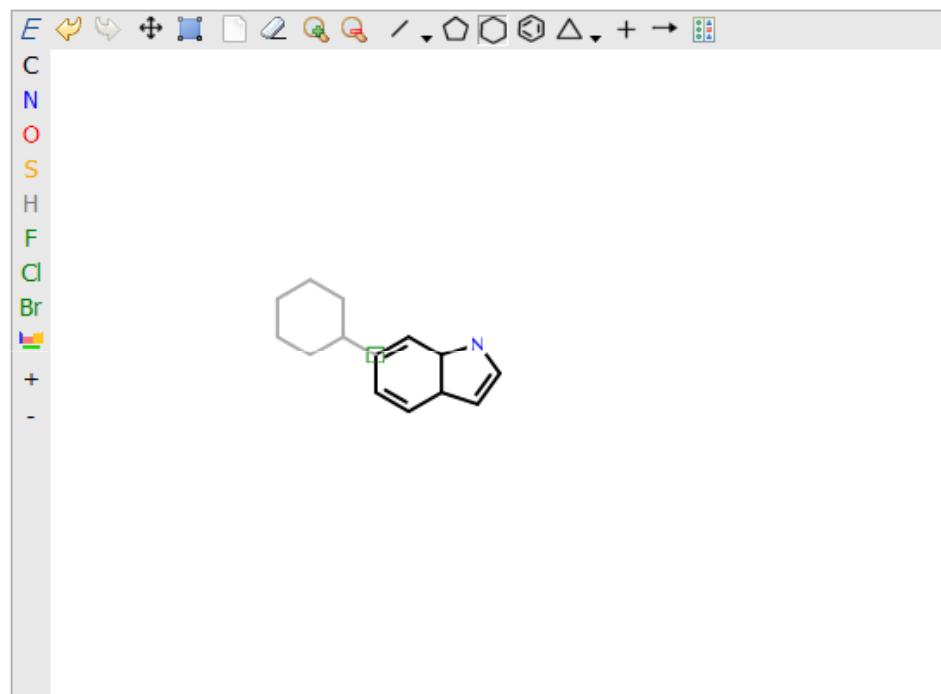


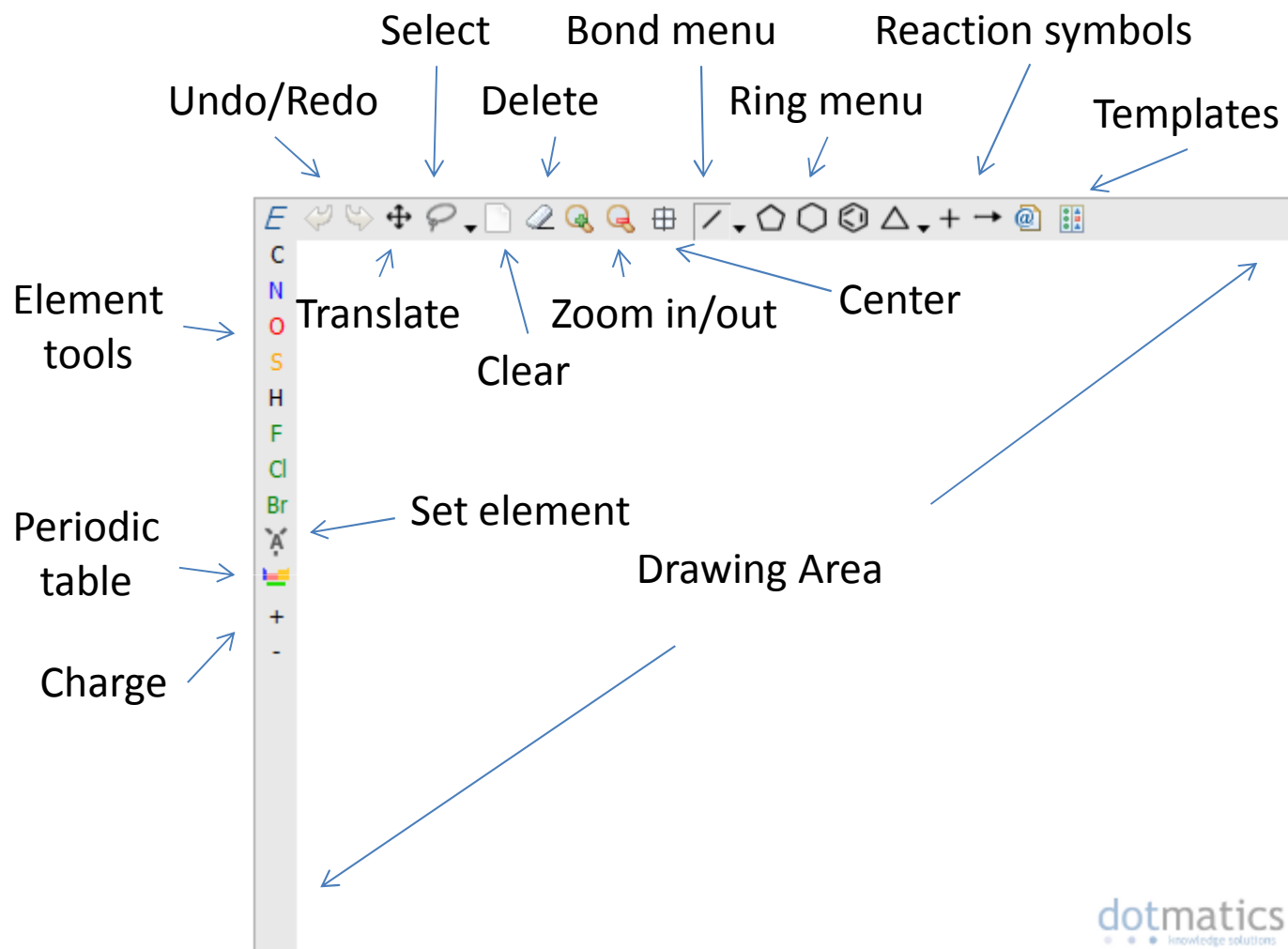
Elemental

User Guide



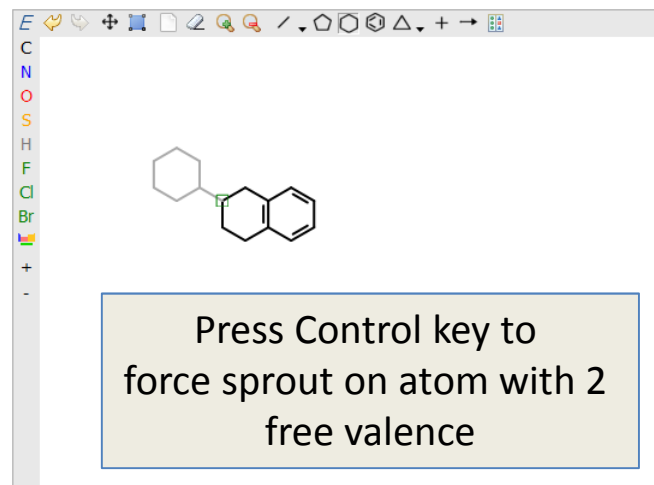
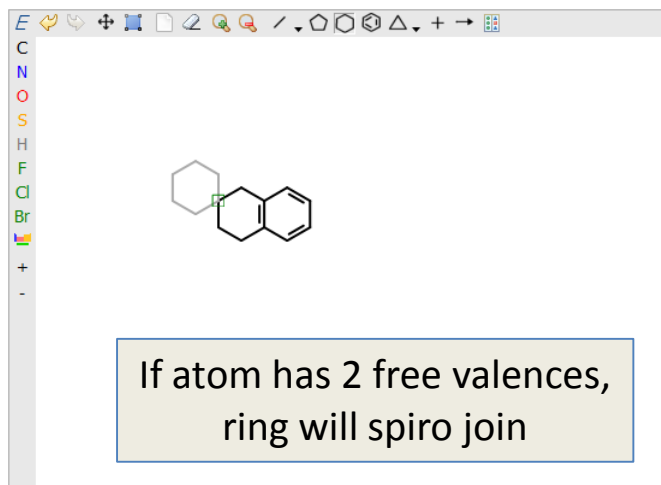
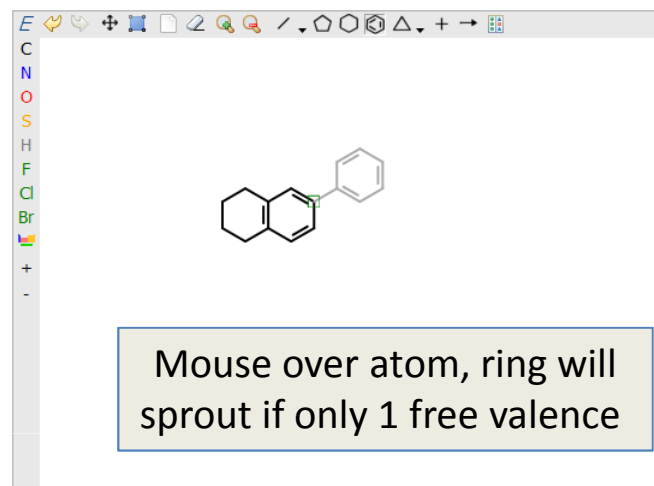
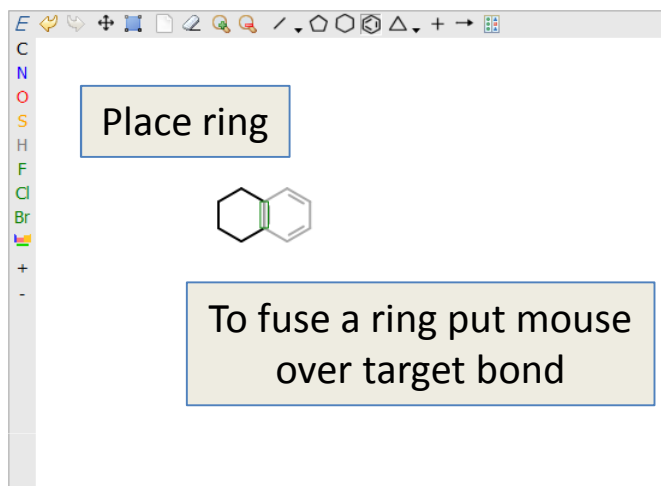
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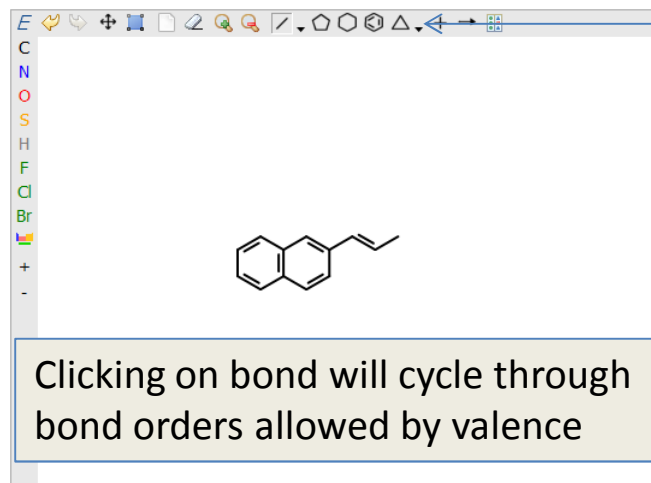
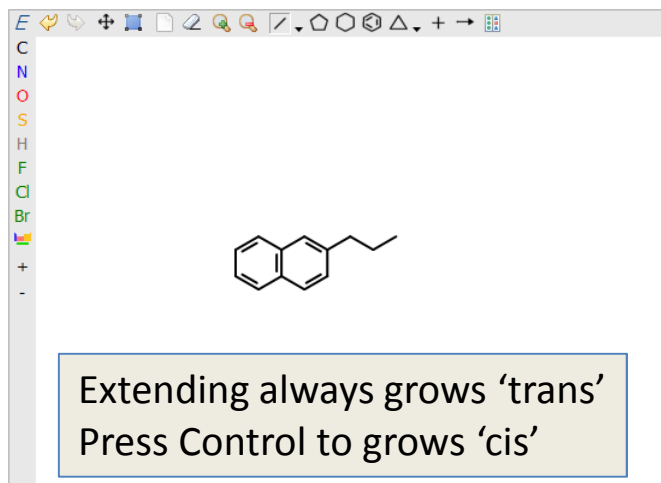
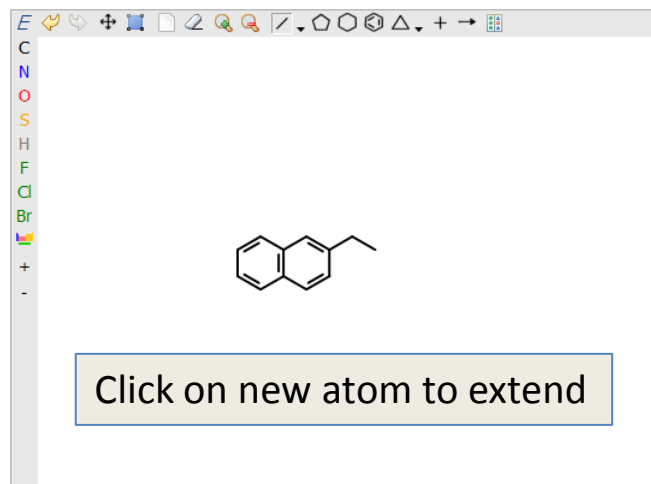
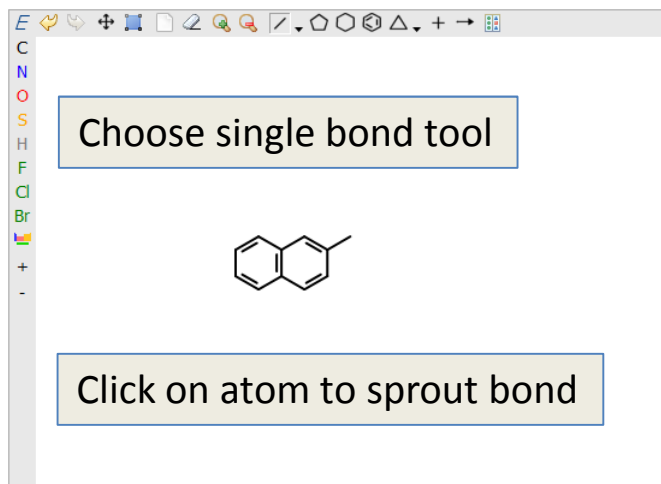
Drawing mistakes can be easily changed by using the undo/redo buttons (also mapped to Ctrl-Z and Ctrl-Y)

Drawing with Rings



Click to place ring

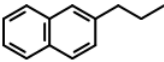
Adding Bonds



Select bond order or wedge bonds from bond menu
Click black triangle to show menu

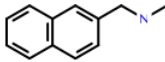
Changing Atoms

Select Element tool e.g. N



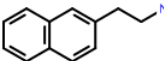
The image shows a software window with a toolbar at the top and a vertical element palette on the left containing C, N, O, S, H, F, Cl, Br, and a plus sign. A text box contains the instruction "Select Element tool e.g. N". Below the text is a skeletal structure of propylbenzene, consisting of a benzene ring attached to a three-carbon alkyl chain.

Click on atom to change element



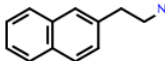
The image shows the same software window. A text box contains the instruction "Click on atom to change element". Below the text is a skeletal structure of N-propylbenzene, where the terminal carbon of the propyl chain is now a nitrogen atom.

Click again if you make a mistake
Then click the correct atom



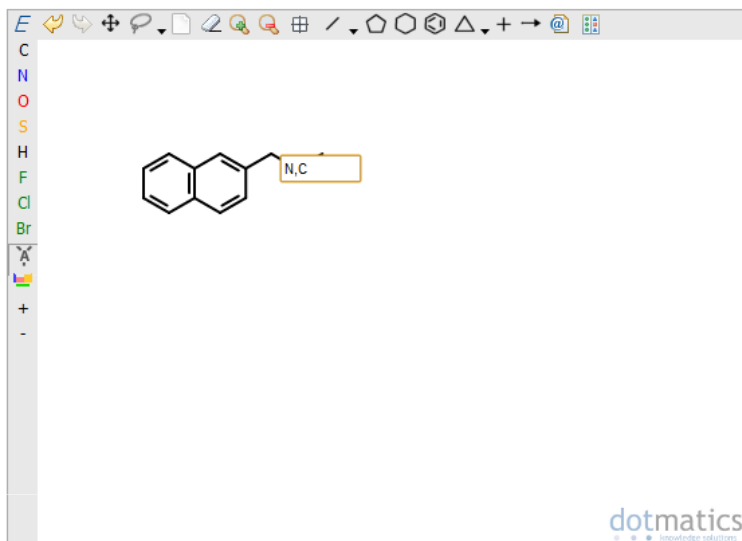
The image shows the same software window. A text box contains the instruction "Click again if you make a mistake Then click the correct atom". Below the text is a skeletal structure of N-propylbenzene, identical to the previous step.

Change charge using the charge tools



The image shows the same software window. A text box contains the instruction "Change charge using the charge tools". Below the text is a skeletal structure of N-propylbenzene with a positive charge (+) next to the nitrogen atom.

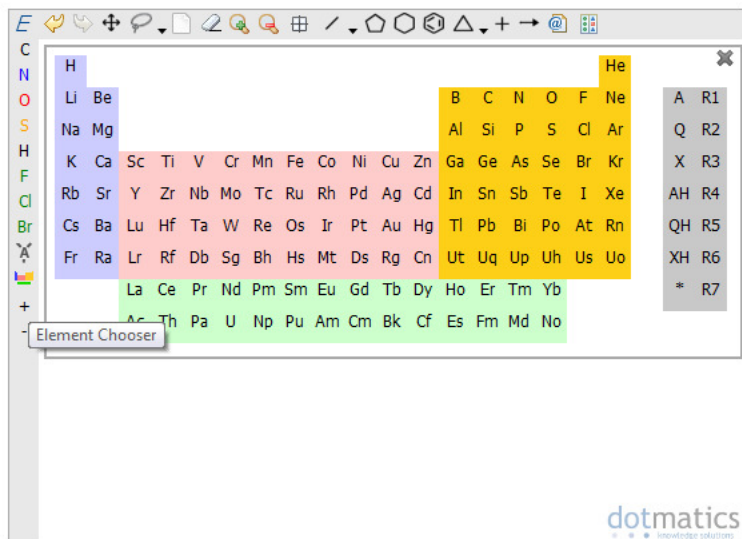
Changing Atoms




Select the 'Set element' tool, and click on an atom.

You can now type the element in the box.

This also allows for the specification of element lists



You can also set uncommon elements by clicking the periodic table 

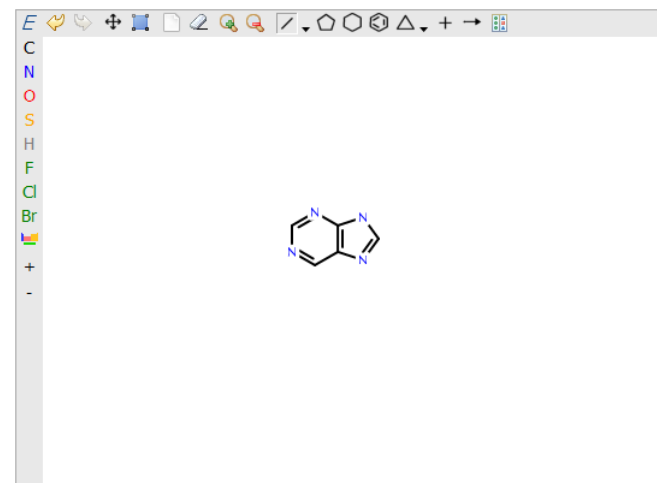
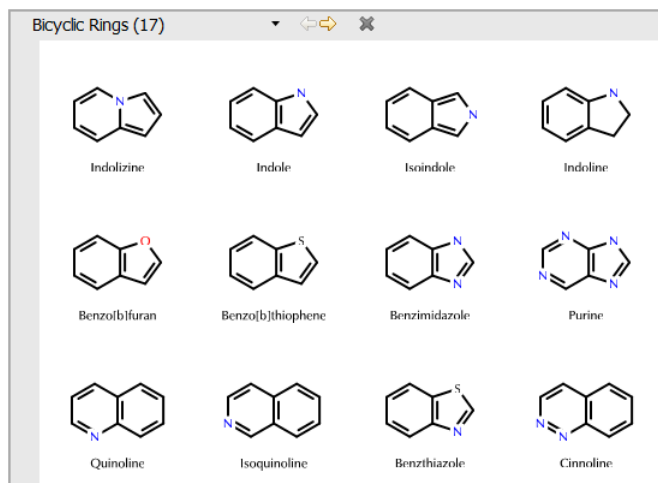
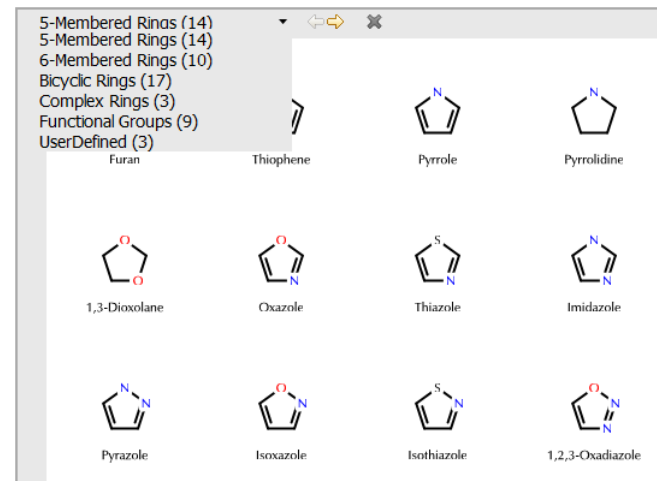
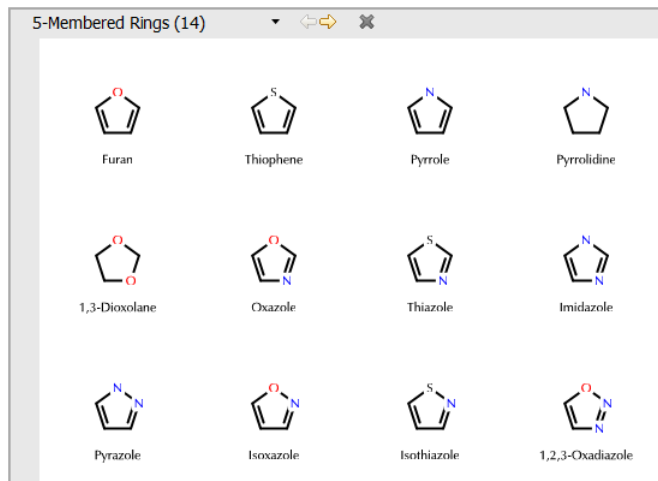
Keyboard short cuts

- Many actions can be performed using short cuts.
 - Copy/delete/paste/undo/redo delete using Ctrl-C,-X,-V, -Z,-Y
- After adding a bond, type on the keyboard to change the element of the atom added with the last bond.
 - Also multi-character elements are supported: 'S' will turn it into a sulfur, 'S' followed by 'i', will turn it into silicium)
- Element modification, and atom/bond deletes from the keyboard are also active on selections or on the (highlighted) atom/bond that the mouse is positioned over (note: selections take precedent). E.g.:
 - Press 'Delete' with the mouse over a bond deletes that bond.
 - Press 'Delete' with a selection deletes all selected atoms
 - Press 'N' with the mouse over an atom changes the element of that atom to nitrogen.

Templates

Select template menu

Choose template group



Scroll with arrows

Pick template by selecting an atom or bond. This will be its connection point

Place template.

The mouse wheel flips the template

User Defined Templates

- User defined templates are stored on the client in 'cookies'
 - Right click on a fragment
 - Choose save as fragment
 - Provide name
- Fragment is saved to User Defined section of template library (click menu to see list)
- To remove template, Right Click on it in template chooser and hit Delete Template

Atom context menu

- Many features are activated by right-clicking.

Right-click on atom:

The screenshot shows a chemistry software interface with a toolbar at the top and a vertical element palette on the left. The palette lists elements: C, N, O, S, H, F, Cl, Br, and a plus sign. A molecule is displayed in the center, and a context menu is open over one of its atoms. The menu items are: Charge, Element, Isotope (highlighted), R-group, Query features, Reaction, Delete, Delete molecule, Copy molecule, Rotate molecule, and Template. A sub-menu for 'Isotope' is open, showing 'Off' with a checkmark, and values 12, 13, and 14. Callout boxes provide the following descriptions:

- Set atom properties:** Points to the 'Isotope' menu item.
- Delete atom:** Points to the 'Delete' menu item.
- Copy/delete whole molecule atom is in:** Points to the 'Copy molecule' menu item.
- Rotate molecule around atom:** Points to the 'Rotate molecule' menu item.
- Save/Use as Template:** Points to the 'Template' menu item. The text in this box reads: "Save the molecule the atom is in to user-defined template library, or use it as a template, using the atom that was clicked on as the connection point."

Bond context menu

Right-click on bond:

The screenshot shows a chemical software interface with a toolbar at the top and a vertical element list on the left (E, C, N, O, S, H, F, Cl, Br, X, +, -). A pyridine ring is displayed with a bond highlighted in green. A context menu is open over this bond, listing the following options: Type, Stereo, Topology, Reaction center, Flip top, Flip bottom, Delete, Delete molecule, Copy molecule, and Template. Callout boxes with arrows point to specific menu items: 'Set bond properties' points to Type; 'Rotate around bond' points to Flip top; 'Delete atom' points to Delete; 'Copy/delete whole molecule atom is in' points to Copy molecule; and 'Save/Use as Template.' points to Template.

Set bond properties

Rotate around bond

Delete atom

Copy/delete whole molecule atom is in

Save/Use as Template.

Save the molecule the bond is in to user-defined template library, or use it as a template, using the bond that was clicked on as the connection point.

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General context menu

Right-click on background:

Standard editor controls

Tidy up layout for reaction or R-group definition

R-group controls

Calculate mass

Edit/add SD data tags

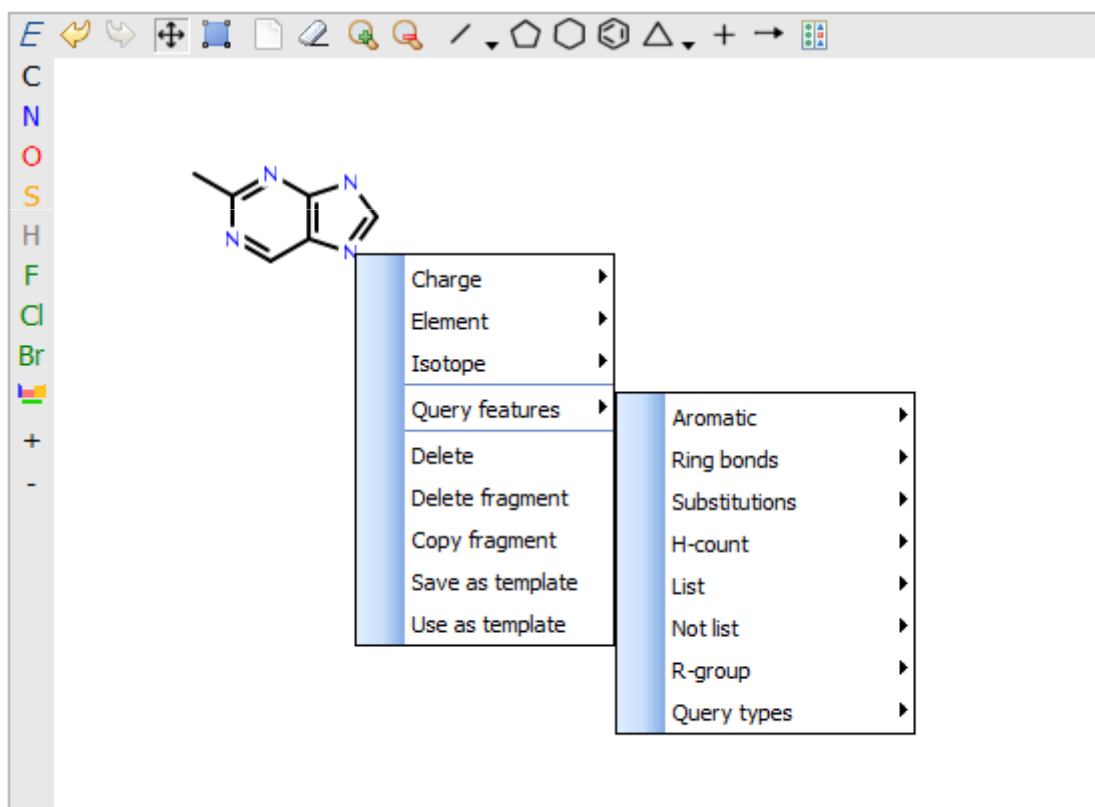
Tidy up sketched geometries

Rotate selection or complete contents around center of geometry

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Atom Query Features

- Query features describe how the atom should behave in substructure searches

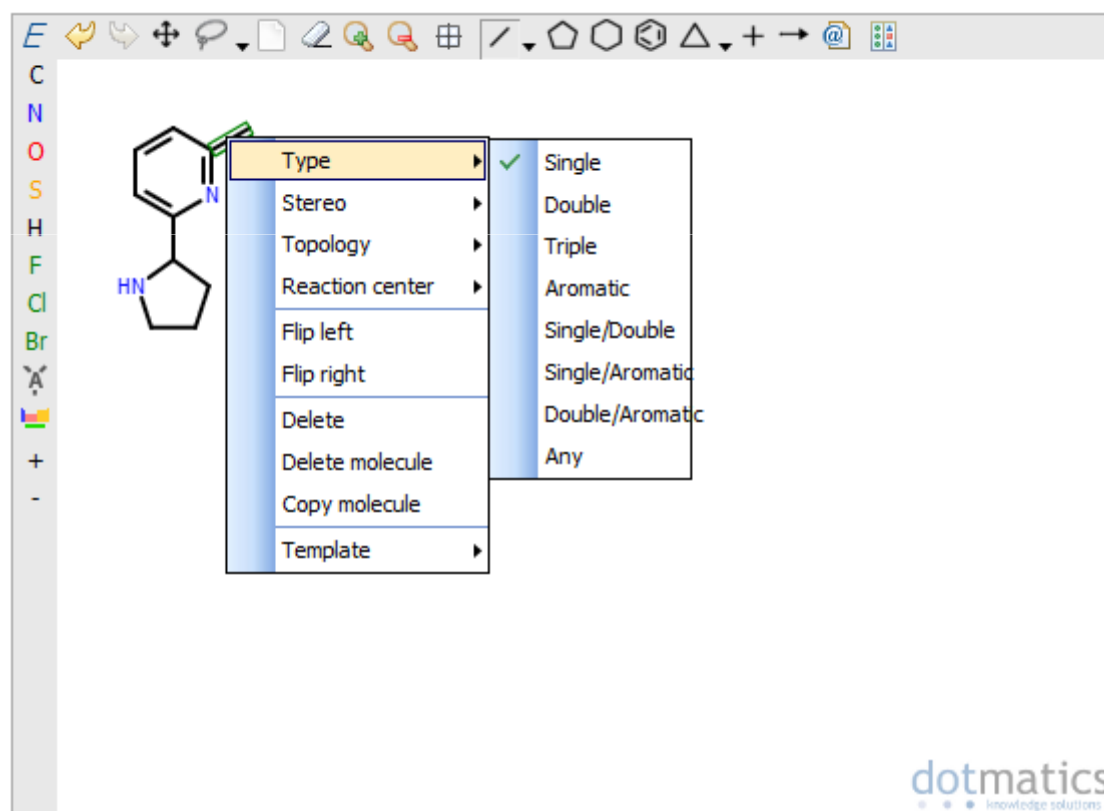


Atom Query Features

- **Aromatic**
 - Should the atom match only aromatic atoms
- **Ring bonds**
 - How many ring bonds the atom should have in matching molecule
- **Substitutions**
 - How many substituents the atom should have
- **H-count**
 - How many hydrogens the atom should have
- **Unsaturated**
 - On requests at least one double bond on atom
- **List/Not list**
 - Element types the atom is (not) allowed to match
 - Select elements from periodic table, press Done to close
- **R-group**
 - An R-group identifier
- **Query types**
 - Built-in atom types

Bond Query Features

- Describe how bond matches in substructure queries

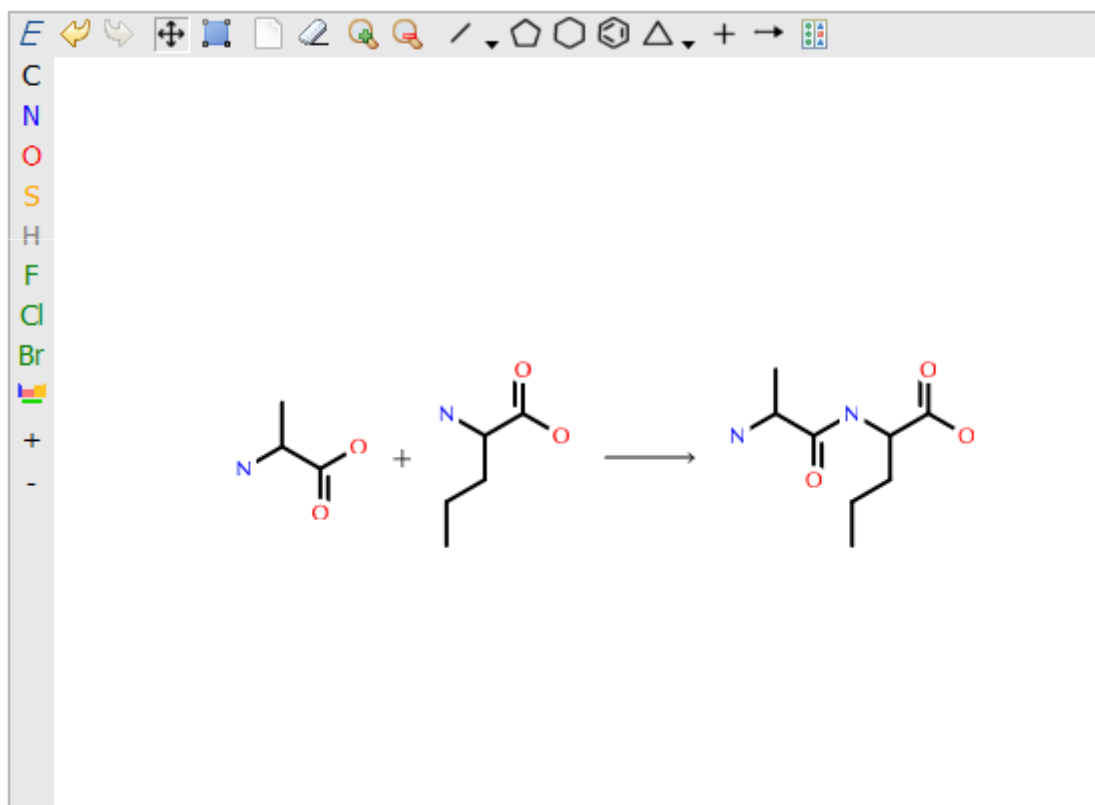


Bond Query Features

- Type
 - Single, Double, Triple
 - Aromatic, Any etc.
- Stereo
 - Up/Down/Either wedge
 - C/T either (cis/trans)
 - Switch ends (swap ends of stereo bond)
 - Molfile stereo care box (C/T double bonds)
- Topology
 - Bond should be in a ring or chain
- Reaction centers

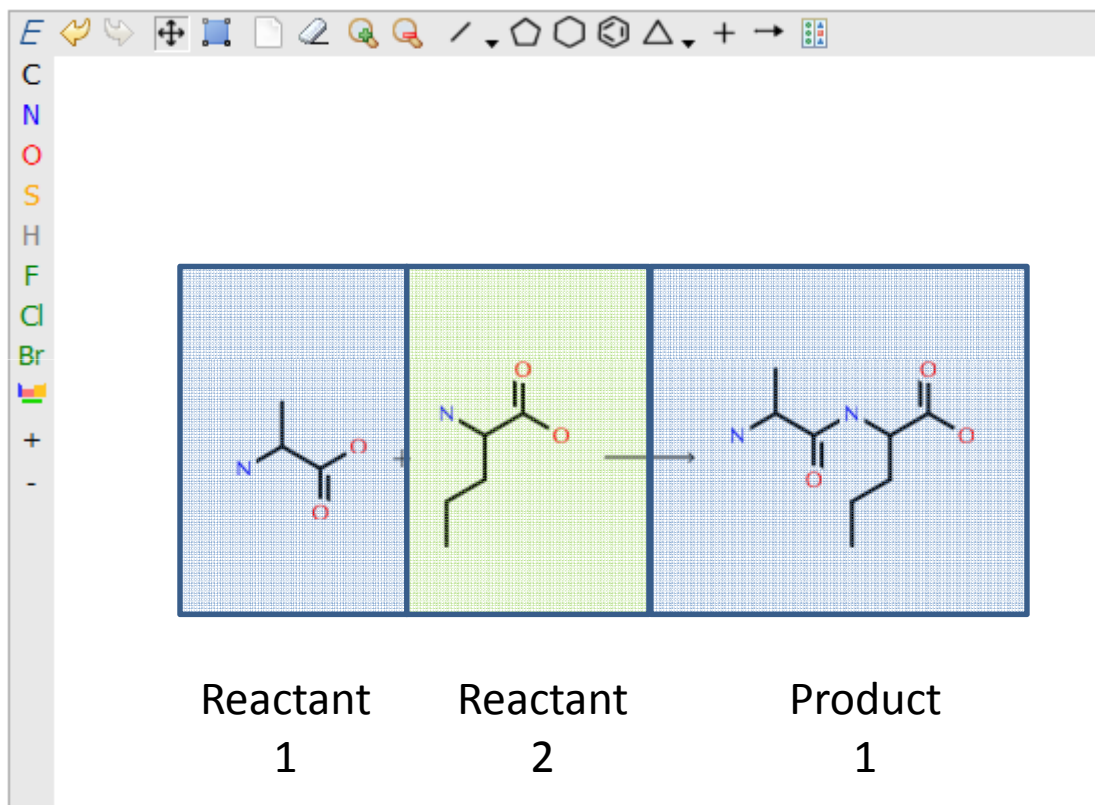
Reactions

- Build reaction using drawing tools and + and \rightarrow symbols

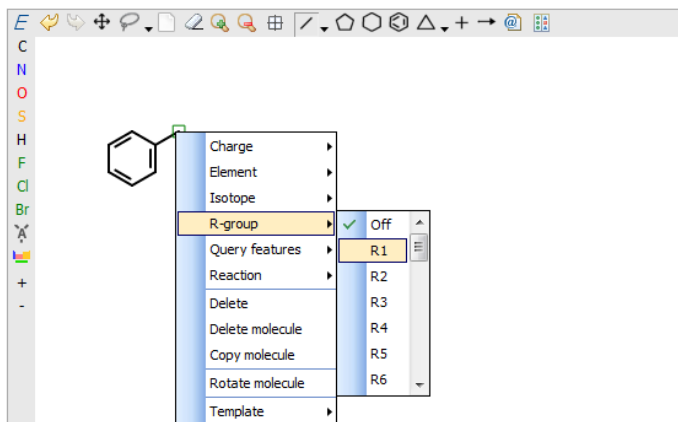


Reaction Perception

- Reactions are split horizontally by + and →

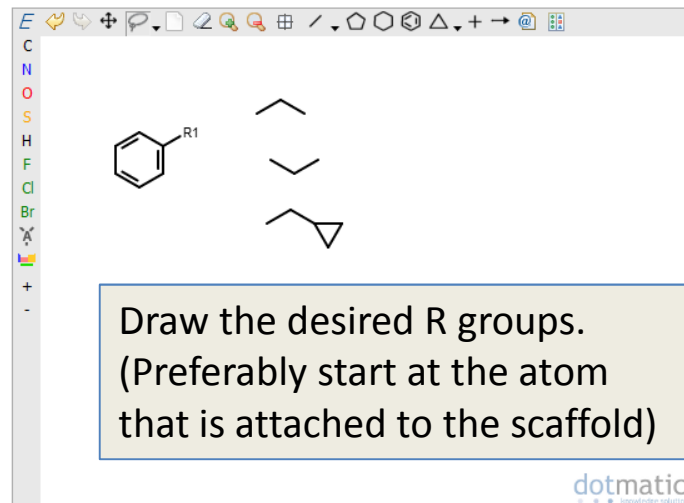


Defining R groups



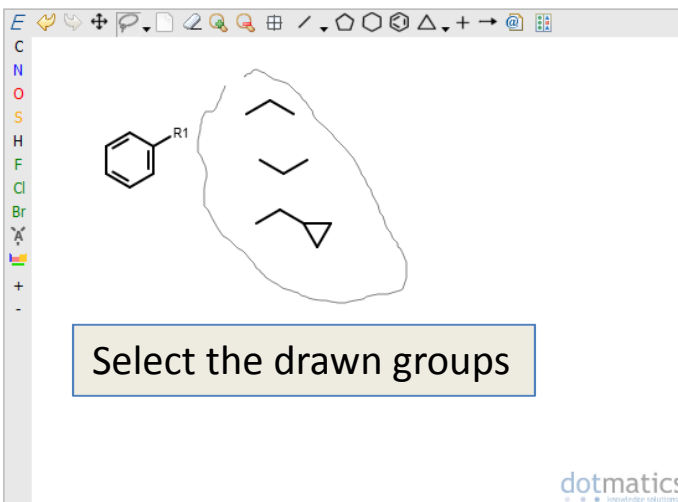
Add an R group to a scaffold
(right-click on atom)

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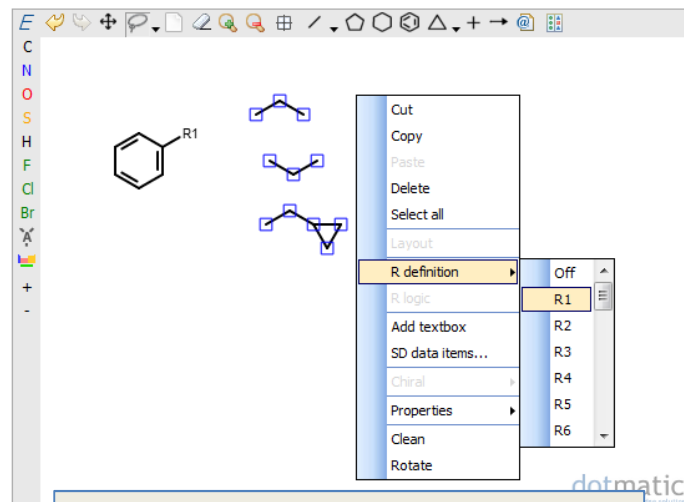
Draw the desired R groups.
(Preferably start at the atom
that is attached to the scaffold)

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Select the drawn groups

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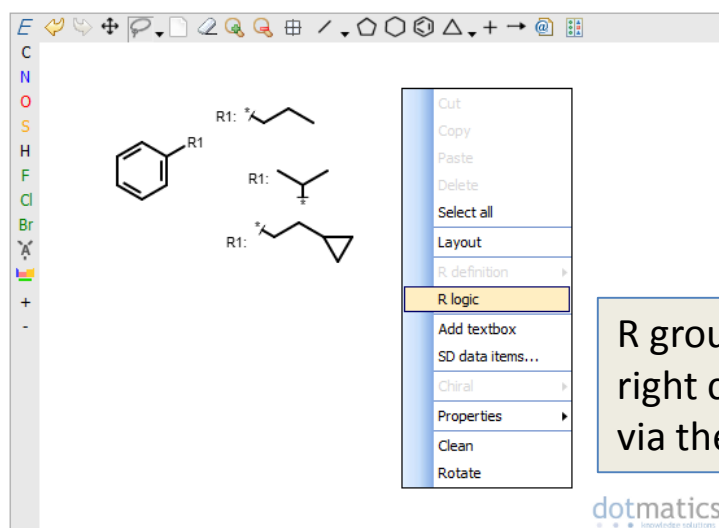
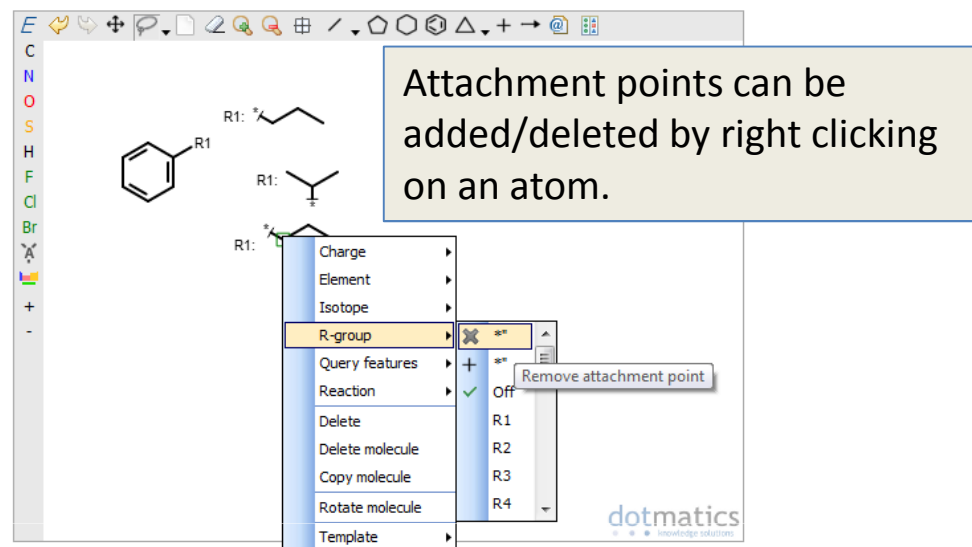
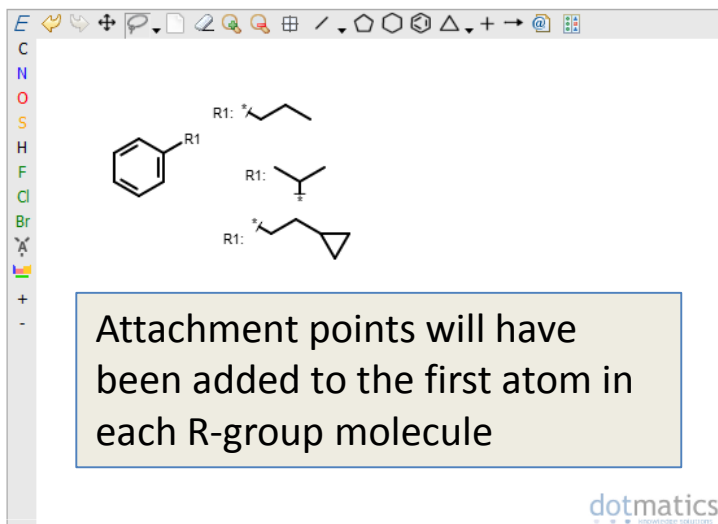


Right-click on background, and
select R definition

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Defining R groups



R group Occurrence range Rest H If R.. then R..

R1 >0 none

OK Cancel

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