are highlighted with a blue border. The 'Pattern' panel shows a skeletal structure of a molecule with a highlighted atom. The 'Environments' panel shows two sub-panels: 'Sub 1' displays a ball-and-stick model of a molecule with a central blue atom and two red atoms, and 'Sub 2' displays a ball-and-stick model of a molecule with a central yellow atom and three red atoms. The status bar at the bottom indicates '4 / 11'.



Enjoy the SMARTSeditor!

