







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)

 $\frac{1}{2} \rightarrow \frac{1}{3}$ $\frac{1}{2} \rightarrow \frac{2}{3}$ H^+  

Marvin JS
by ChemAxon

Hide Drawing Panel Clear All Smart Search (default) Submit

Heteroatom Metal Halogen

Any atom

Add groups (e.g., NO₂, 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)

A	Q	M	X
AH	QH	MH	XH
?	query prop.		

Any heteroatom/metal/halogen OR hydrogen

Not currently applicable in SOS

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

Smart Search (default)
Exact Search
Substructure Search
Smart Search (default)

Hide Drawing Panel Clear All

A	Q	M	X
AH	QH	MH	XH
?	query prop.		

Submit

Convert trivial, trade or systematic name Not yet applicable in SOS ✕ Clear NAME Convert

Clear Save Undo/Redo Cut Copy/Paste Zoom 3D Rotate Settings Show all hydrogens

Upload structure/reaction

Add group: type abbreviation for a group (e.g., NO₂) and click OK, then click on place where you want to add this group to your molecule

Common ring templates


Search type


Hide Drawing Panel Clear All Smart Search (default) Submit


Marvin JS by ChemAxon

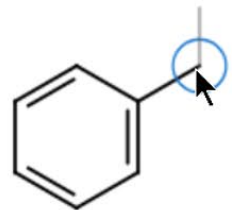
H
C
N
O
S
F
P
Cl
Br
I
A

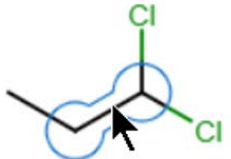
- **Tip!** Common keyboard shortcuts such as Ctrl+C (copy) and Ctrl+V (paste) can save you time when drawing reactions

Convert trivial, trade or systematic name ✕ Clear NAME  Convert






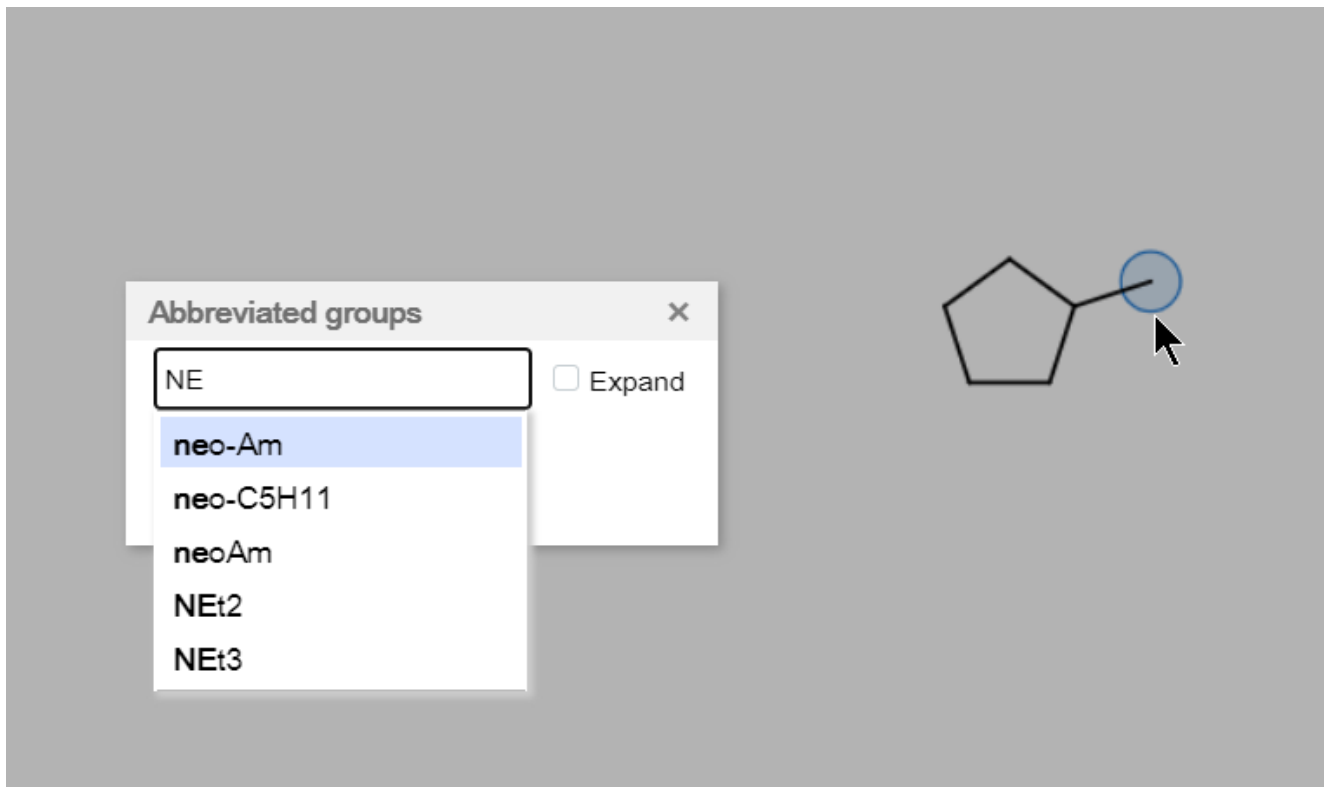




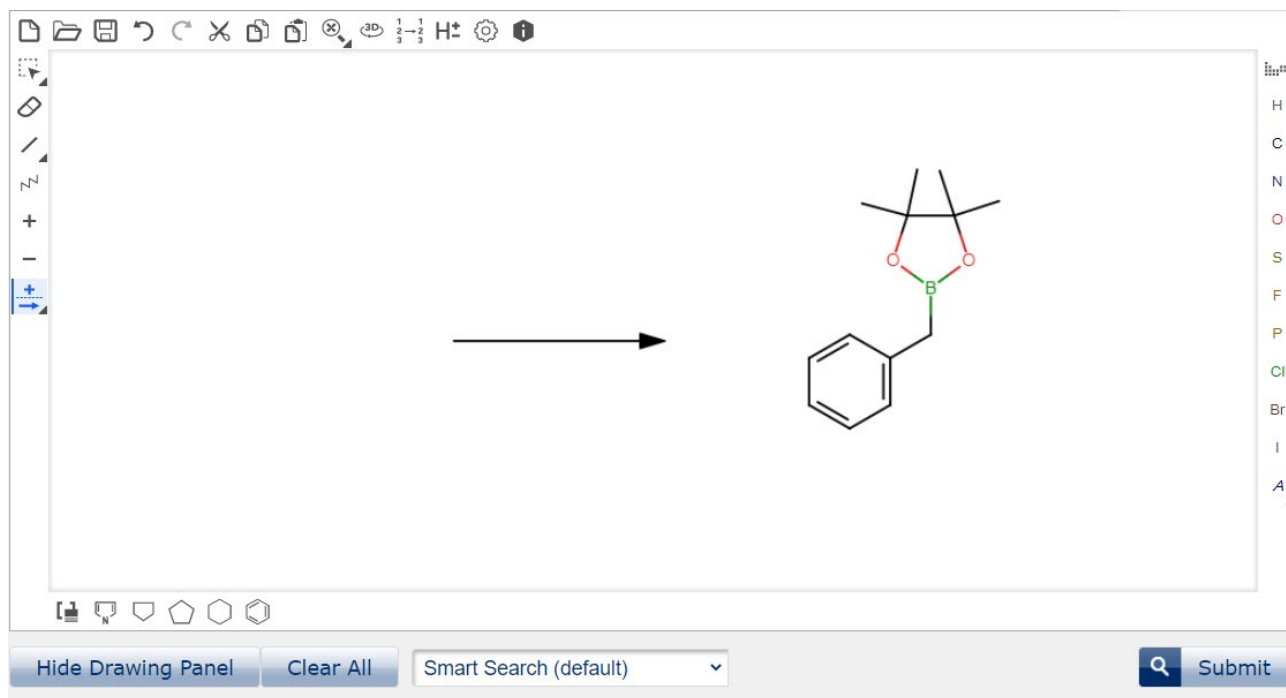
- The blue circle, which appears when you move your mouse over an atom or bond, shows the “active” atom/bond.
- You can change the element or groups simply by typing the symbol/abbreviation (e.g., F, Br, Tos, NO2) and hitting enter.
- When a bond is highlighted, you can change the bond order by typing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



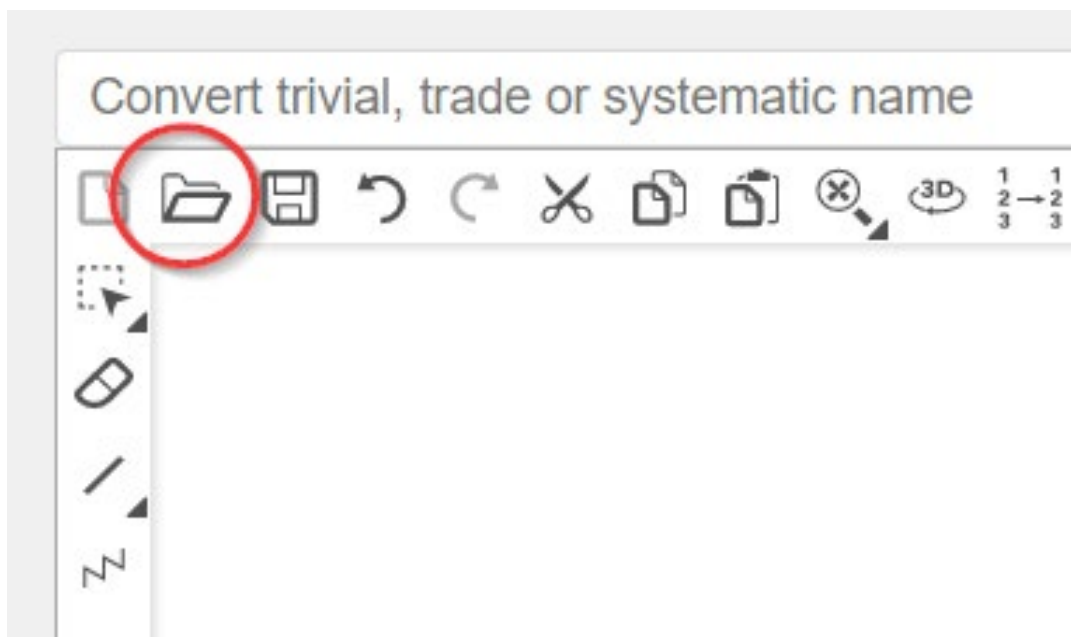
Hide Drawing Panel Clear All Substructure Search Submit



- 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)

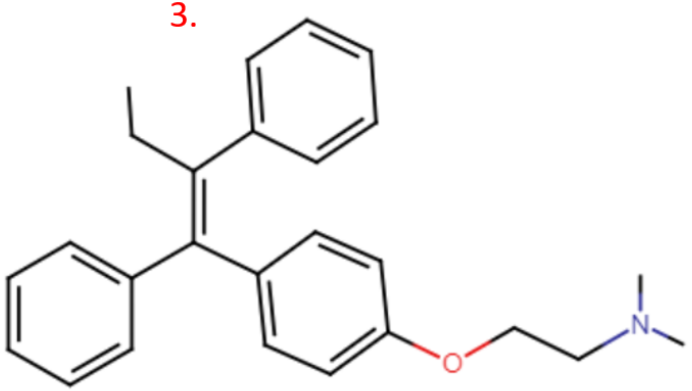
tamoxifen 1.

Clear Convert

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

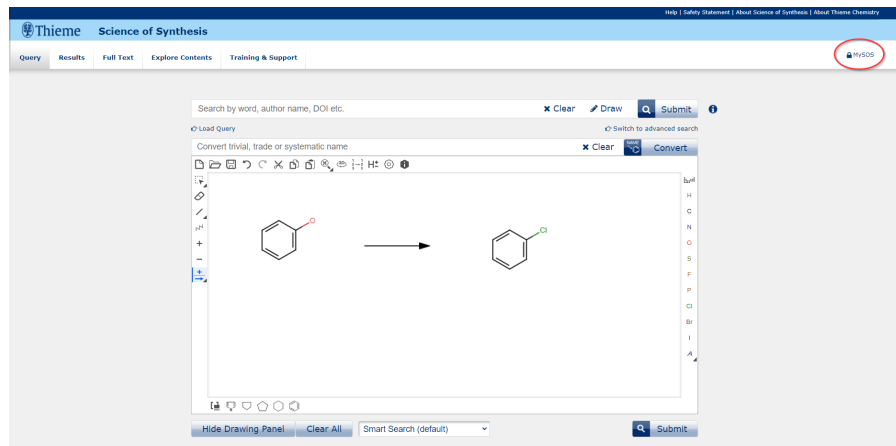
3.



The chemical structure of tamoxifen is displayed, showing a central carbon-carbon double bond. One carbon is bonded to a phenyl ring and an ethyl group. The other carbon is bonded to a phenyl ring and a 4-(dimethylaminoethoxy)phenyl group.

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

Thieme Science of Synthesis

Query Results Full Text Explore Contents Training & Support [Log out]

REFINE

FILTER BY:

☒ Reaction (46)

FILTER BY MATCH TYPE:

☒ Exact (3)

☒ Reaction substructure and reaction type (3)

☒ Reaction type (32)

☒ Similar reaction type (14)

SORT HITLIST:

☒ By relevance

☐ By publication date

[Update]

MySOS FUNCTIONS

☒ Save Query

☒ Save hitlist

☒ Load hitlist

Results (Articles found containing your search term, structure or reaction)

Hide All Reactions [Select Page] [Update Hit List] [Delete Hits After This Page] [Reset Hit List]

Page: 1 of 10

Synthesis of Product Class 2

31.2.1.1.4 Method 4: Substitution of a Phenolic Hydroxy Group

Stapfer, S. K. Science of Synthesis, (2007) 31, 1497.

Hide Reaction Show Full Text Show TOC Show Single Step Reactions

Phenol derivative reacting with PhPCl_2 at 180°C to form a chlorinated aromatic compound.

$\text{R}^1 = \text{H}$ 78%

$\text{R}^1 = 3\text{-Cl}$ 71%

$\text{R}^1 = 3\text{-OMe}$ 80%

$\text{R}^1 = 4\text{-F}$ 81%

Diaryldiazones

31.25.1.1.8.3.3 Variation 3: Displacement of Hydroxy Groups by Phosphoryl Chloride

Rück-Braun, K.; Dietrich, S.; Kempa, S.; Priewisch, B. Science of Synthesis, (2007) 31, 1497.

Hide Reaction Show Full Text Show TOC Show Single Step Reactions

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

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

