Style for chemical structures in *Nature Chemical Biology*

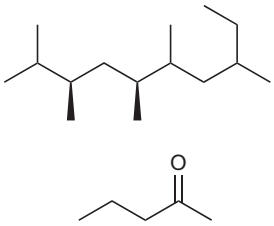
Though there are a number of ways that chemicals can be drawn based on individual preferences, we are hoping to standardize the presentation of small molecules both to improve consistency in our publications and to ease the burden on our production team in managing these images. What follows is a list of *Nature Chemical Biology* preferences. There is also a ChemDraw template available that will assist you in following our journal style. Please see the *Nature Chemical Biology* author page to download the template (http://www.nature.com/nchembio/authors/index.html).

If after reading this, you have any questions, please contact your manuscript editor for more information.

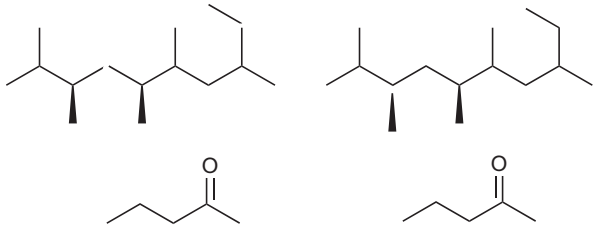
CONNECTIVITY

- All bonds should be connected to each other (no gaps between bonds).

Correct:

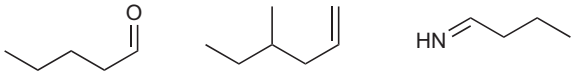


Incorrect:

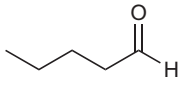


The primary exception is when a double bond is at the end of a chain.

Correct:

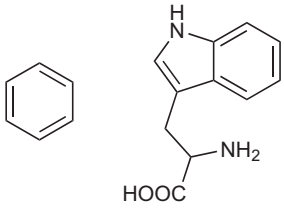


Not preferred:

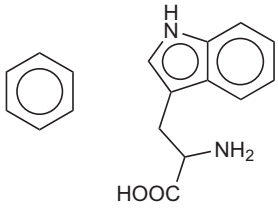


- Discrete bonds should be shown rather than rings. The primary exception is for the cyclopentadienyl anion (right).

Correct:



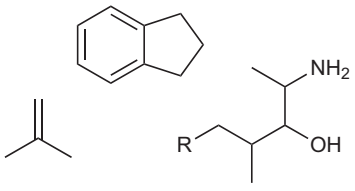
Incorrect:



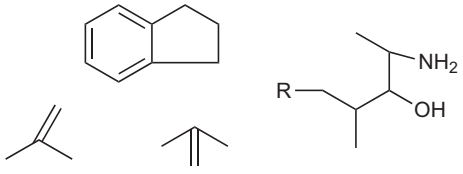
An exception:

- Standard bond angles should be used and made consistent when possible.

Correct:

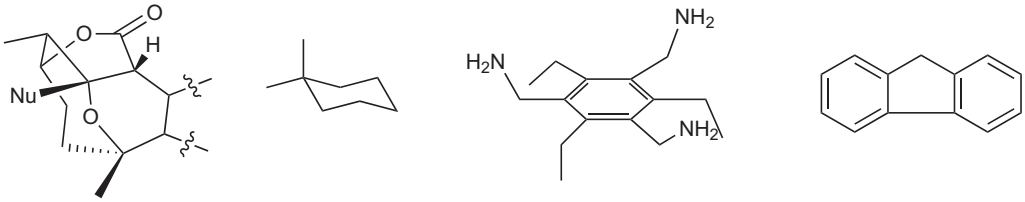


Incorrect:

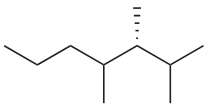


Obviously, there are exceptions, such as for 3D representations or in the context of a larger molecule:

Acceptable:

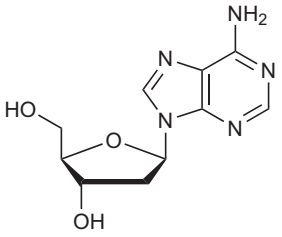


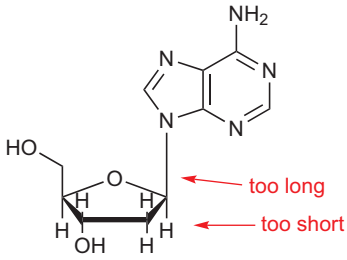
- Avoid using bond thickness for emphasis; instead, use color.
- Bond lengths should be consistent when possible.

Correct: 

Incorrect: 

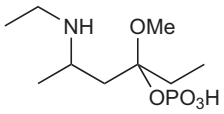
Particular attention should be paid to structures generated by ChemDraw templates.

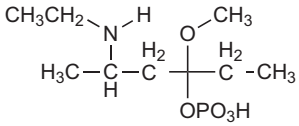
Correct: 

2'-deoxyadenosine from the Chemdraw template: 

LABELS

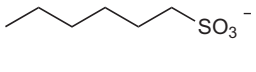
- Only heteroatoms or substructures that are altered during the course of a reaction should be labeled.

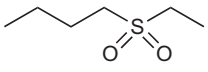
Correct: 

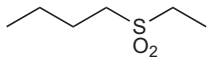
Incorrect: 

Acceptable: 

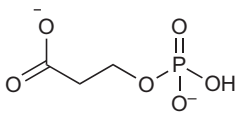
- As in the example above, methyl groups should be labeled as Me when attached to a heteroatom and left as an unlabeled bond when attached to another carbon. Me/H/other text labels when attached to heteroatoms are not separated by a bond.
- Preferred abbreviations of common functional groups are: CO_2H, NO_3, NO_2, SO_2, N_2, N_3, OPO_3H (Pi and 'P' in a circle are also acceptable in reaction schemes), Ph, Ac, Bn, Me, Et, *i*-Pr, Bu, *n*-Bu, *t*-Bu, Fmoc, Boc, Bz, Cbz, PG, LG, R, Nu, E (or E^+), X. Non-standard abbreviations should be defined. When an abbreviation looks 'bad' (such as the internal group below/right), it should be drawn out (center).

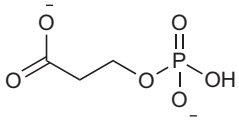
Correct: 

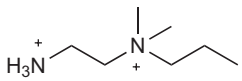


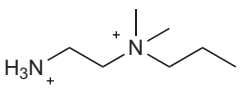
Incorrect: 

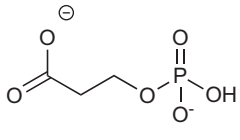
- Charges: no circles around charges. Charge should reside on charged atom (i.e., not R_3NH^+), although specific placement around the atom is flexible (see examples below). For the positive charge ("+" symbol), use the charge tool rather than including the charge within the atom label. The negative charge can be placed either way, but if in the text box, it should be a superscript en dash (i.e., "–". Note that "-" (the minus sign) is too short).

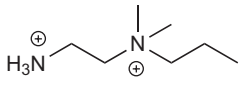
Correct: 



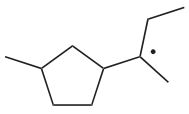


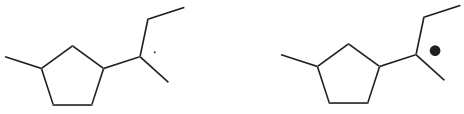


Incorrect: 

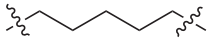


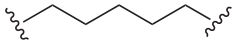
- Radicals should be visible but not too large. Use radical tool.

Correct: 

Incorrect: 

- Wavy lines that indicate truncation of a molecular structure should be placed in the middle of the bond

Correct: 

Incorrect: 

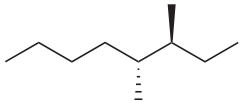
STEREOCHEMISTRY

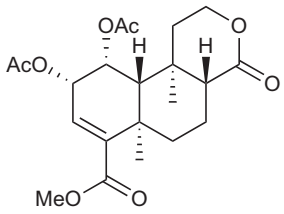
Compounds that need extra definition include: enantiomers, diastereoisomers, and geometric isomers (i.e., *cis* and *trans*).

A cautionary note: If you need to redraw a chiral molecule in a different orientation/arrangement or flip it in either dimension, be careful that the new configuration is the same as the original!!

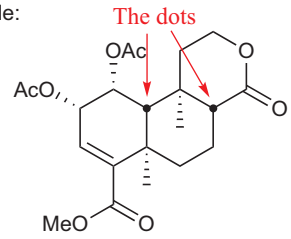
- Stereochemistry must be specified with wedges (preferred) or dots (sometimes required). In general, do not draw H's unless absolutely necessary.

Correct:

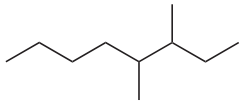


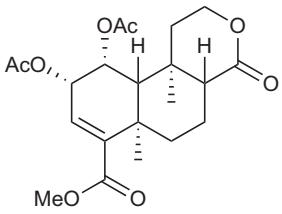


Also acceptable:



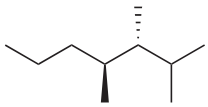
Incorrect:



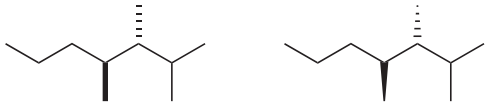


- Use wedges instead of thick bonds.

Correct:

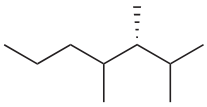


Incorrect:

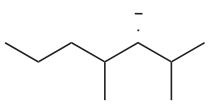


- For clarity and consistency, the number of hashes in hashed wedges and bonds should be at least 3.

Correct:

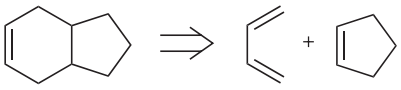


Incorrect:

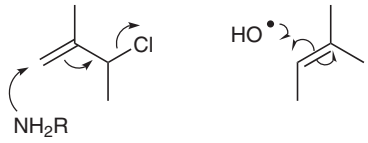


SPECIAL TOPICS

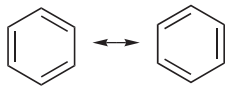
- Arrows: please use these arrows instead of other similar options.



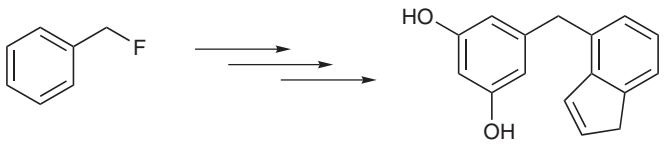
Retrosynthetic arrow



Reaction arrows



Resonance arrow

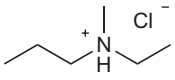


Multistep synthesis/reaction arrows

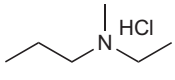
Equilibrium arrow

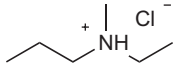
- Salts should be shown with counterions in dissociated form.

Correct:



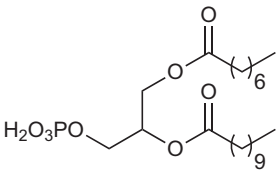
Incorrect:



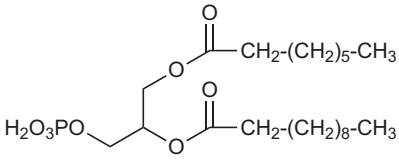


- Long alkane chains, if abbreviated, should be abbreviated with parentheses as follows:

Correct:

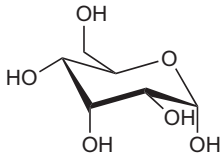


Incorrect:

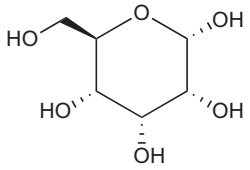


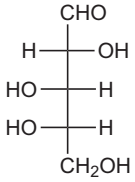
- Sugars: please check that these conform to our preferred structure.

Correct:



Also acceptable:
(but discouraged)





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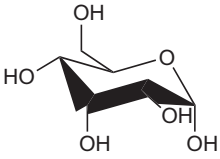

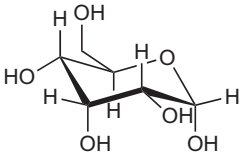

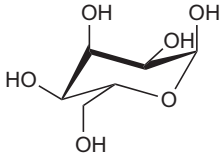

MOVING TOWARD PUBLICATION…

- Fonts/formatting (these preferences are already set in the *Nature Chemical Biology* template):
  Please use Arial, 8 pt font for all atom labels.
  "Show labels on Terminal Carbons" and "Hide Implicit Hydrogens" should be UNCHECKED.

- Please use the following drawing settings:
  chain angle, 120°
  bond spacing, 18% of width
  fixed length, 14.4 pt
  bold width, 2.0 pt
  line width, 0.6 pt
  margin width 1.6 pt
  hash spacing 2.5 pt

- Warnings
  Chemdraw has the option of using several warnings to alert the user that there are too many or too few bonds to an atom, unbalanced parentheses, and similar. These are currently turned on in our template, and can be helpful in identifying places where there might be problems (although identifying the cause of the warning is up to you!). However, this warning system does not catch every problem, so please confirm the correct appearance of your structures with the previous preferences or your chemical intuition.