

# Guidelines for Structure Drawing

The two accepted formats for submitting structures to the BU-CMD are:

ChemDraw (ACS style)

– or –

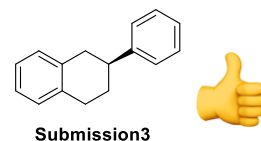
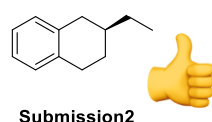
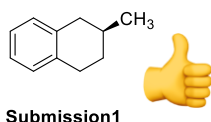
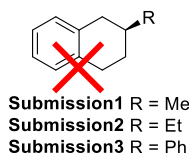
SMILES text strings

**TIP:** SMILES strings can be accessed via the clipboard by (1) drawing a structure in ChemDraw, (2) selecting the structure, and (3) choosing Edit → Copy As... → SMILES (Ctrl+Alt+C on Windows)

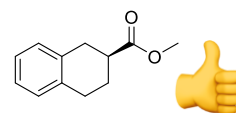
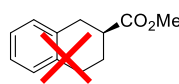
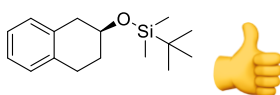
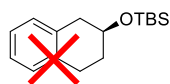
Whichever format you choose, please always follow these guidelines when preparing your initial structures in ChemDraw:

- 1) Label the structures clearly with a **unique name**. This name should also be written on the vial.
- 2) Draw the structures out completely.

This means don't use R-groups. Draw out each structure separately.

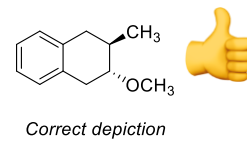
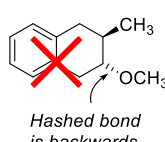
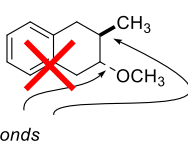
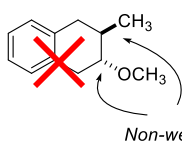


Avoid using condensed formulae or abbreviations for functional groups.  
Draw each non-hydrogen atom explicitly.



- 3) Depict the **stereochemistry** appropriately.

ChemDraw needs to be able to assign each stereocenter correctly. Unfortunately, there are many representations of stereochemistry that are easy to interpret for a human, but that a computer might find ambiguous.



**IMPORTANT:** The best way to check your stereocenters is to select the structure and go to Options → Show Stereochemistry. ChemDraw will assign the stereocenters it can interpret, and will place a red box on any stereocenter it can't figure out. **Fix all red boxes you see before submission.** Sometimes ChemDraw will (incorrectly) assign R/S on a red-boxed stereocenter it finds ambiguous, so check carefully for the appearance of those red boxes and make sure the R/S assignments are right!

- 4) Structures should be "cleaned up" unless doing so seriously distorts the structure

- 5) Chemdraw often has a really hard time interpreting three-dimensional projections of stereochemistry. Whenever possible, structures should be drawn from the clearest possible 2D perspective.

