Introduction to ChemDraw JS in Reaxys

Reaxys®

PerkinElmer®
For the Better

What's new in ChemDraw 18.0

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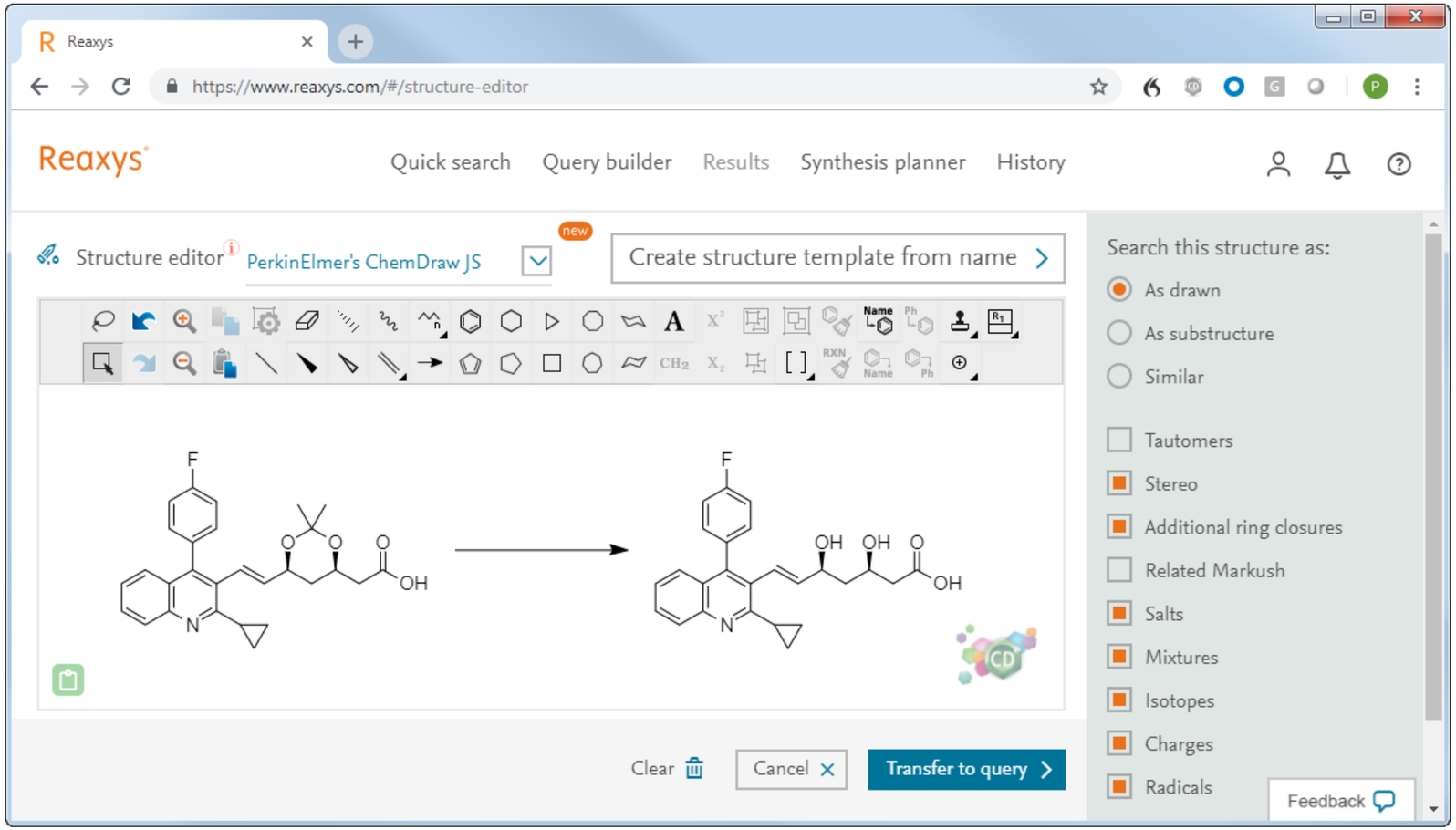
PerkinElmer's partnership with Elsevier in 2018

- PerkinElmer and Elsevier have engaged in a long-term partnership
  - ChemDraw JS as a drawing editor on new Reaxys website (June 2018)



What's in a name ? (that which we call ChemDraw)

- Leading Chemical Research Application for more than 30 years.

- ChemDraw stands for:
  - ✓ Publication-grade Quality
  - ✓ User Friendliness and Ease of Use
  - ✓ Chemical Intelligence

- ChemDraw is the chemical heart and brain of PerkinElmer Informatics solutions

More than ever, ChemDraw 18's chemical intelligence and new integrations, now including Elsevier Reaxys, let scientists spend less time drawing, and focus on what really matters: their Research.

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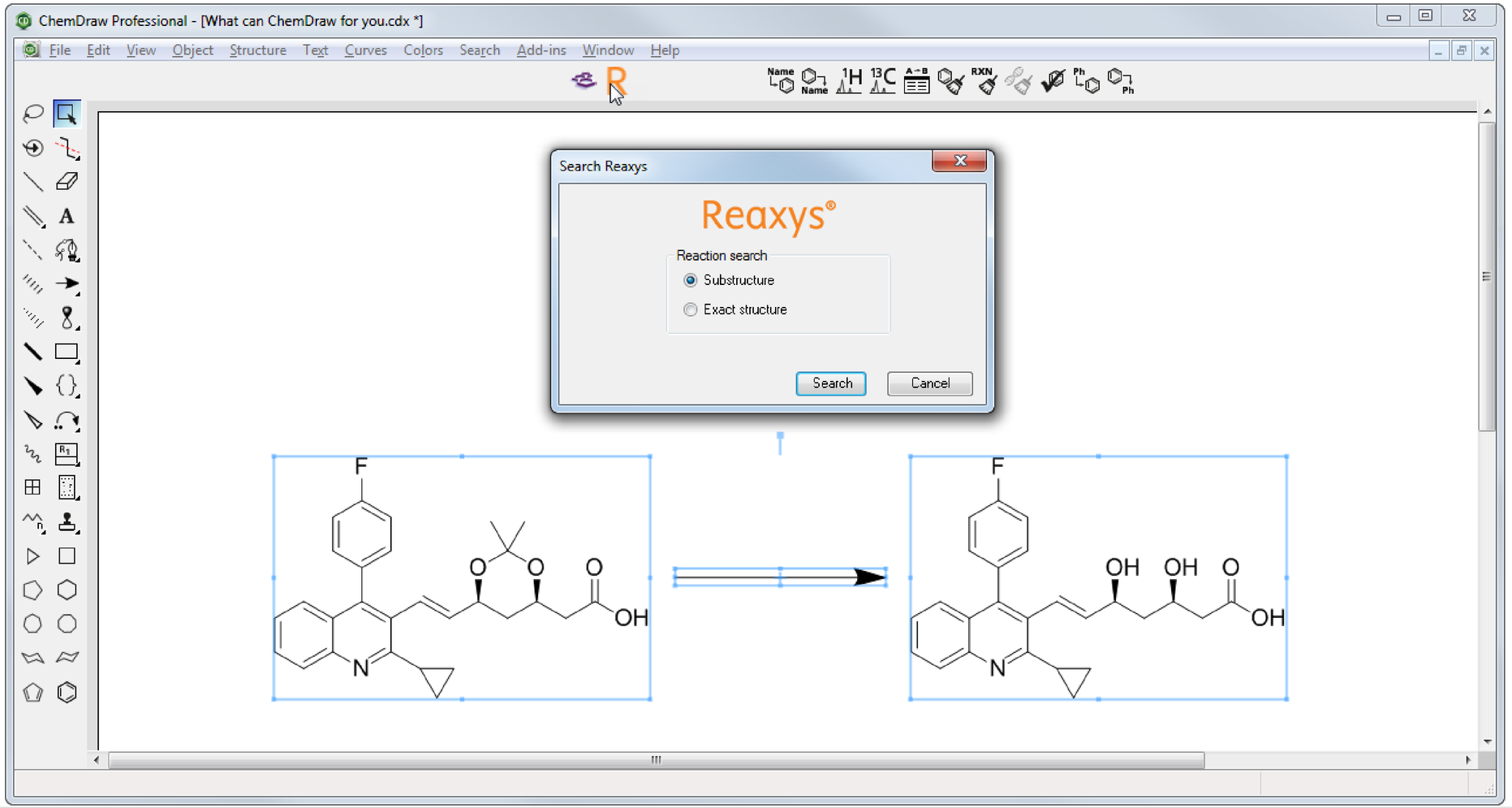
PerkinElmer's partnership with Elsevier in 2018

- ChemDraw 18.0 provides a search integration with Reaxys (Oct 31st 2018)



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ChemDraw JS Basics: Quick selection and duplicates

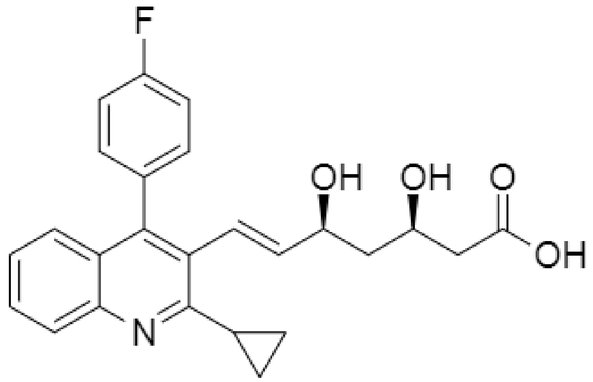
With Marquee tool selected:
Double-click on a molecule to select it

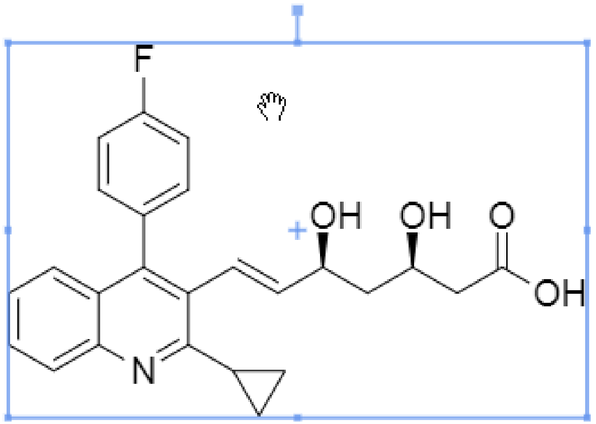
To quickly select several molecules:
hold « **Shift** » and double-click on molecules

While an object is selected:
hold « **Ctrl** » and drag to quickly copy it

While moving an object:
hold « **Shift** » to move in horizontal
or vertical lines

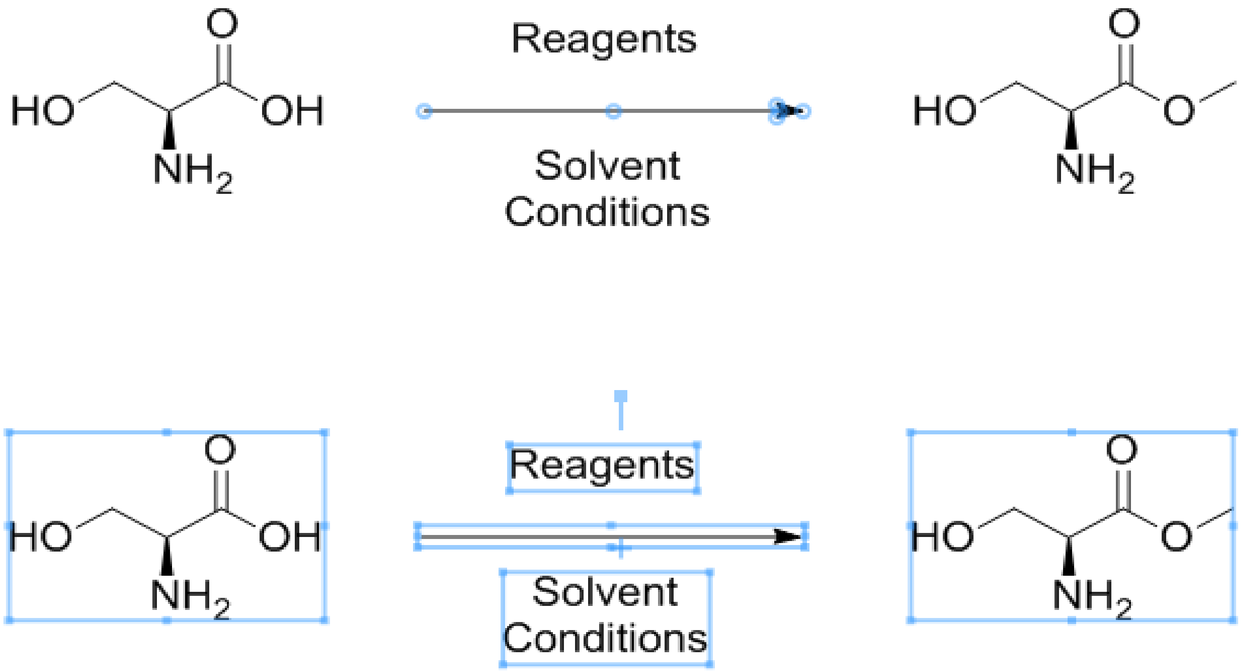
Hold « **Shift** » « **Ctrl** » and drag
to make aligned copies





Reaction selection

Double click on a reaction arrow to quickly select:
Reagents, Reactants, Products and Conditions



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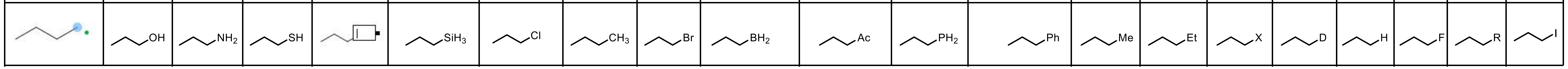
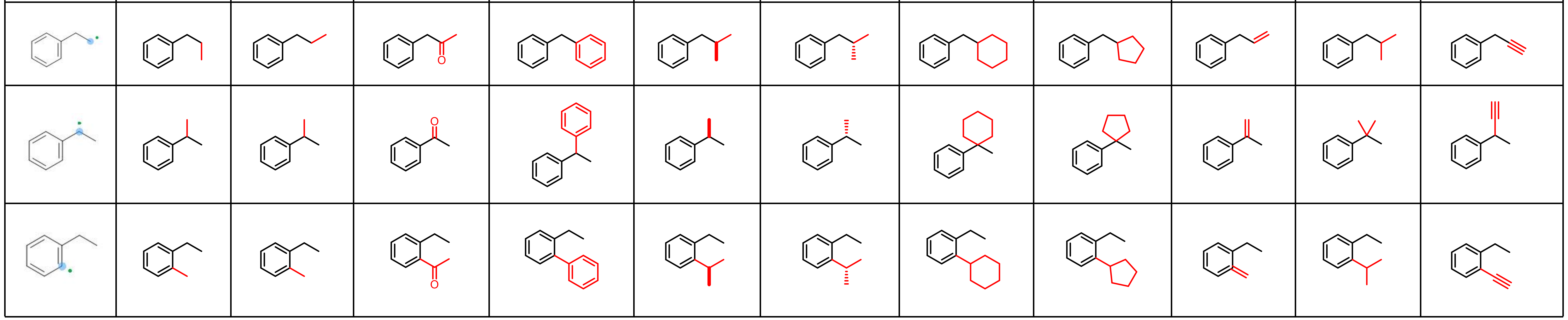
Overview of all hotkeys (touch molecule, move away, and use arrows to navigate)

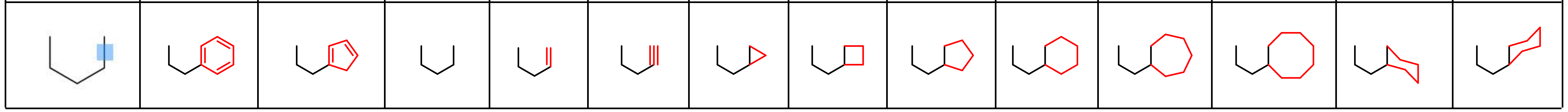
Atom Hotkey	o ; q	n ; w	s	Enter	Shift + s	I or Shift + c	c	b	Shift + b	Shift + a	p	Shift + p	m	e	x	d	h	f	r	i



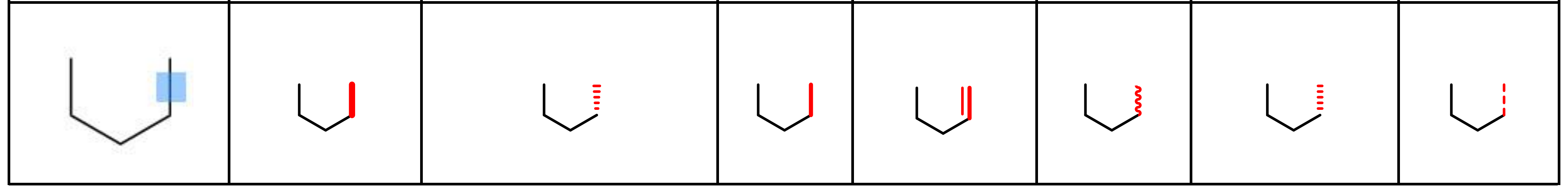
Atom Hotkey	0	1	2	3 ; a	4	5	6	7	8	9	z



Bond Hotkey	a	z	1	2	3	v	4	5	6	7	8	9	0



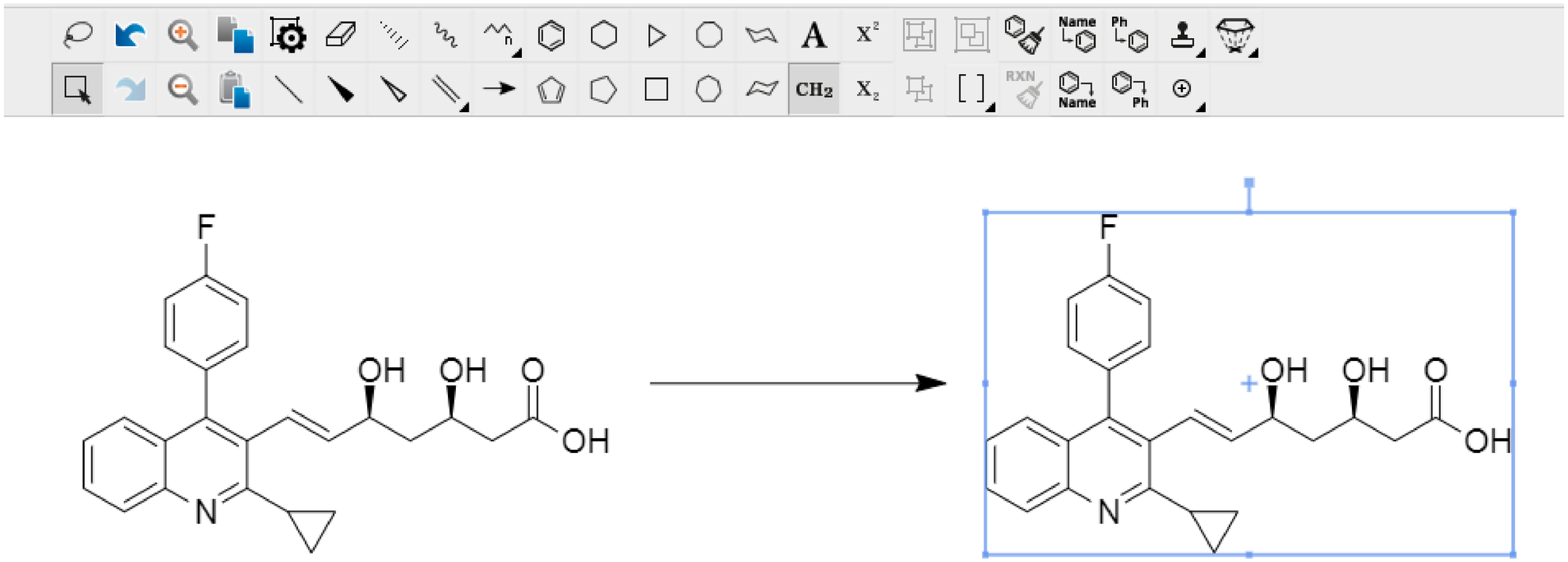
Bond Hotkey	w	h or Shift+w	b	Shift+b	y	Shift+h	d



To increase/decrease charges, hotspot over an atom and press “+/-”as many time as needed

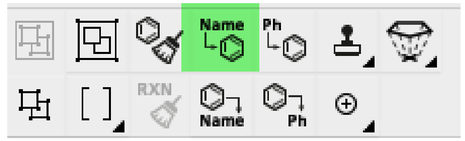
Reaction Shortcut

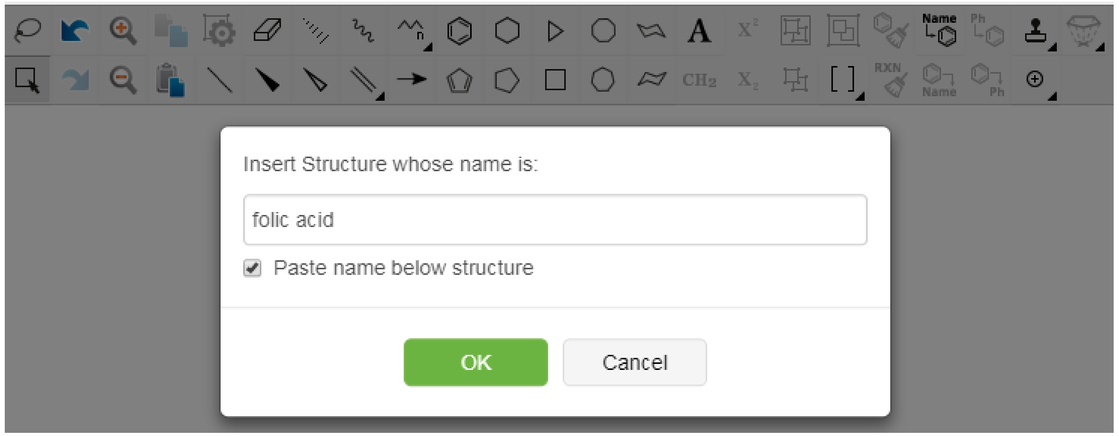
- When you finish drawing a molecule, press “Space” (select), then “Ctrl + → ” **(Keyboard arrows)**

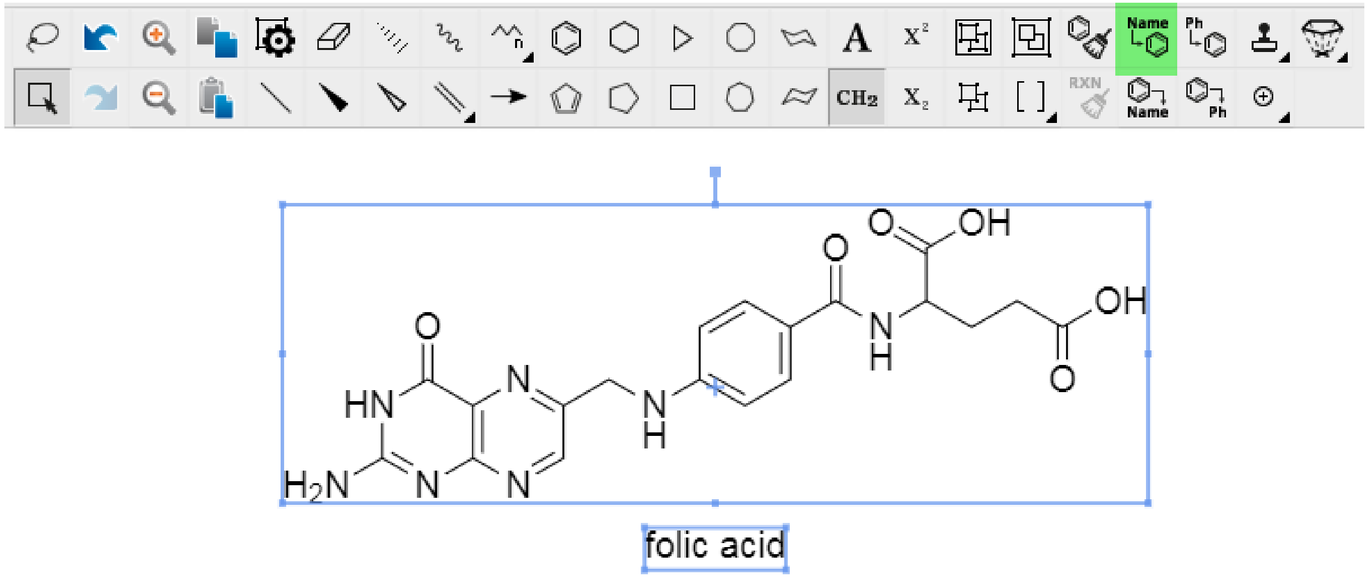


Name-to-Structure (N2S)

- Press the icon to bring up the N2S dialog

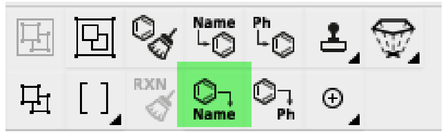


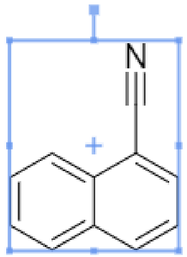




Structure-to-Name (S2N)

- Select Molecule, then press « Ctrl+Alt+N » or press





1-naphthonitrile

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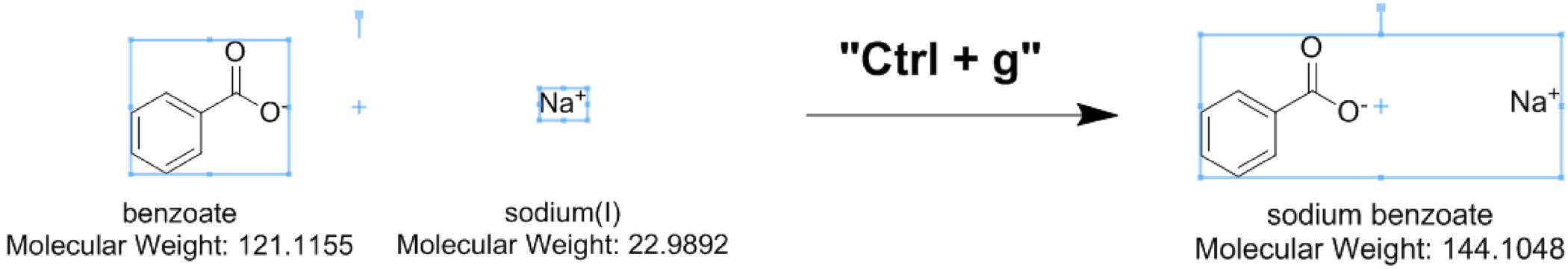
Grouping / Ungrouping (for salts)



Ctrl + g to group

Ctrl + Shift + G to ungroup

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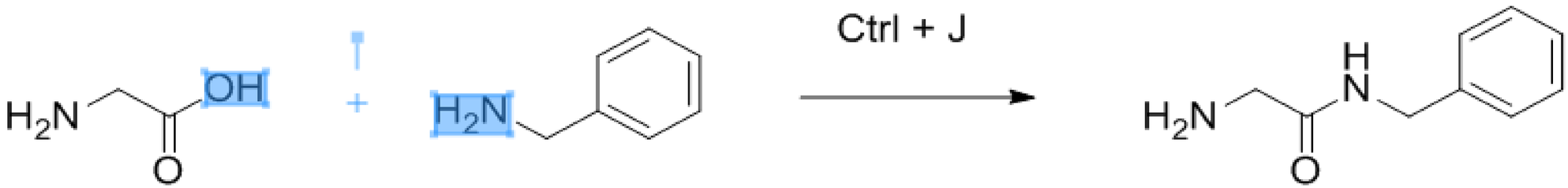
Joining shortcut: Ctrl + J (there is no icon)

Join molecules together: select two atoms/bonds on different molecules

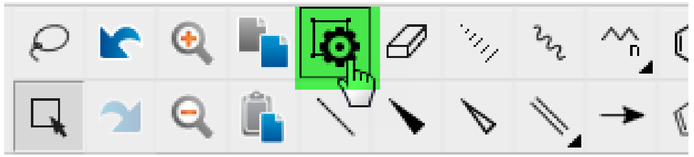
Click on one, hold « **Shift** », click on the second one, then press « **Ctrl + j** », first atom does not move



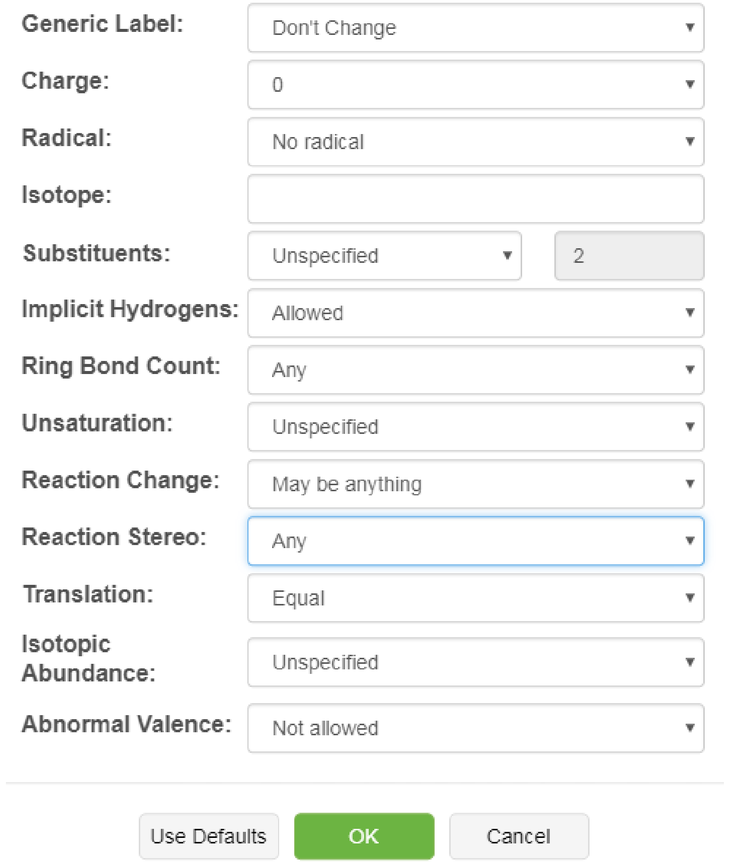
Works with 2 Bonds as well

Atom and Bond Properties
(Reaxys labels, # of Susbtituents, Reacting sites etc.)

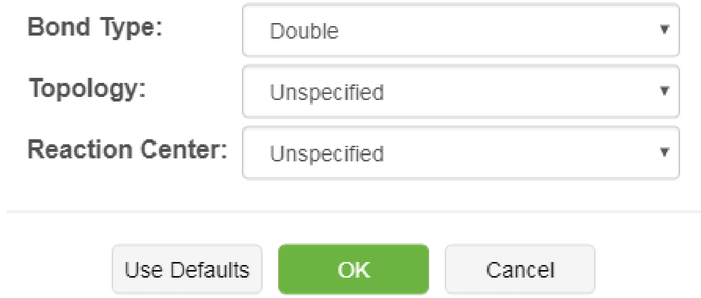
- While an atom or a bond is active press « / » or



Atom Properties

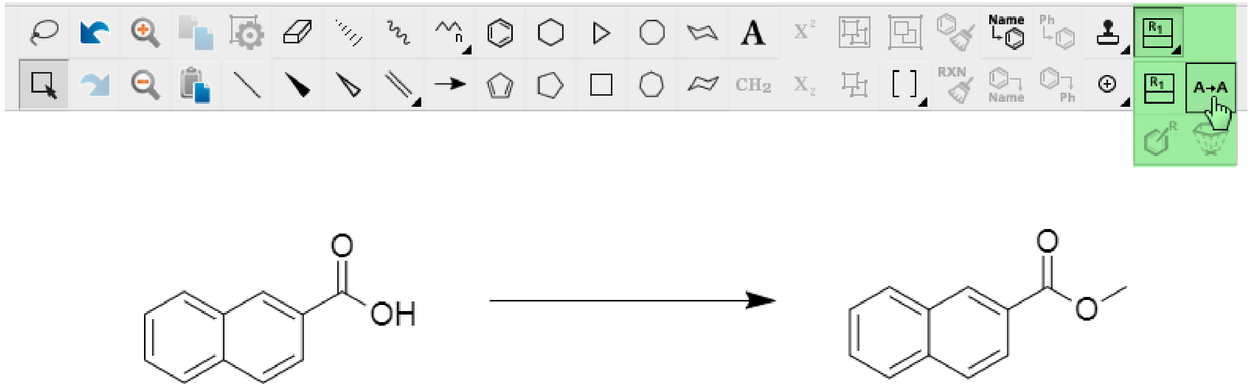


Bond Properties

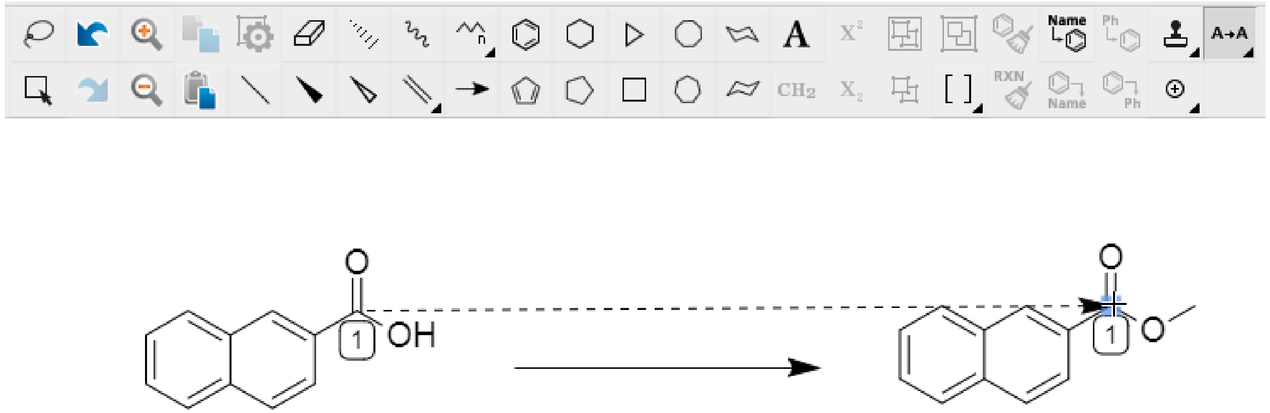


Manually Map Reaction

- Hold Left click Down on tool to reveal sub-menu

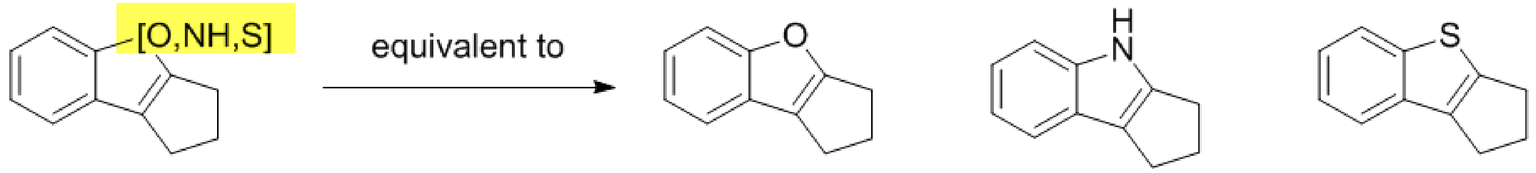


- Click and drag between atoms on reactant and product. Repeat as needed

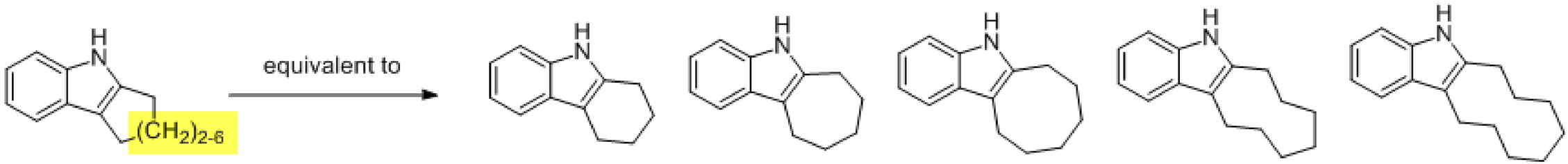


Atom/Label lists, Ranges of Repeating Units

Atom/Nickname lists are entered as labels between brackets, separated with commas
They can be single atomic elements, but also labels and nicknames



Single repeating units between parentheses followed by a range of numbers: 2-6



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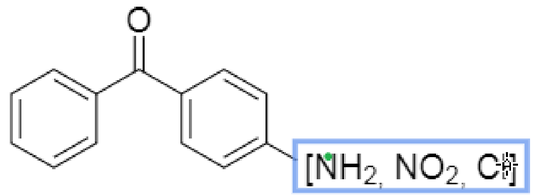
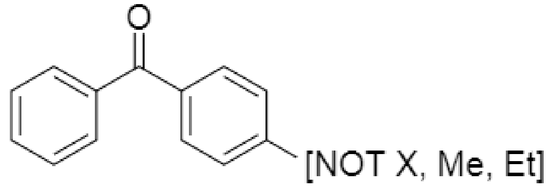
Atom/Label lists

- Use Text Tool or Press « Enter » over an atom to start the text tool, « Enter » again to close it
- Insert groups between brackets, separated by commas
- Generic groups like « X » for halogens are understood
- Logical operator « NOT » is understood





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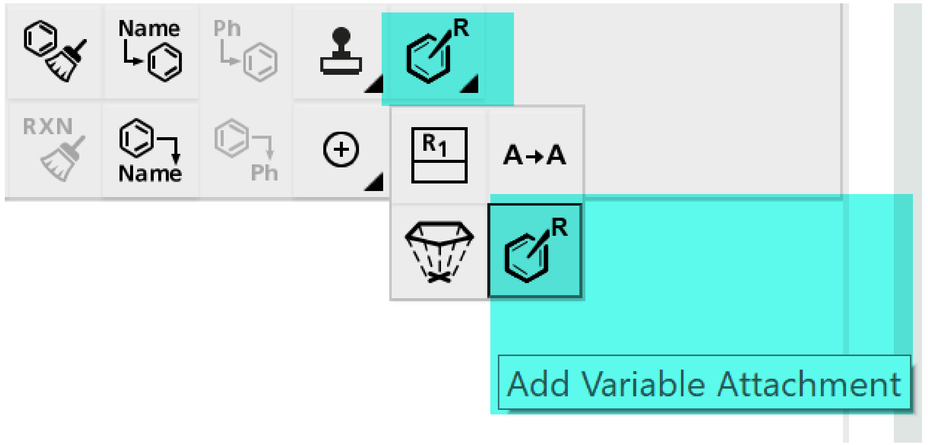
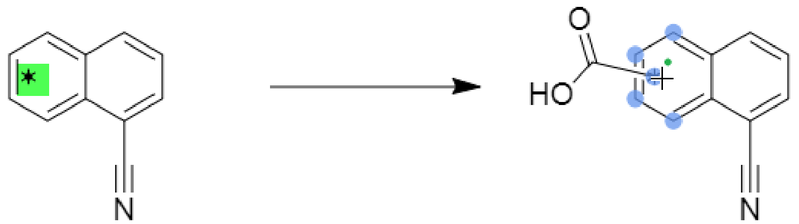
Variable Attachments

- Select multiple atoms (hold **Shift** while clicking for additive selection)
- Click on the Var. Attachement Icon
- An asterisk will appear
- Draw a bond from it with the C-C Bond tool



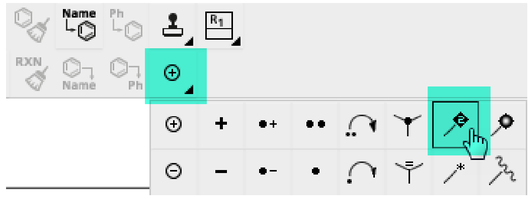


R-group lists (one connection)

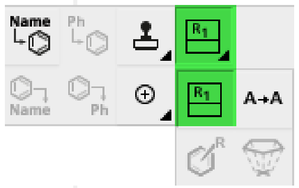
Use R-group tool to draw a table, and add components inside

Use the Text tool or Press « Enter » to type $R_{1\text{-}n}$

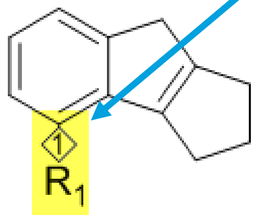
Define connecting point by pressing « . » (dot) or use attachment point tool

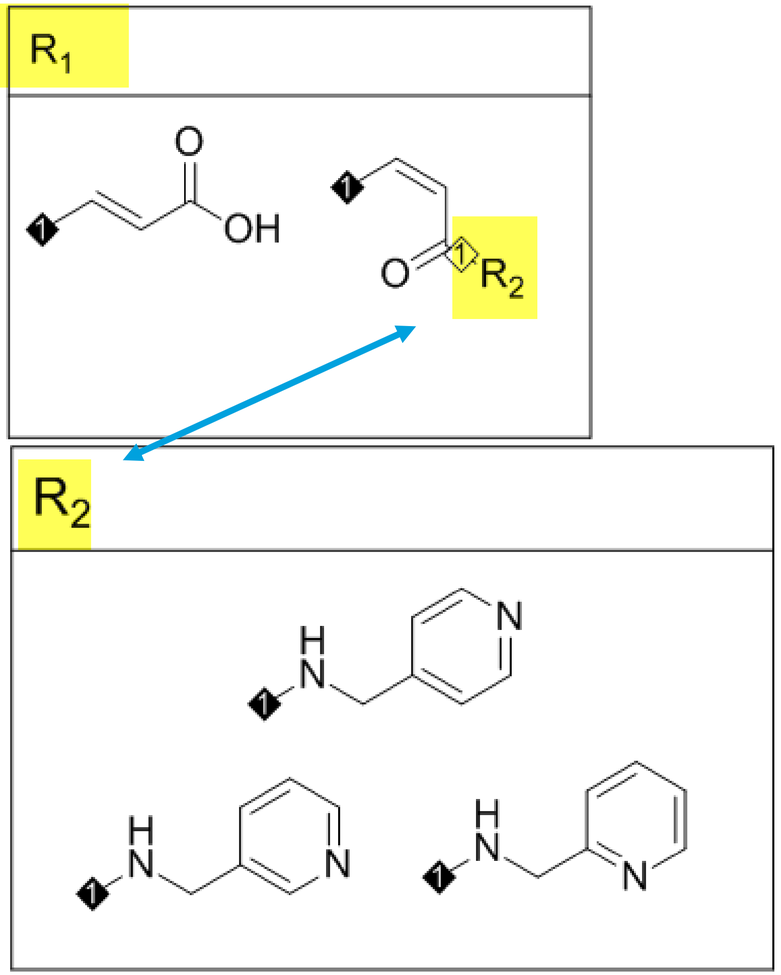


The generic label on the molecule **must match** the label in the table (R_1 and R_2 here). If they match, white squares with corresponding numbers will automatically appear



MUST MATCH





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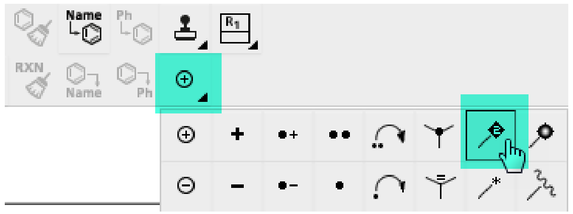
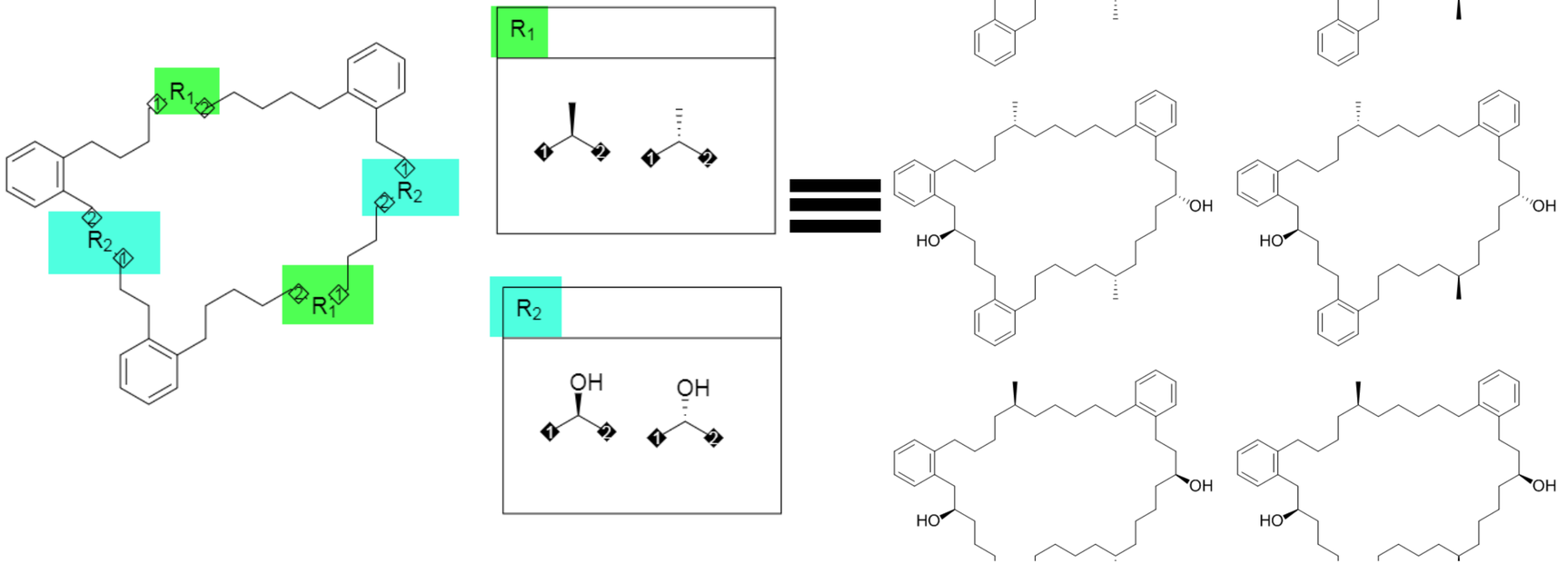
R-group lists (2 or more connections)

Use the Text tool
or
Press « Enter » to type $R_{1\text{-}n}$

For each component, define connecting point
by pressing « . »
Or
use **attachment point tool**





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