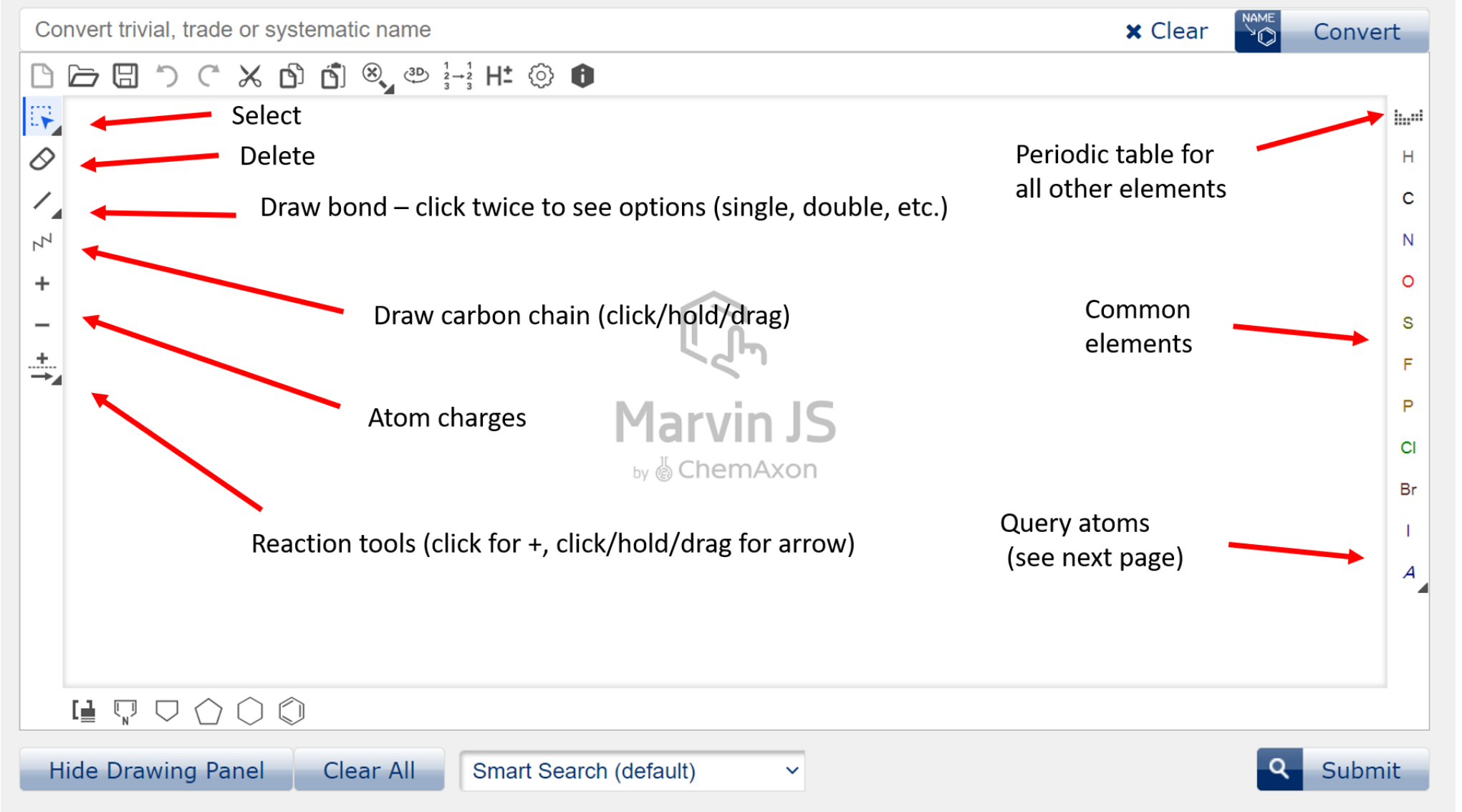
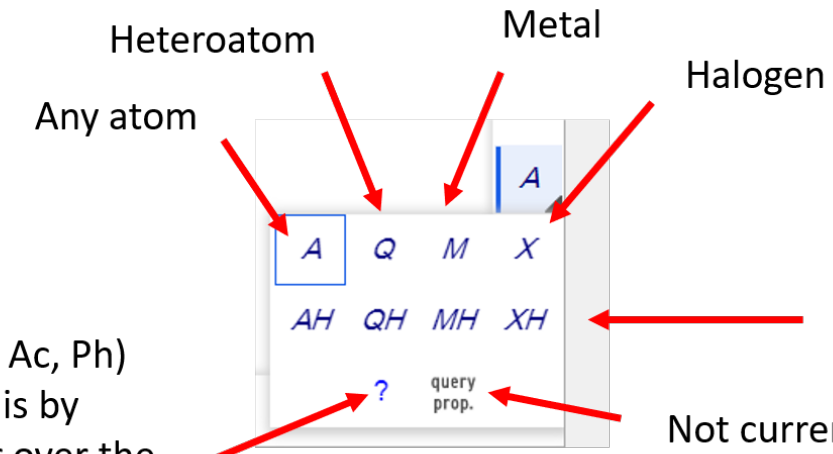
Structure and Reaction Searching in Science of Synthesis

Cheat Sheet


Convert trivial, trade or systematic name
Clear
NAME
Convert
Select
Delete
Draw bond – click twice to see options (single, double, etc.)
Draw carbon chain (click/hold/drag)
Atom charges
Reaction tools (click for +, click/hold/drag for arrow)
Periodic table for all other elements
Common elements
Query atoms (see next page)
H
C
N
O
S
F
P
Cl
Br
I
A
Marvin JS
by ChemAxon
Hide Drawing Panel
Clear All
Smart Search (default)
Submit

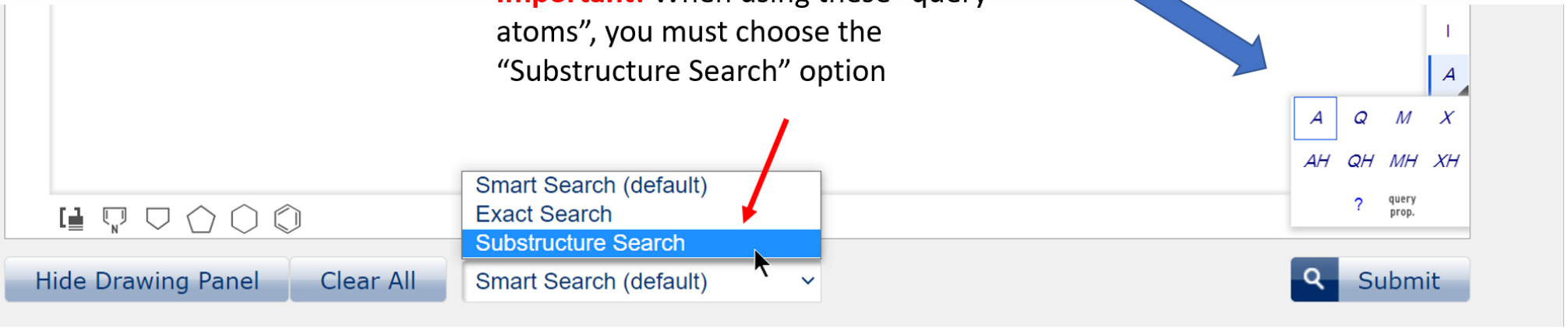


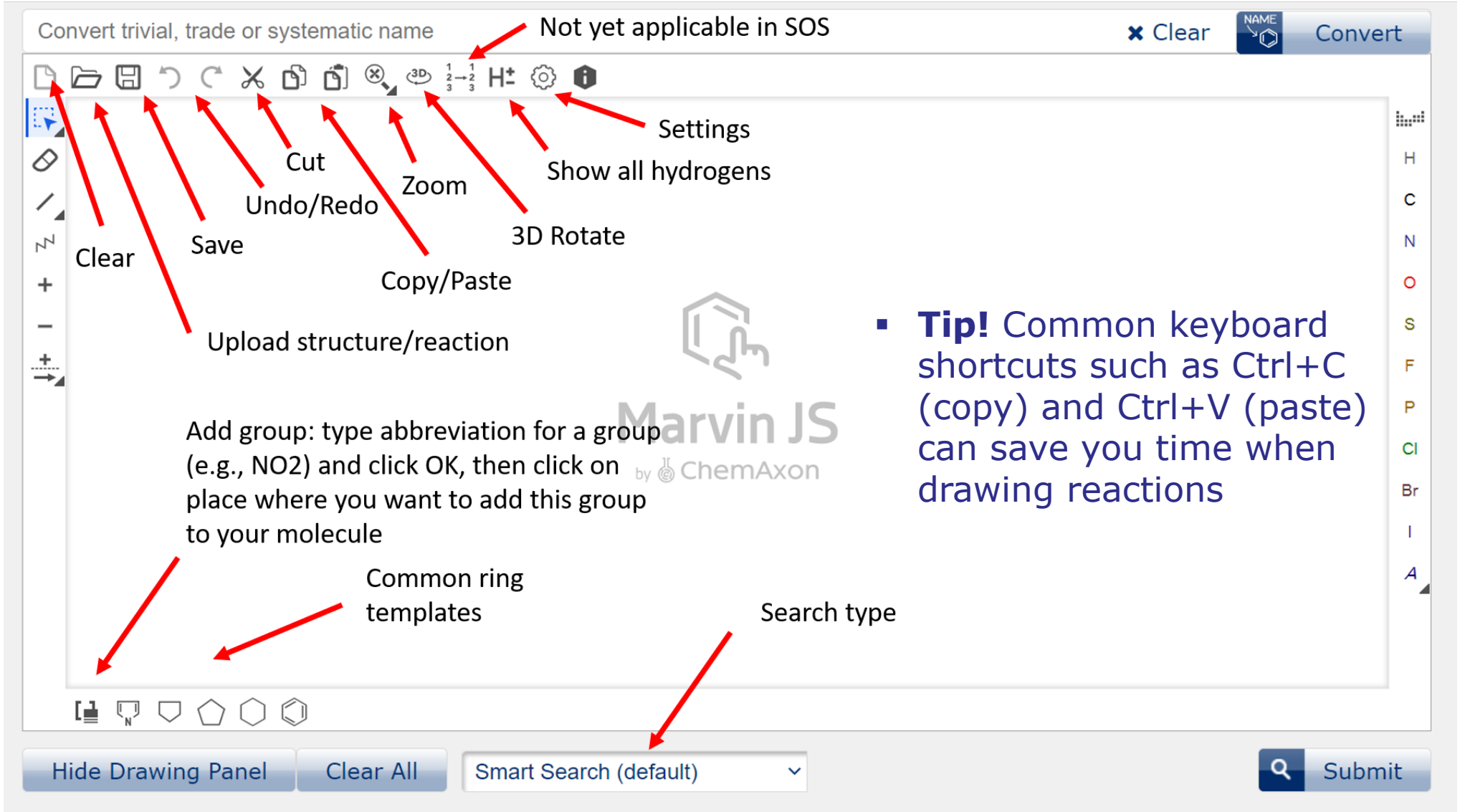
Any heteroatom/metal/halogen OR hydrogen

Add groups (e.g., NO_2, Ac, Ph)
Tip: you can also do this by pointing mouse cursor over the place where you want to add the group and typing the group abbreviation (case sensitive)

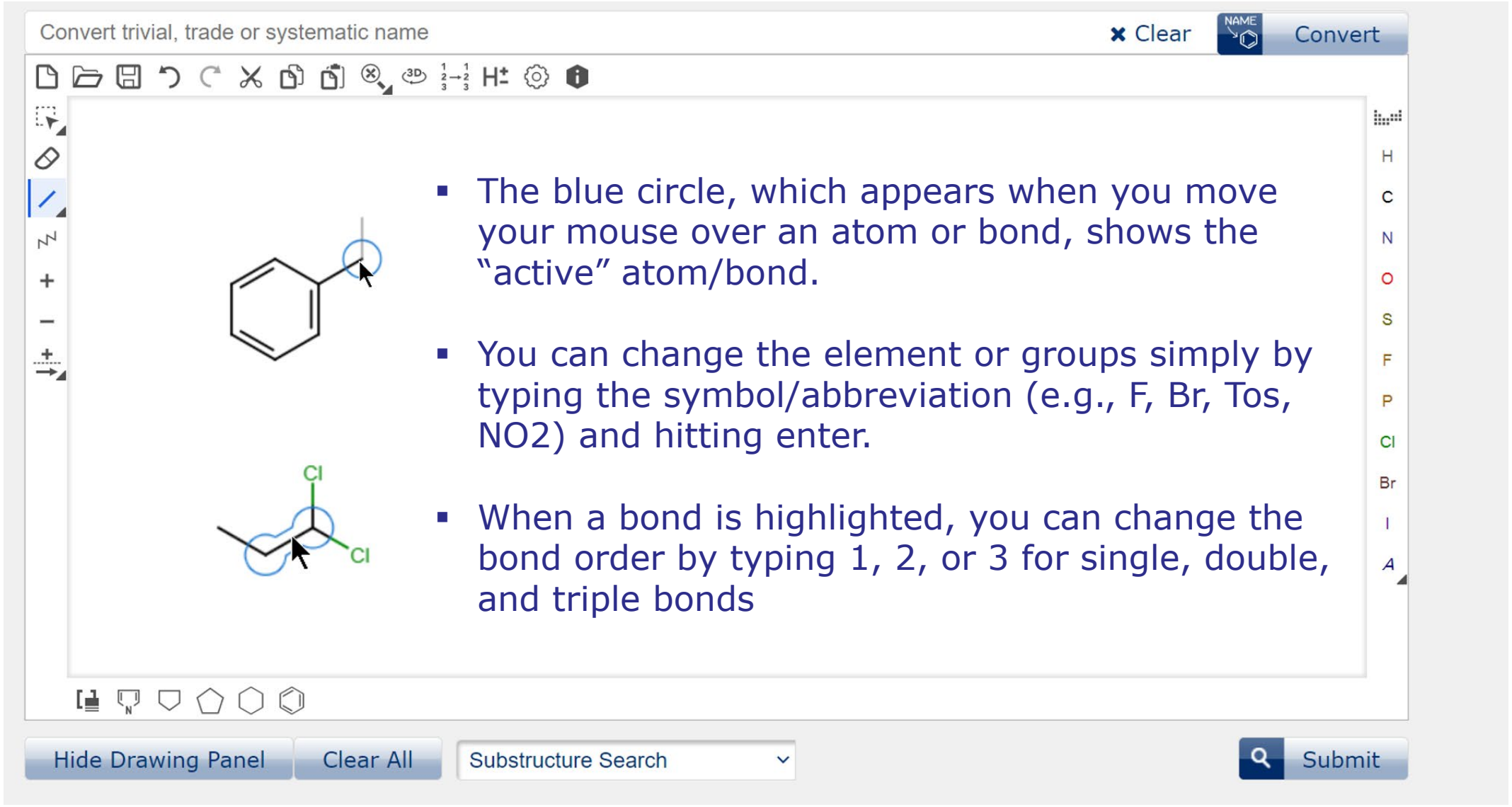
Not currently applicable in SOS

Important! When using these "query atoms", you must choose the "Substructure Search" option

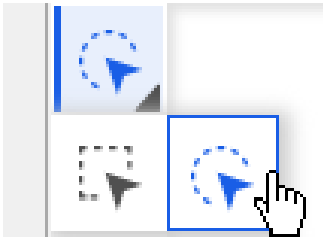


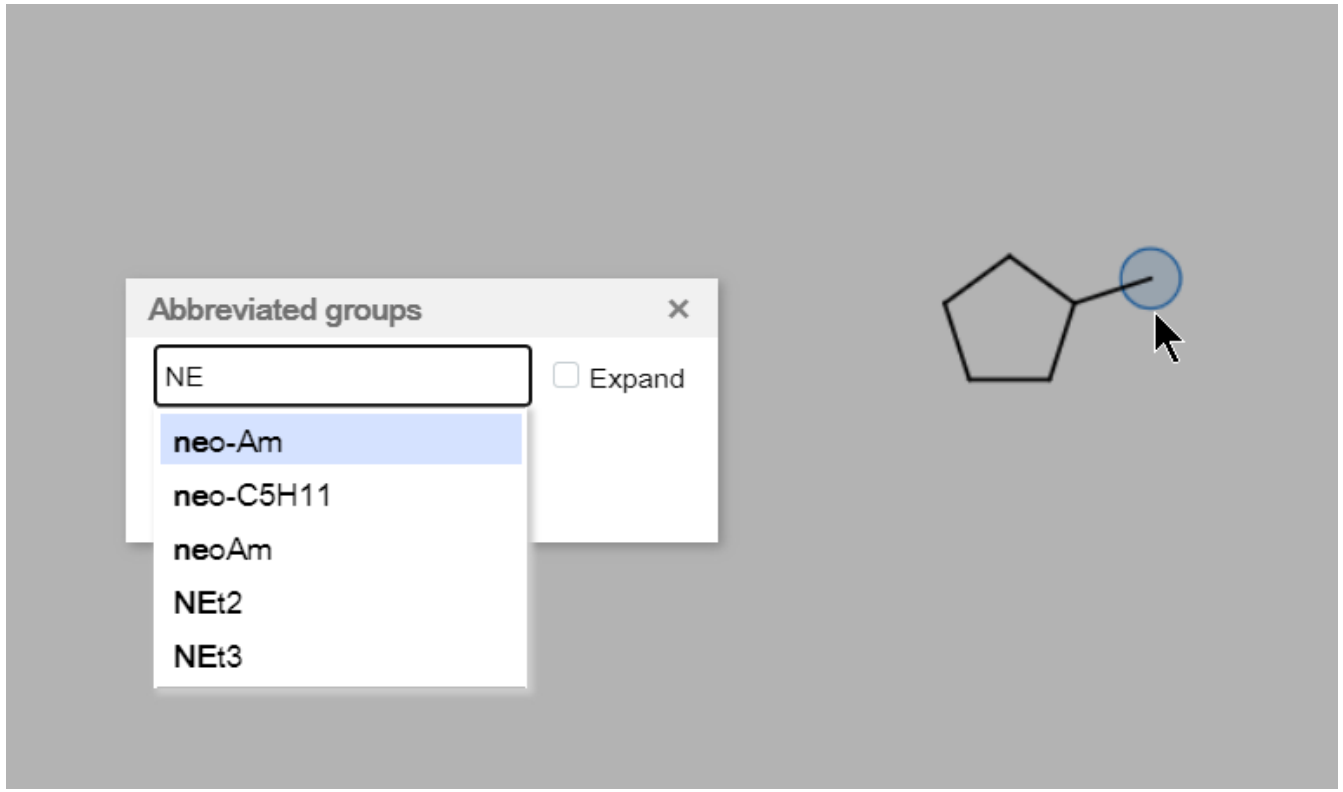


- **Tip!** Common keyboard shortcuts such as Ctrl+C (copy) and Ctrl+V (paste) can save you time when drawing reactions

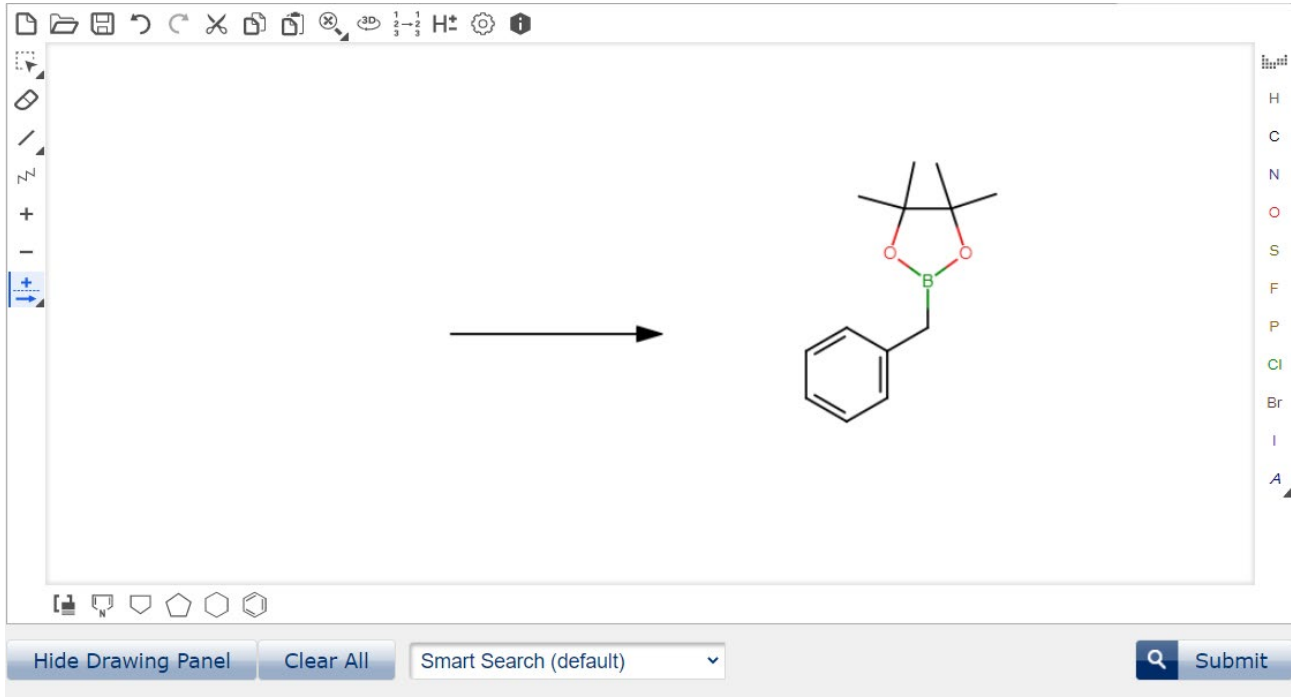


- The blue circle, which appears when you move your mouse over an atom or bond, shows the "active" atom/bond.
- You can change the element or groups simply by typing the symbol/abbreviation (e.g., F, Br, Tos, NO2) and hitting enter.
- When a bond is highlighted, you can change the bond order by typing 1, 2, or 3 for single, double, and triple bonds

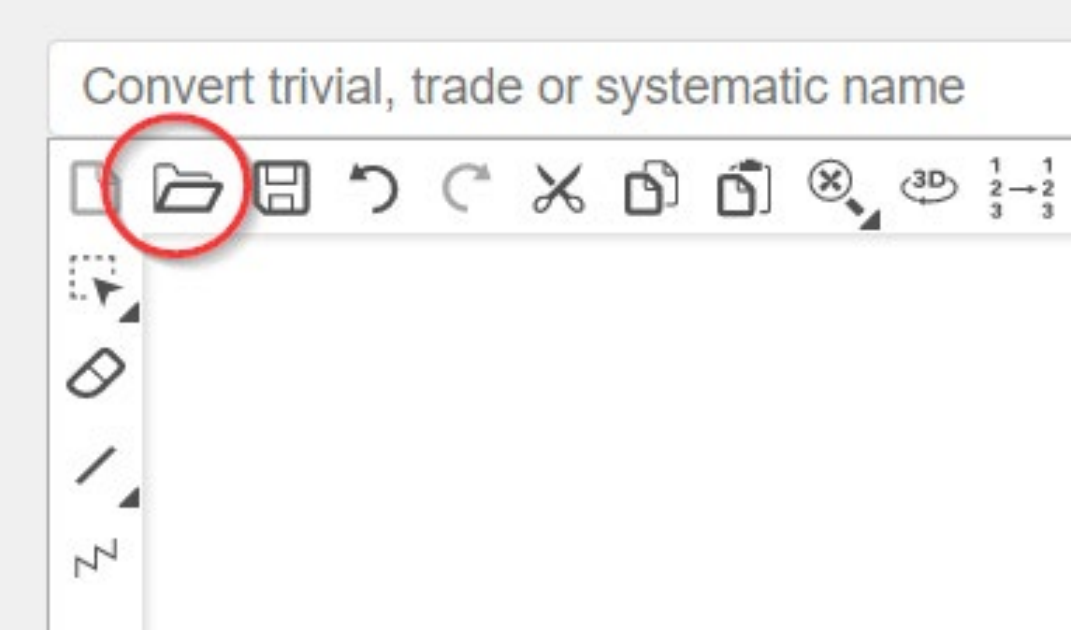




- When an atom is selected with the select tool, you get a shaded blue circle. Then, hitting space brings up a window allowing you to select abbreviations from suggestions in “as you type” list



- Use “half reactions” to prefilter the results with the drawn molecule as a product (or starting material, if the molecule is drawn before the arrow)



- Select the molecule/reaction in ChemDraw
- In the “Edit” menu of ChemDraw, choose “Copy As” then “SMILES” (or just use ALT+CTRL+C)
- In SOS, click once in the drawing panel, then hit CTRL+V (NOTE: Using right mouse click then “paste” does not work)
- You can also upload saved cdx files (and many other chemical information file formats, e.g., MOL, SMILES, InChI) using the upload function (circled below)

tamoxifen 1.

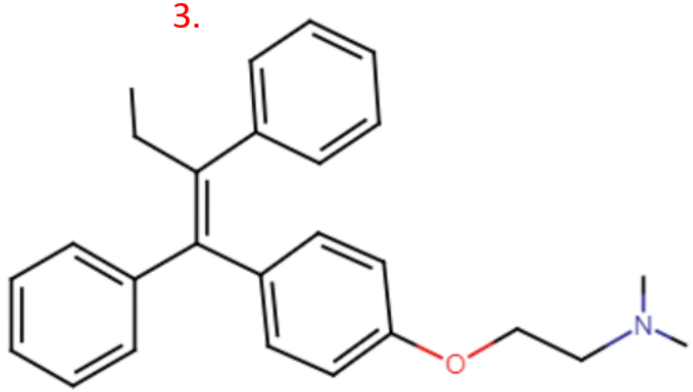
Clear | NAME Convert

2.

Want to save time drawing a complex structure?

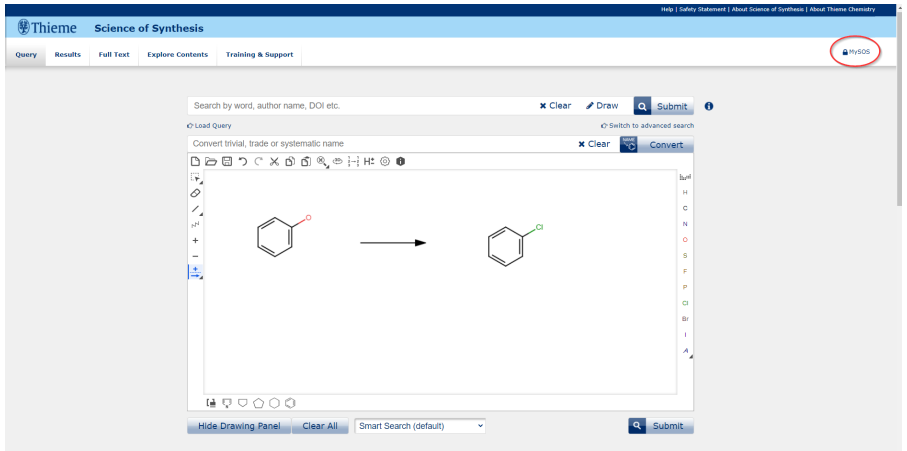
1. Type the name in the bar at the top of the drawing window
2. Click “Convert”
3. The structure appears so you can modify it or directly do a structure search

3.

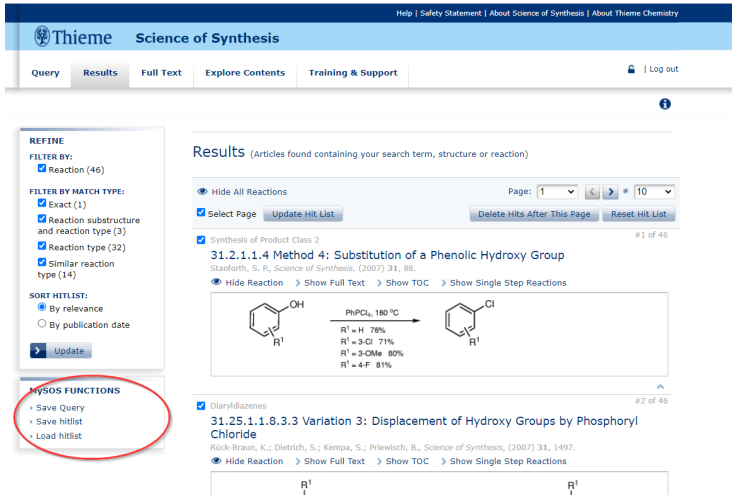


Hide Drawing Panel | Clear All | Substructure Search | Submit

- Keep it simple! Focus on the transformation you want to achieve and only include relevant functionality
- When using query atoms (A, X, M, etc.) remember to select the “Substructure Search” option
- If you get too many hits, try limiting your search by adding a relevant keyword to the text search bar (e.g., “hydrogenation”, “palladium”)
- Use of atom mapping is not necessary – the search engine will automatically identify the difference between starting material and product.
- For π-bonded organometallics we recommend a text search or browsing the table of contents



- Register for MySOS to be able to save your searches (or hitlists) so you can repeat and/modify them later



- When logged in to my SOS, the save query/hitlist options appear on the Results page after doing a search

Exporting Searches

- You can save/export your structure or reaction in many common formats (e.g., MOL, SMILES, cdx, InChI) using the save function