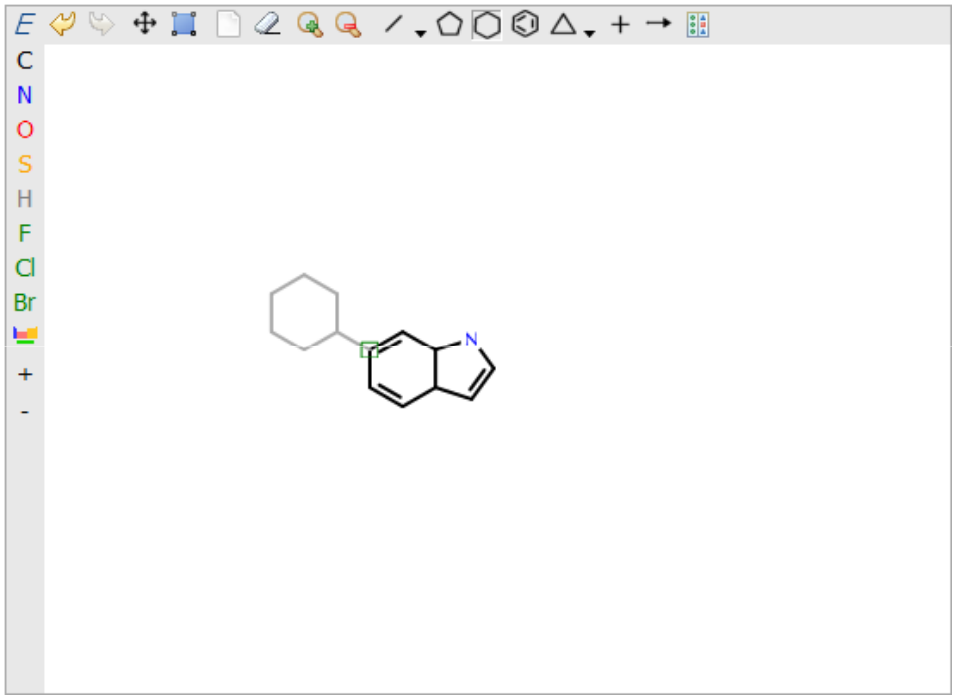
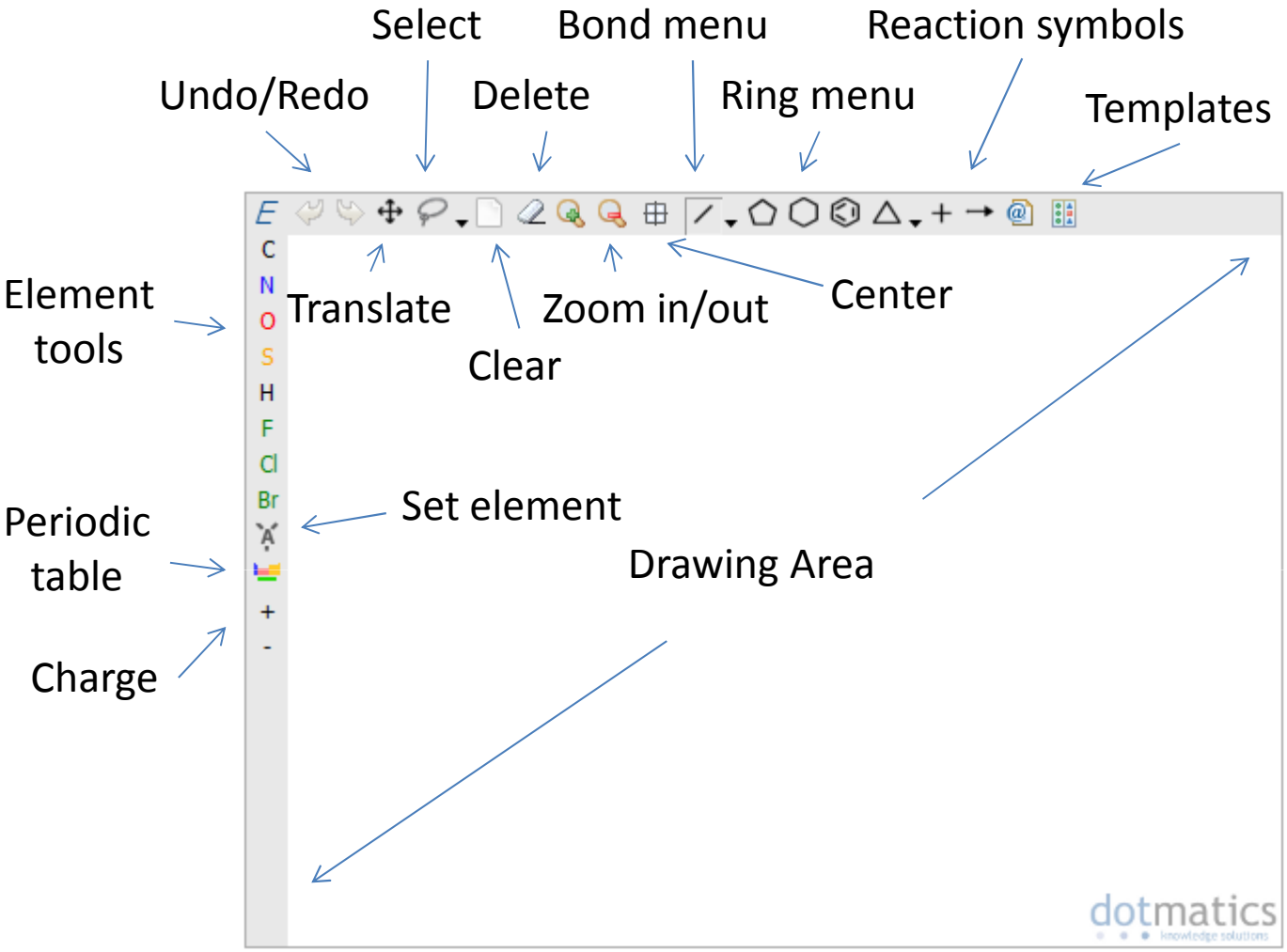
Elemental

User Guide



Dotmatics Limited



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

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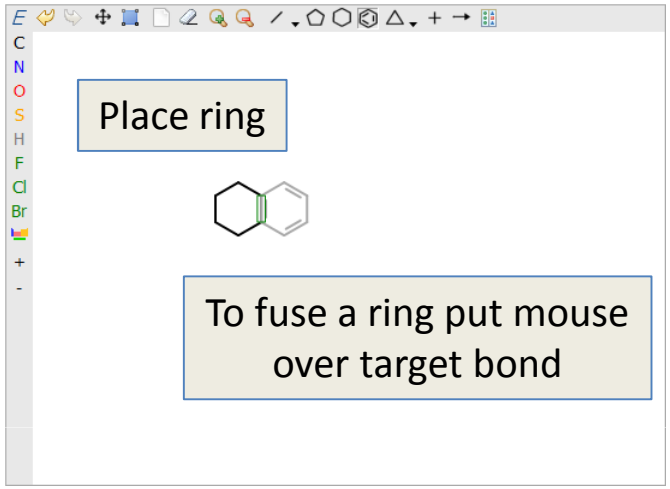
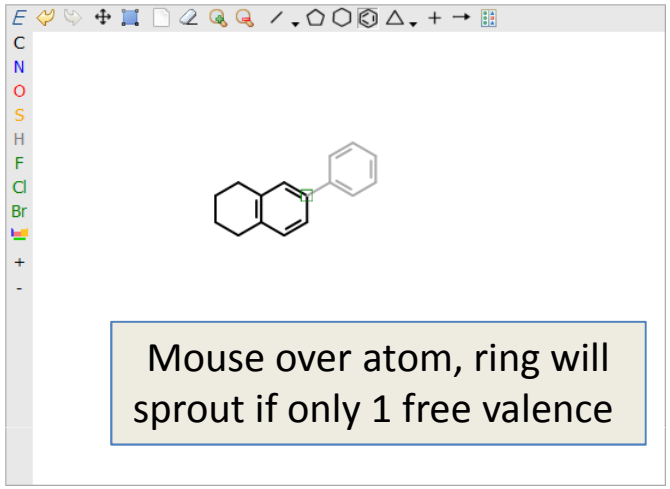
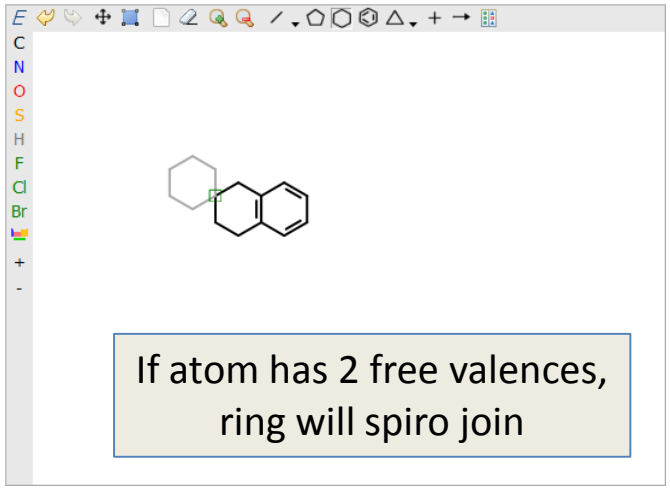
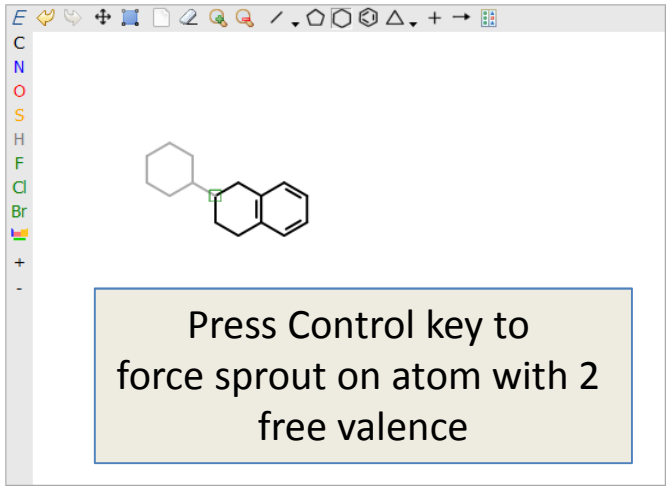
Drawing with Rings









Click to place ring

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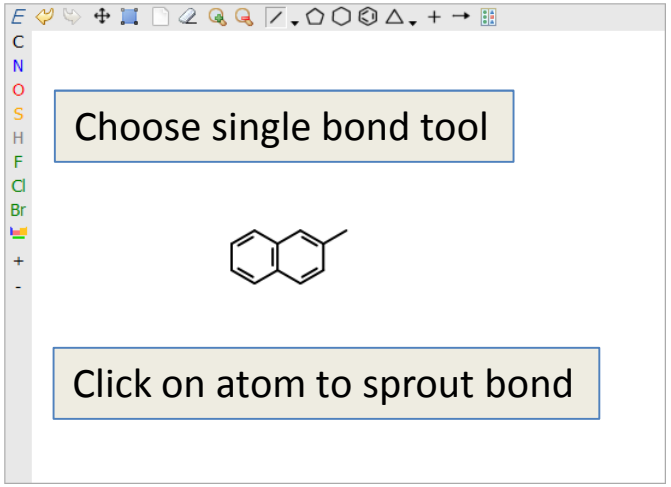
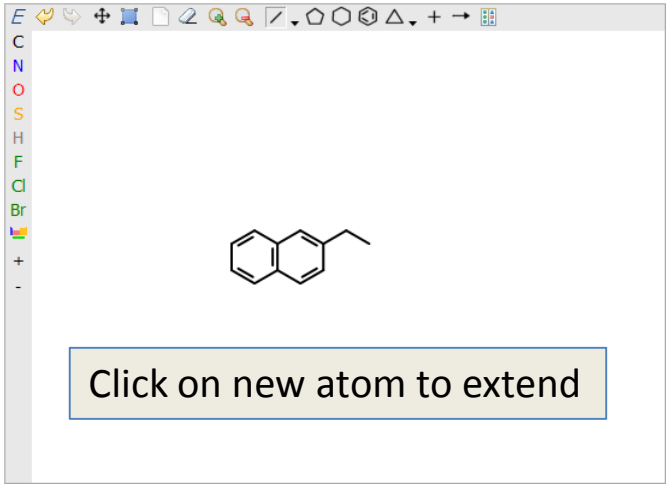
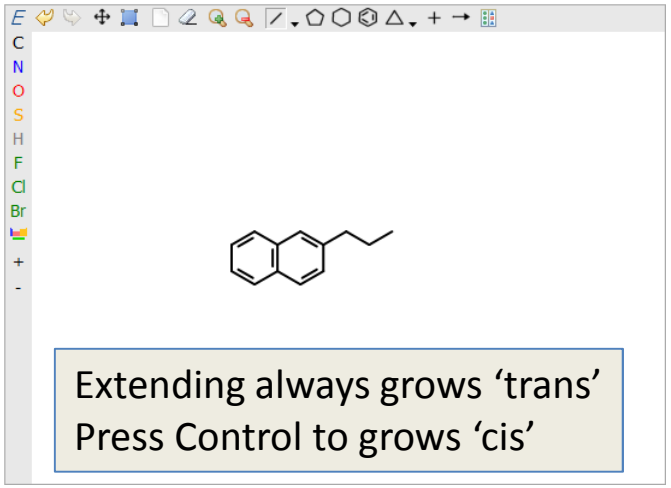
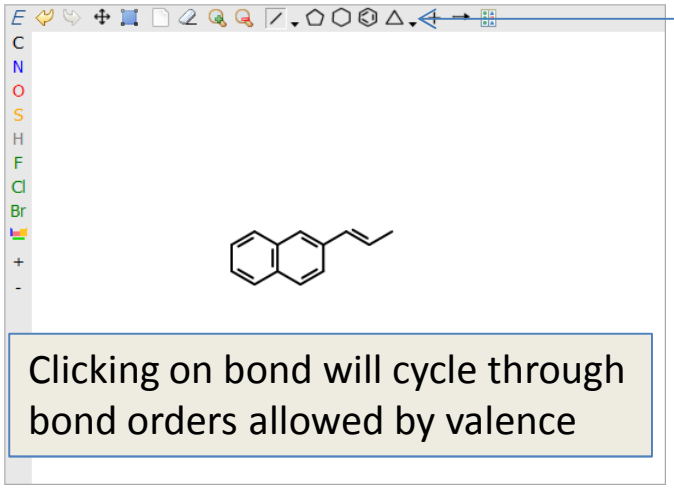
Adding Bonds









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

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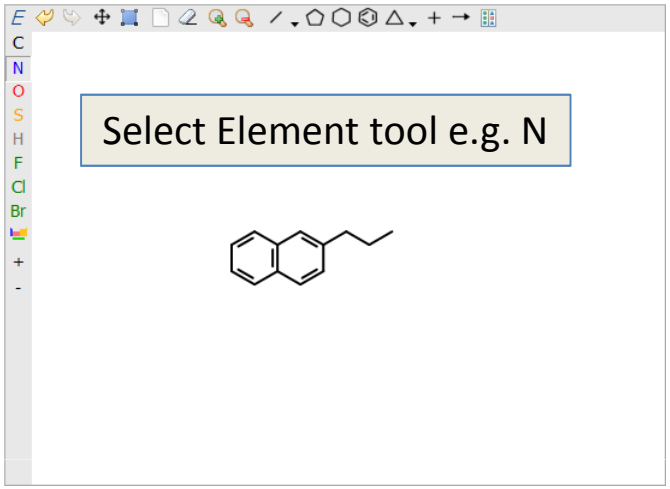
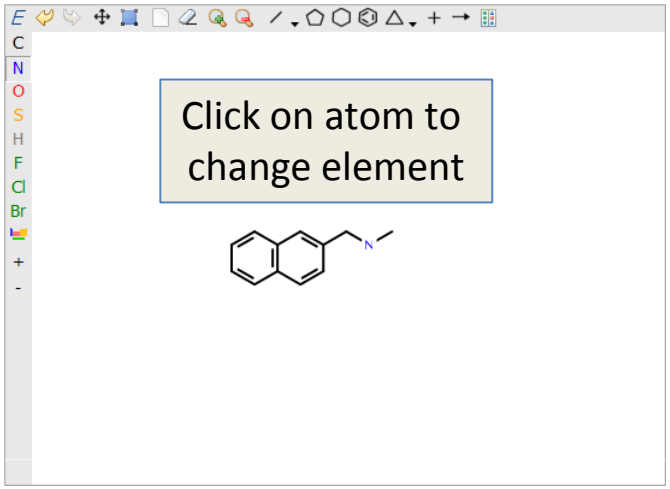
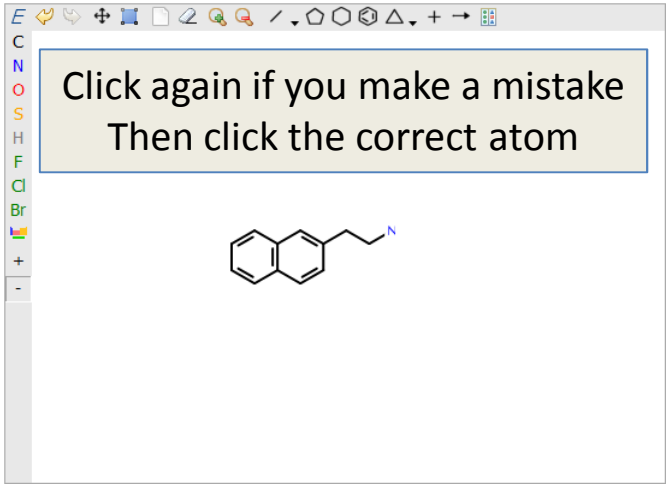
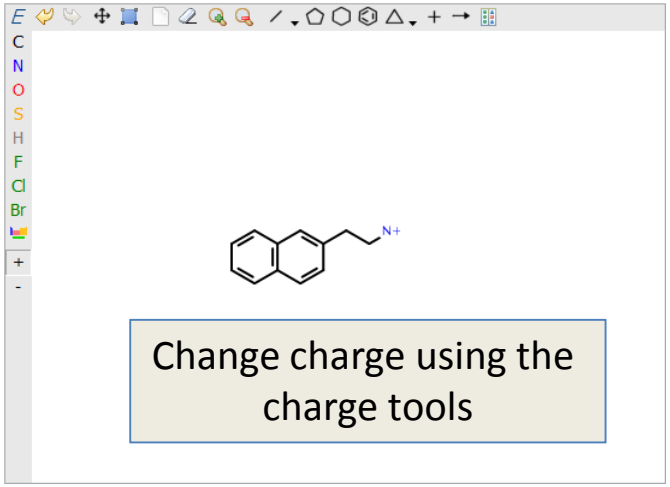
Changing Atoms









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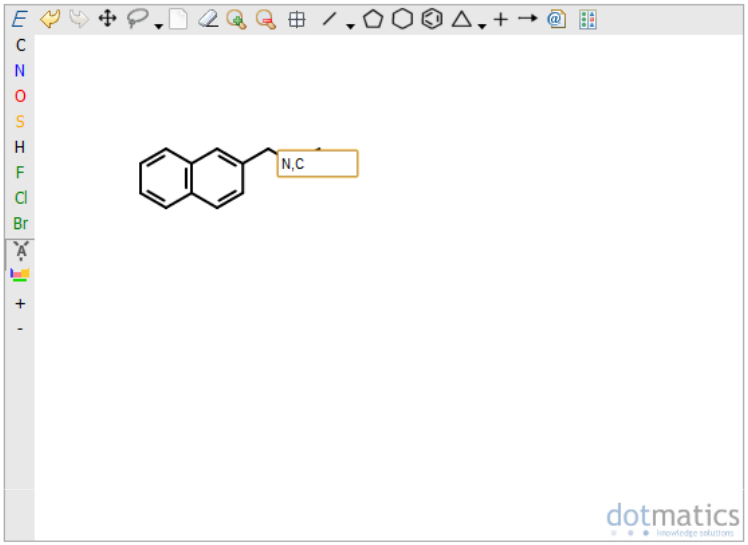
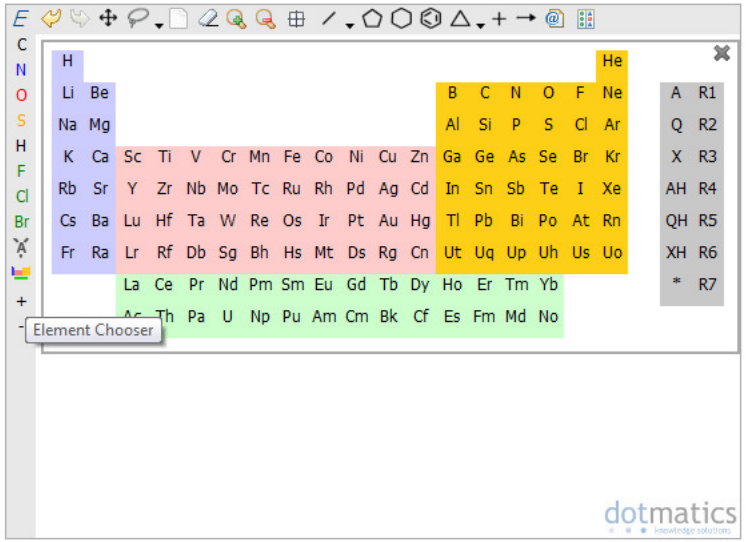
Changing Atoms



Select the ‘Set element’ tool, and cllick 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

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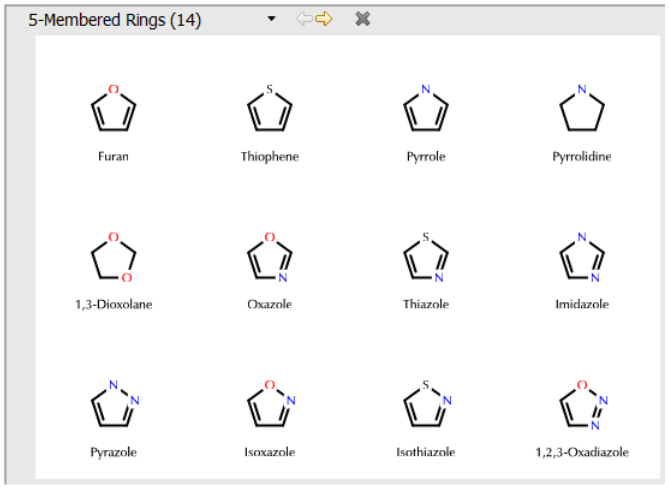
Keyboard short cuts

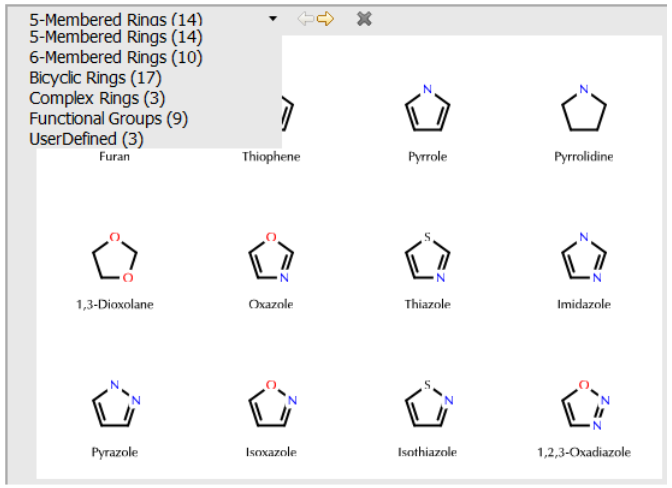
- Many actions can be performed using short cuts.
  - Copy/delete/paste/undo/redo delete using Ctrl-C,-X,-V, -Z,-Y
- After adding a bond, type on the keyboard to change the element of the atom added with the last bond.
  - Also multi-character elements are supported: ‘S’ will turn it into a sulfur, ‘S’ 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.

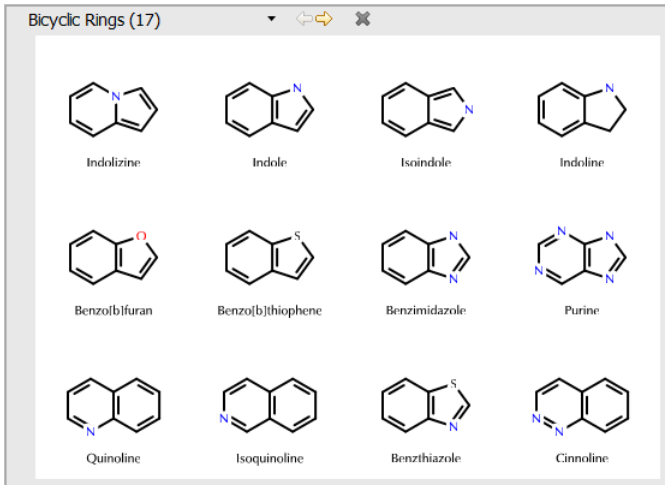
Templates

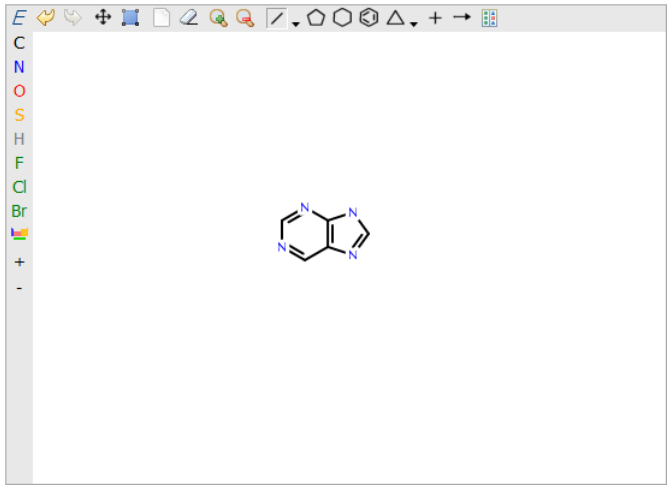
Select template menu



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

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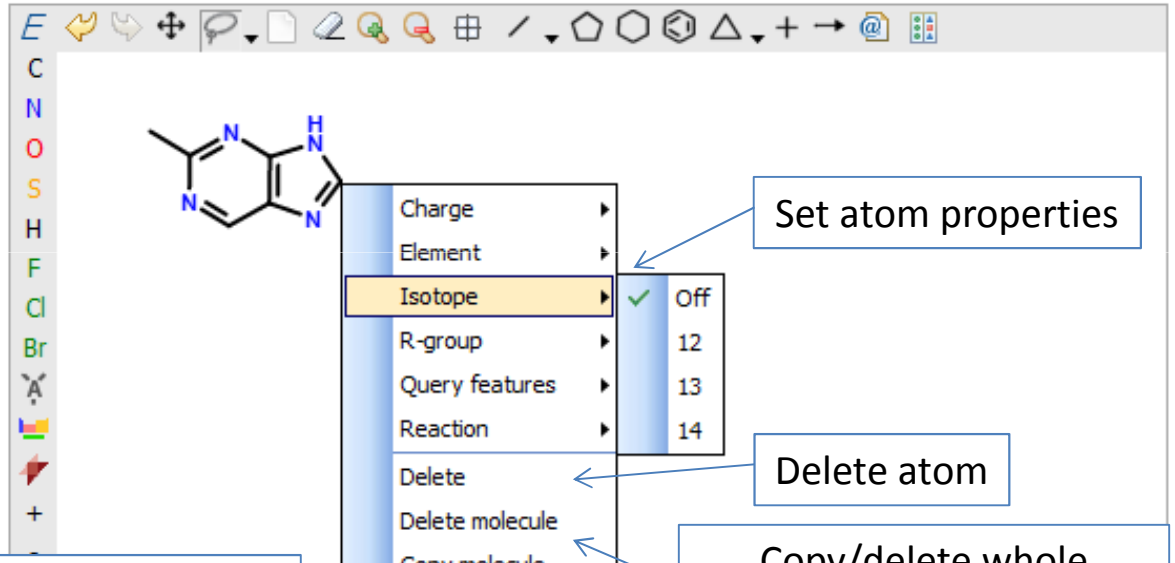
User Defined Templates

- 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:



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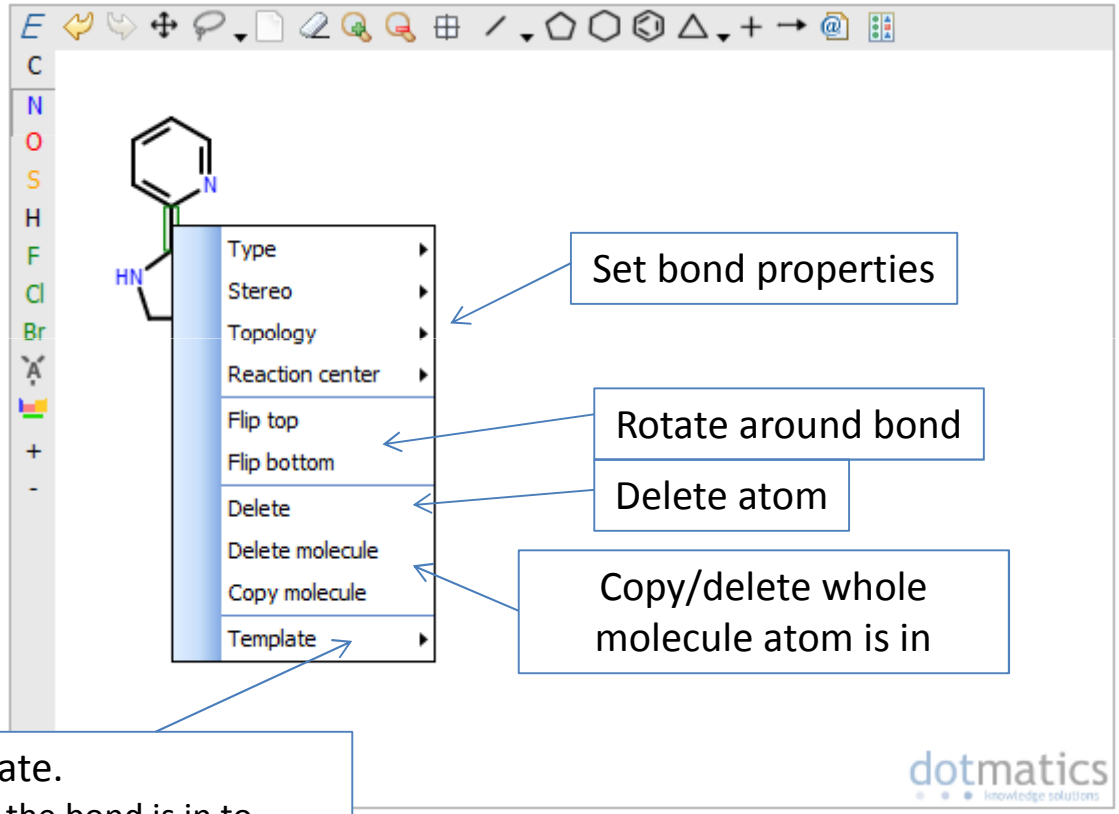
Bond context menu

Right-click on bond:



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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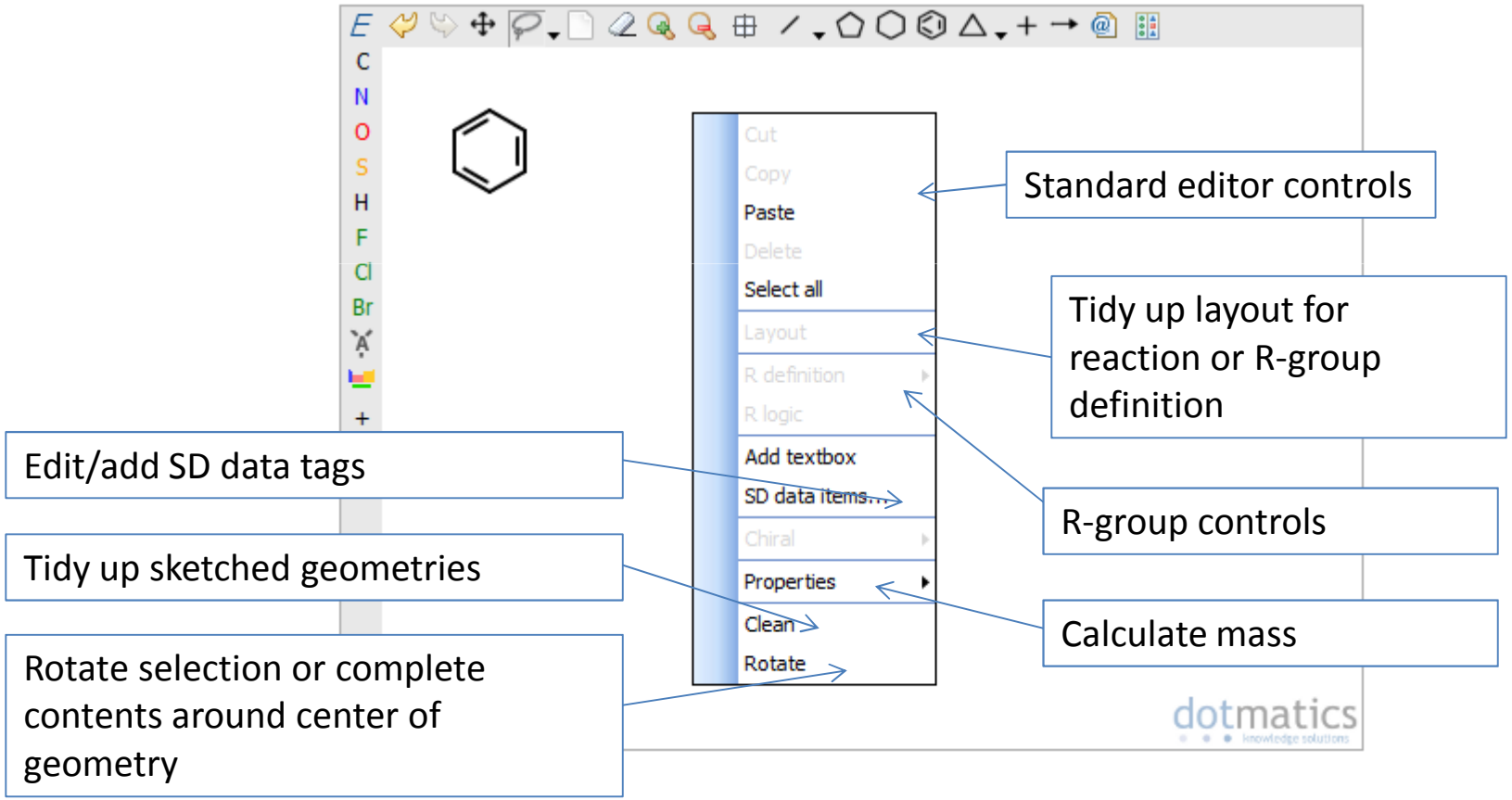
General context menu

Right-click on background:



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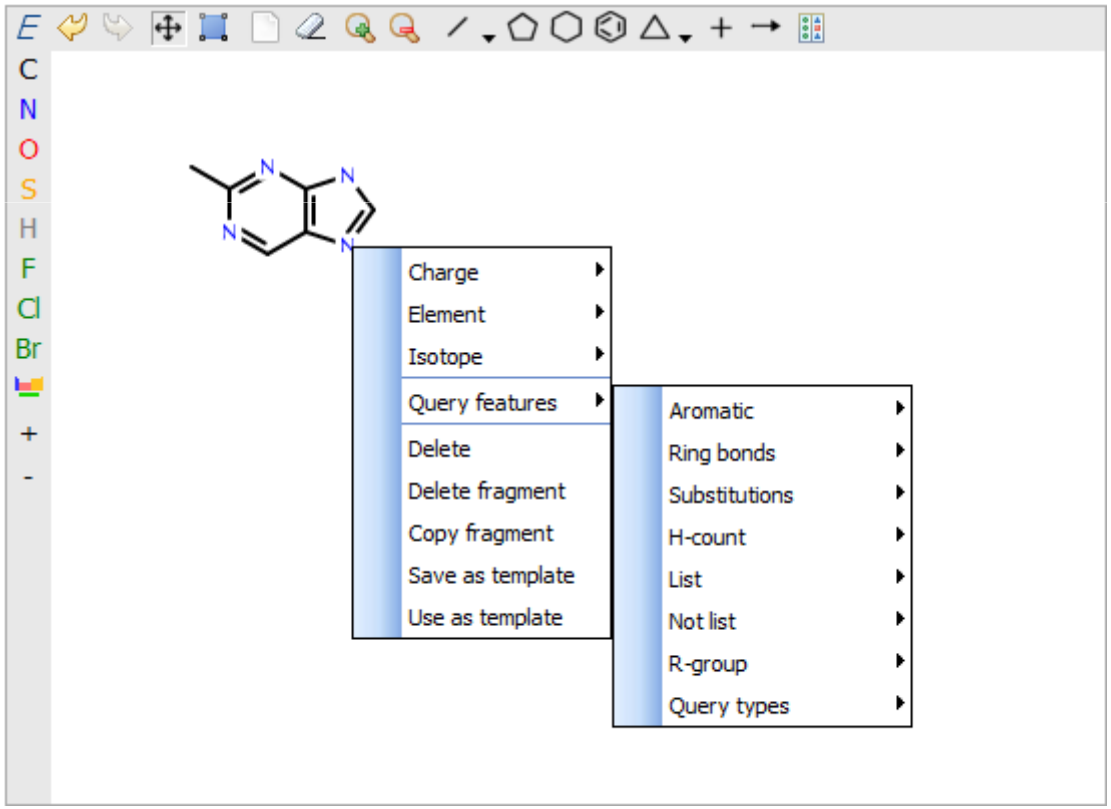
Atom Query Features

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



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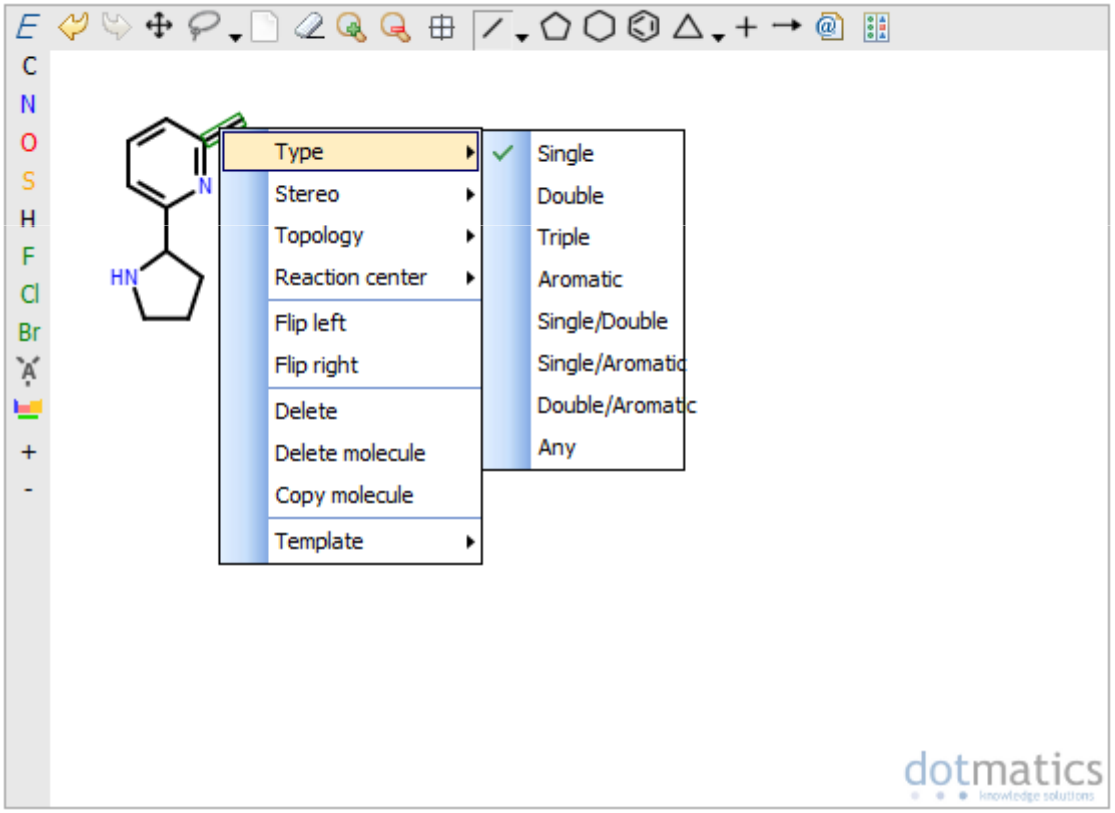
Atom Query Features

- 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



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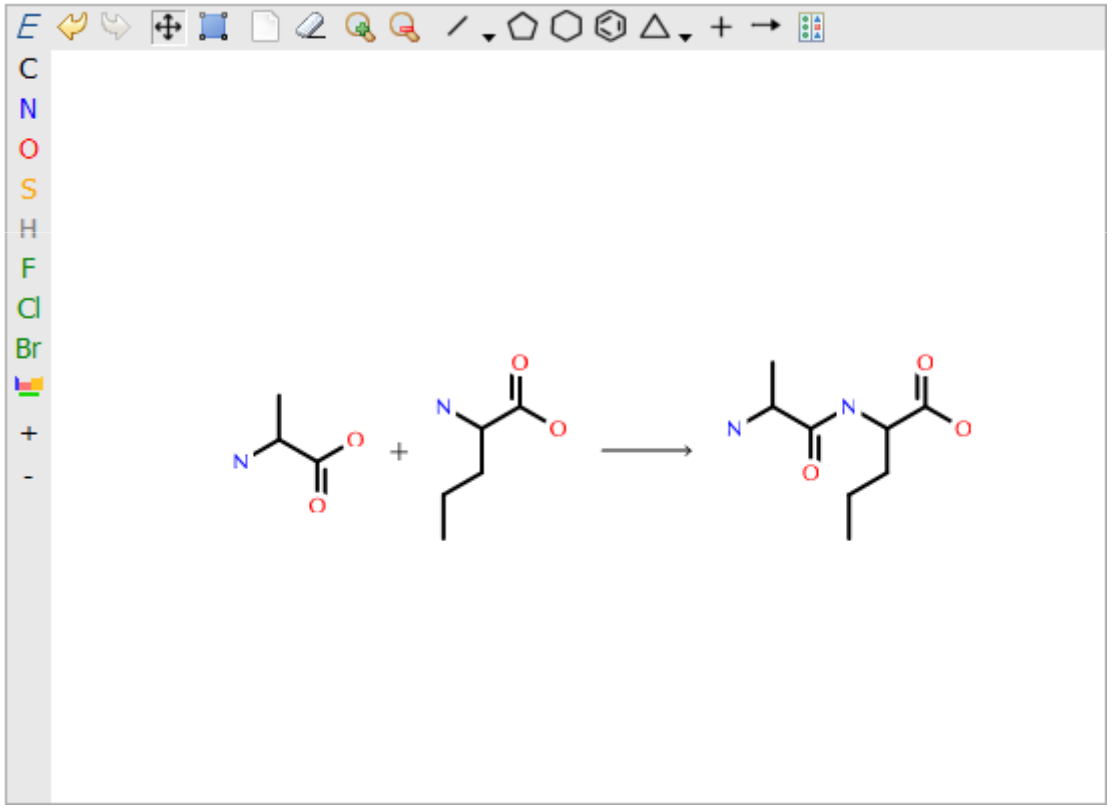
Bond Query Features

- 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 → symbols



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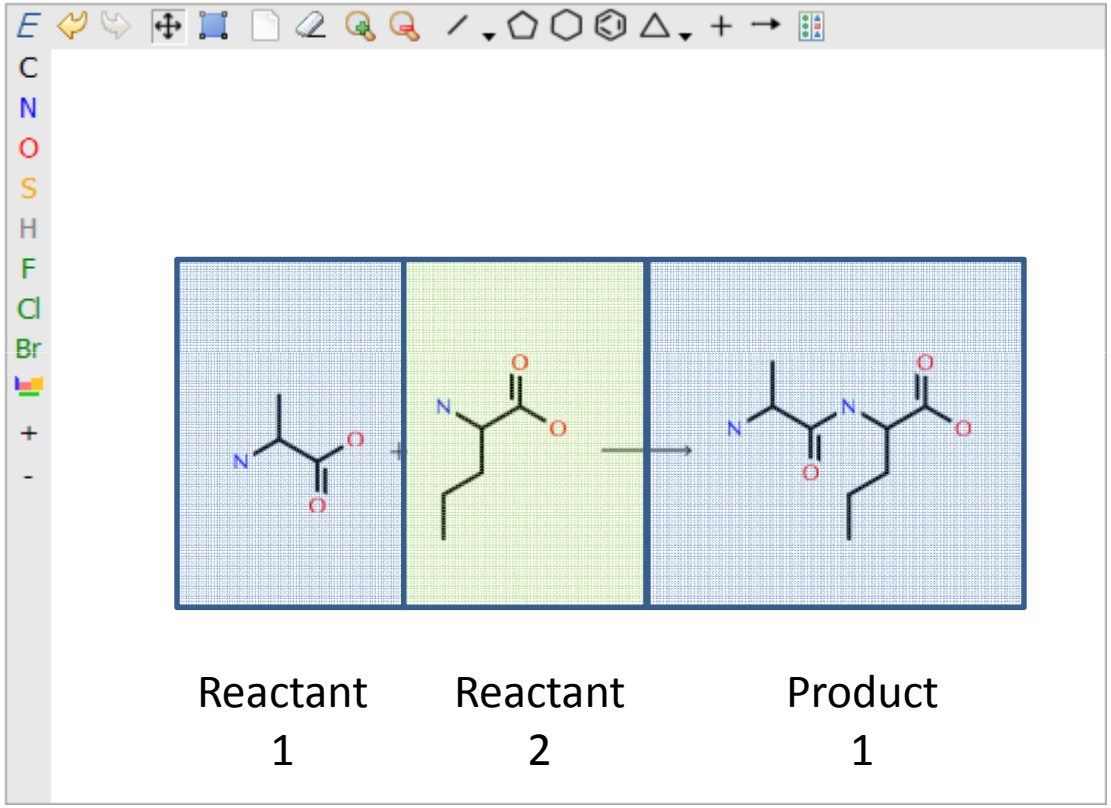
Reaction Perception

- Reactions are split horizontally by + and →



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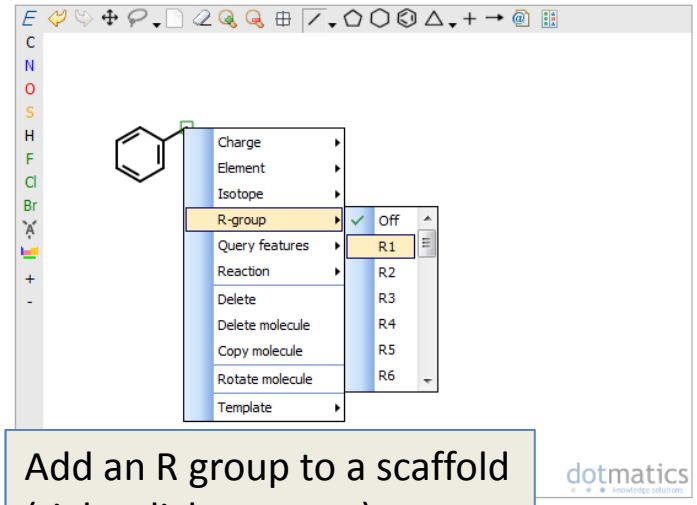
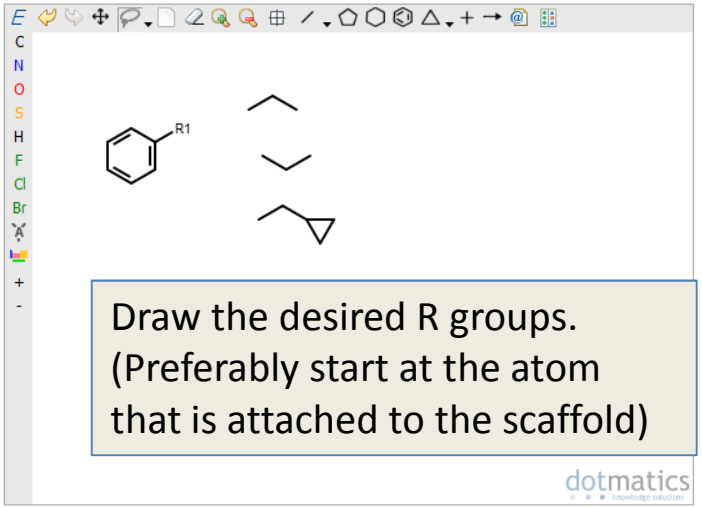
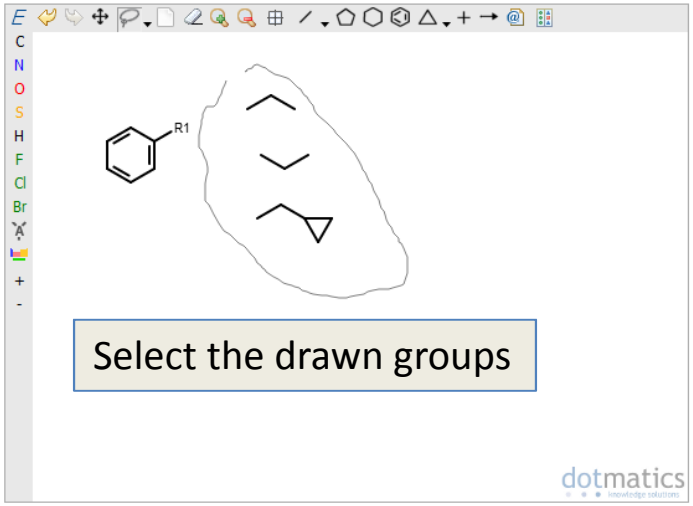
Defining R groups



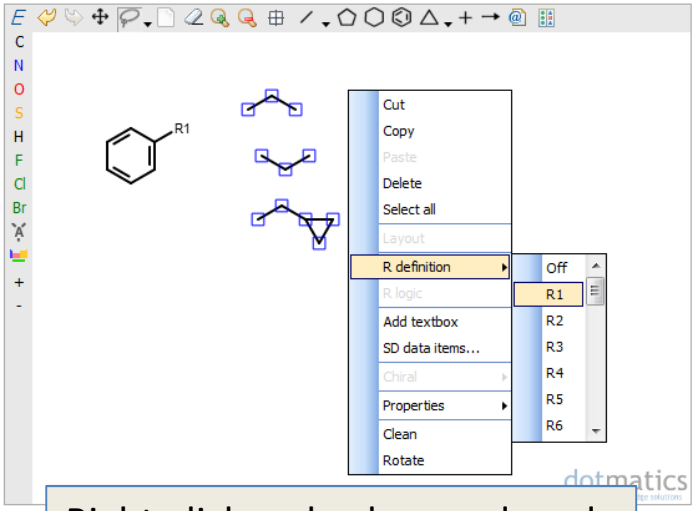
Add an R group to a scaffold (right-click on atom)



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



Select the drawn groups



Right-click on background, and select R definition

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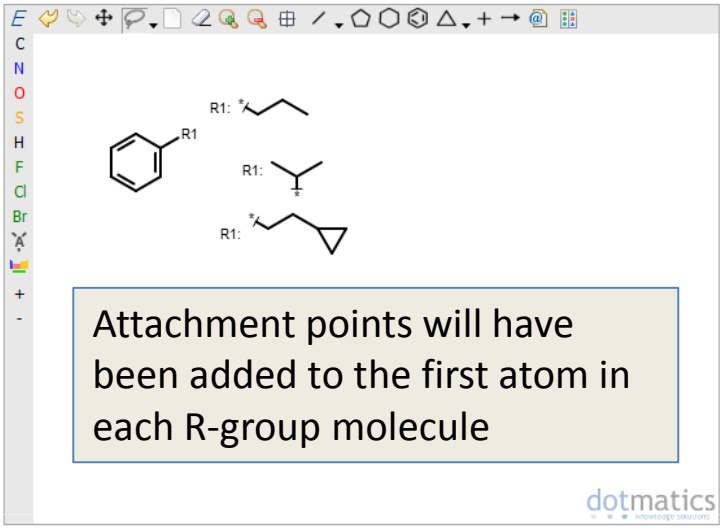
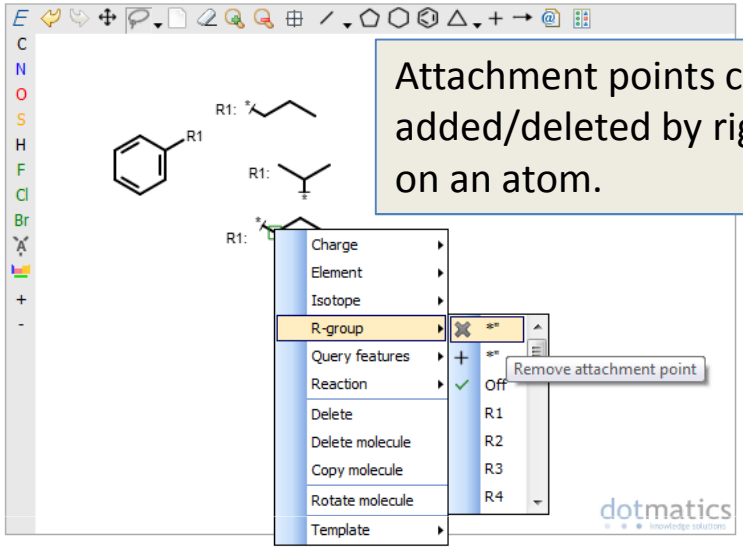
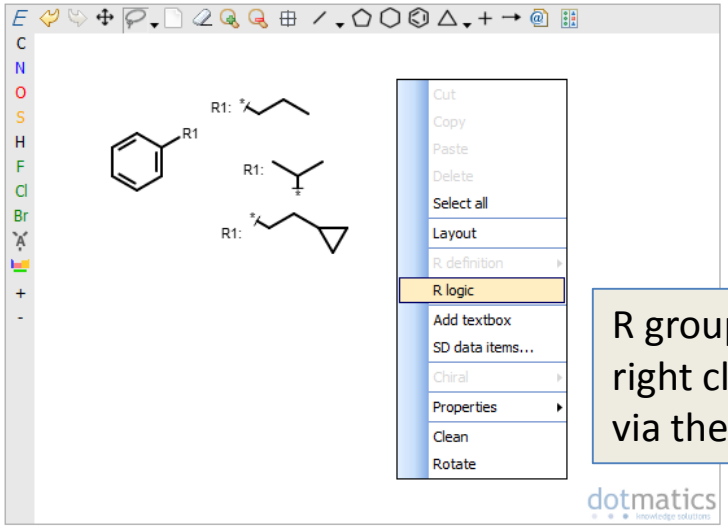
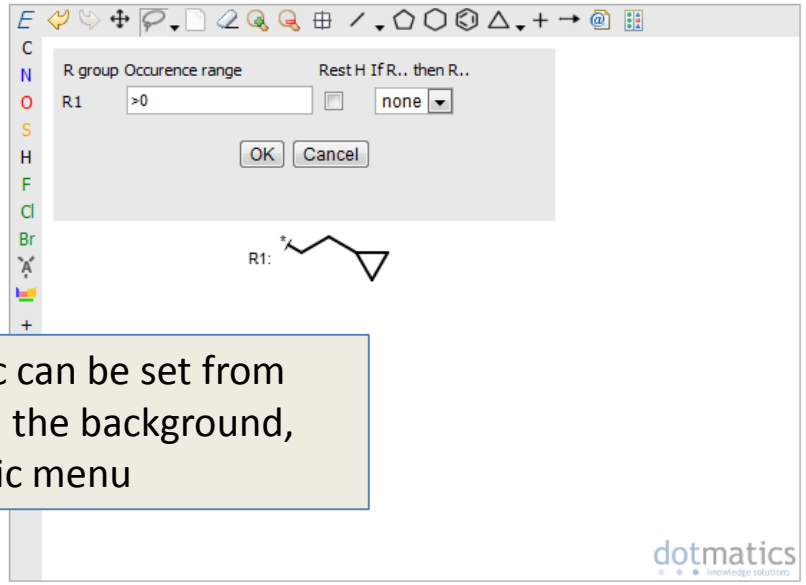
Defining R groups









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