ChemSketch:
A Guide to Drawing Chemical Structures

Freeware Version

ACD/ChemSketch

http://www.acdlabs.com

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ChemSketch Version 5

ChemSketch: A Guide to Drawing Chemical Structures

ChemSketch, freeware from [ACD Labs](#), is a chemical structure drawing program. Two-dimensional chemical structures are the common representation in textbooks and other print materials in chemistry, biology, and the health sciences. They display the interconnectivity of atoms in the structure. Knowing how to draw structures is required to understand them and helpful as they are converted into three-dimensional structures. Forming a three-dimensional mental image from a two-dimensional drawing is an advantage for scientists. Chime and RasMol are great aids to help develop this.

When ChemSketch opens (as shown in the screen below), it is ready to draw carbon by default and places the appropriate number of hydrogens needed on the carbons. The three default functions are circled in green. If you place the cursor over a button on the toolbar, its function will appear. Comments and reactions can be
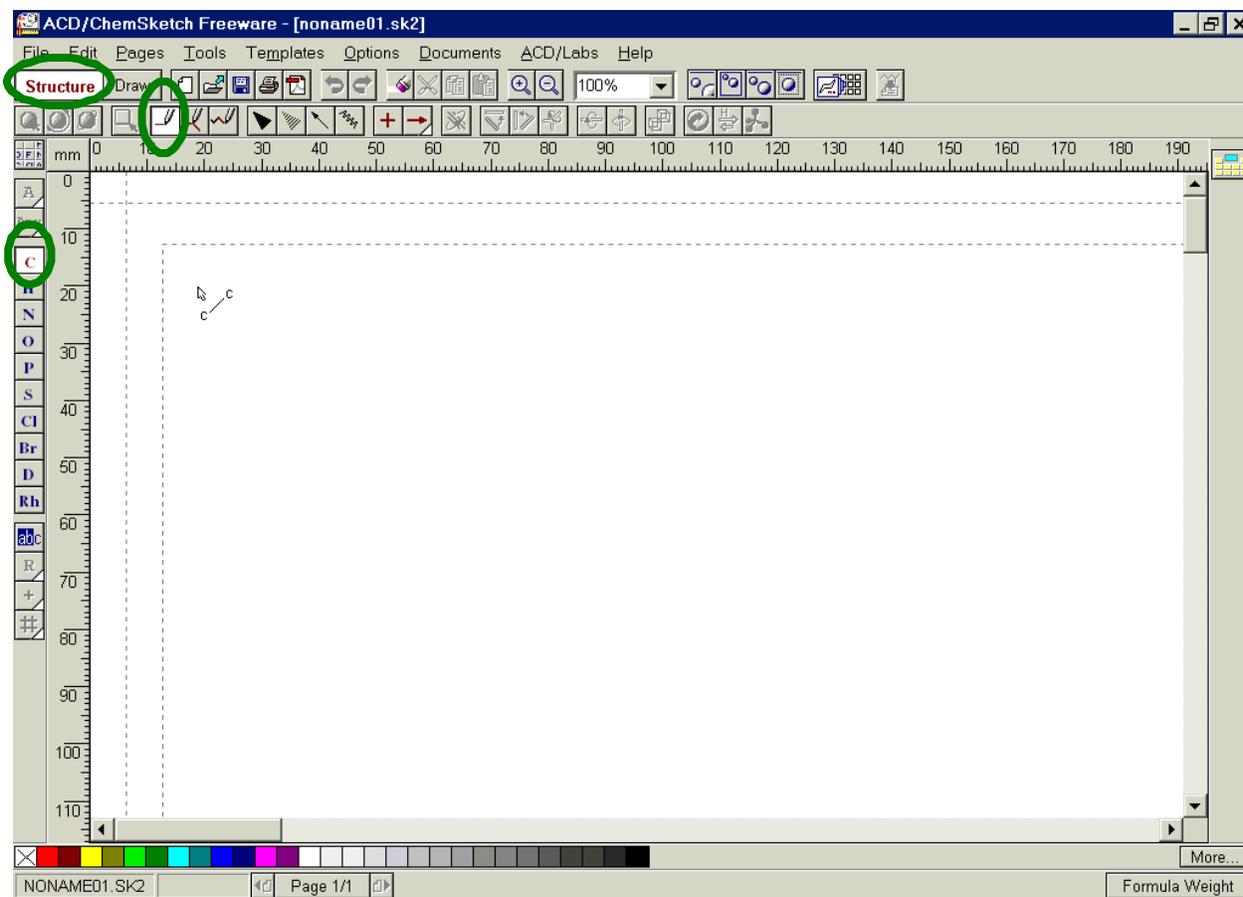

added to the screen as well as laboratory glassware. A number of common drawing

tools are available if you click on "Draw" on the toolbar. As you toggle between the "Structure" and "Draw" modes, you will notice that the toolbars change.

Drawing Chemical Structures

To start drawing, just click the cursor and a CH_4 appears on the screen. If you click on this first CH_4 another carbon will add to it. The next carbon added will be at the carbon that is highlighted with the box (as shown to the left). You can position the cursor at any of the carbons to form branches or side chains. The program defaults to show hydrogens only on the terminal carbons (at the end of the chain). Where the lines meet (or corners), there are carbon atoms with additional hydrogens (unless four lines meet).
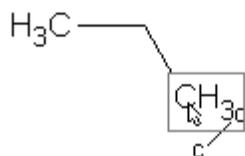
If you place the cursor over a "corner" in the chain you will see the –CH_2- group appear highlighted in a box as shown below.
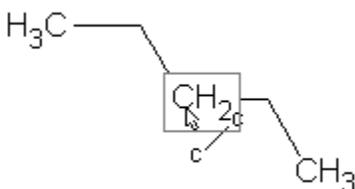
Now if you want to add a double or triple bond, you select the bond position with the cursor. A box will highlight it as seen to the right, and then click it once for a double; click it again for a triple bond, and again to go back to a single bond.

H_3C——CH_3 H_2C==CH_2 HC≡CH
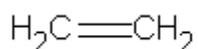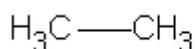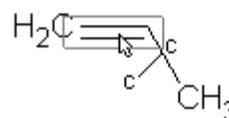
one click   two clicks

The number of hydrogens on each carbon adjusts automatically as multiple bonds form or as side chains are added to a structure. The carbon atoms in a molecule must always have FOUR bonds.

If you want all the carbons and hydrogens to be displayed on the structure, click on the tool circled in green on the toolbar, and then place the cursor on the carbon and double click it. The "Properties" box will appear with the "Atom" tab. On this

window, click the C and then select by clicking "Show" and then click the "Apply" button. The –CH_2- group will appear in the structure. Move to the other carbons, and click on them and then click the "Apply" button to repeat the procedure.

Here are four representations of pentane, C_5H_{12} (shown below). The last one is an attempt to show a three-dimensional structure. Being able to go from one of
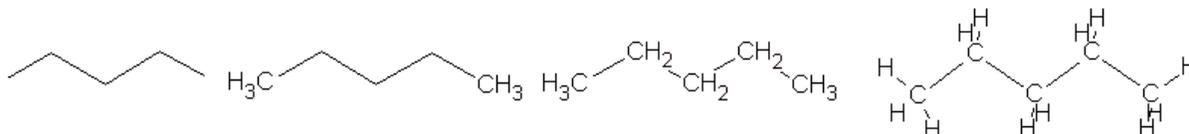
these forms to any one of the others is a good skill to obtain. And it is important to remember that around any carbon atom are probably hydrogens too!

To have the chain lay in a horizontal position; we can use the rotate function which is circled in green below. Click on the structure to get the red circle with the plus sign placed on the structure, and then click on the end of the structure and drag it to rotate.
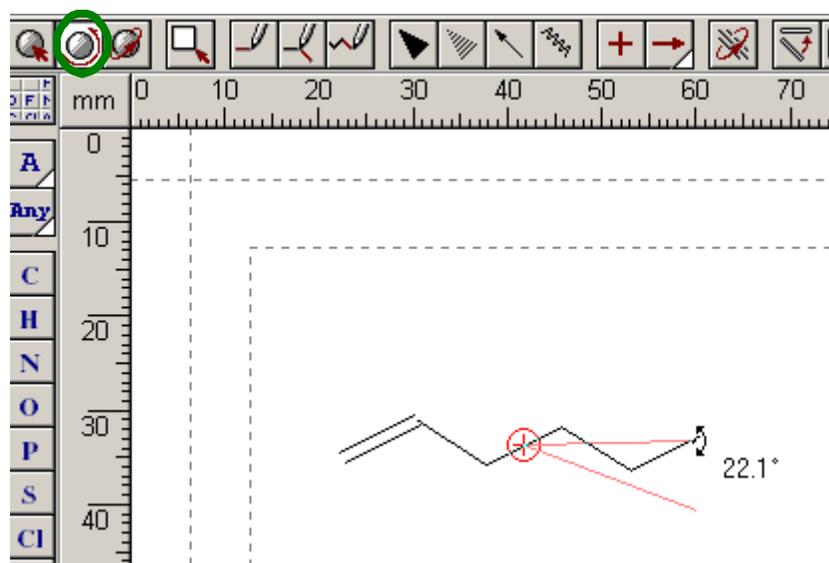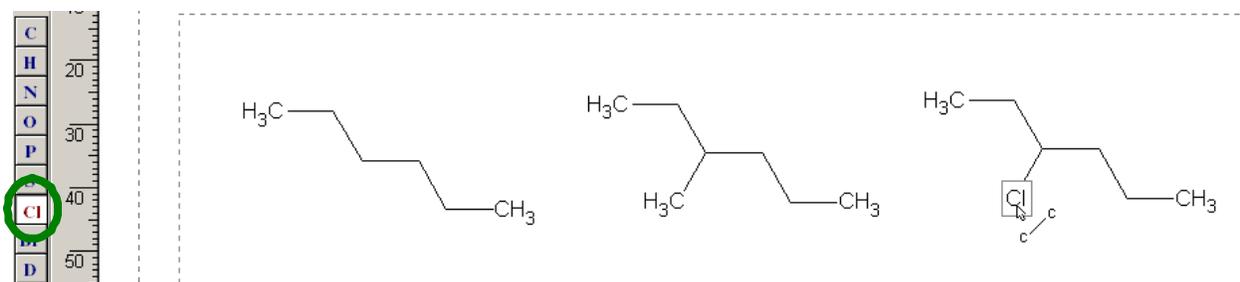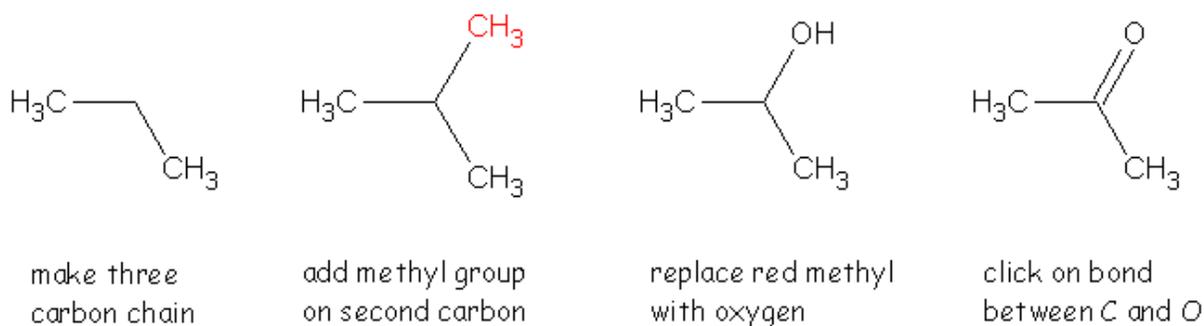

How about if you want to insert an atom other than carbon? The easiest way to do this is to add a carbon at the site where you want the other atom and then substitute the new atom for the carbon. Here it is explained in steps. Build the six carbon chain. Then go to the third carbon and click on it again to add the $-CH_3$ side chain.

Now go to the menu bar on the side and click on Cl (circled in green above), then place your cursor on the carbon of the side chain and click. The carbon becomes chlorine and the hydrogens are adjusted appropriately.

If you selected the O instead of Cl, you would have placed an –OH group on the chain. Click on the C-O bond and the –OH (an alcohol) becomes a C=O (a ketone). The stages for drawing acetone, $(CH_3)_2CO$, are given on the next page.

CH₃ OH O

| make three carbon chain | add methyl group on second carbon | replace red methyl with oxygen | click on bond between C and O |

You can try your hand at drawing the various functional groups in organic chemistry by following the steps in the table given at the end of guide.

There are two other draw tools that may prove useful at various times. One is the continuous draw, , which allows you to draw rings or place connecting bonds between any two carbons. The style of the cursor changes as shown below. After using this tool, you may want to use the "Clean Structure" tool, , to optimize the structure especially for rings (standardizes all bond lengths and angles, especially trigonal and linear for a 2D drawing).

new cursor

continuous draw of 4 C's   after use of clean structure tool
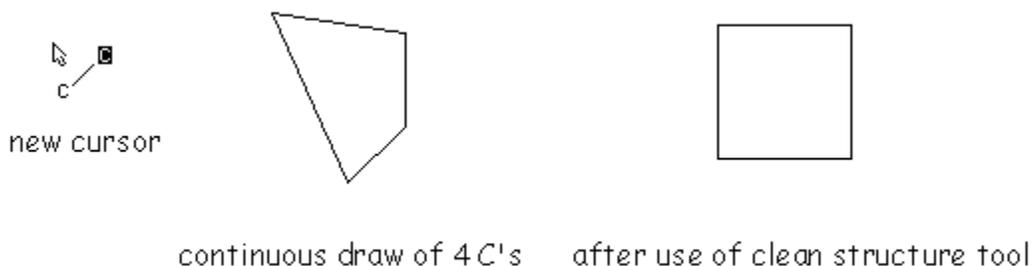
If you do not like the results after using the Clean Structure tool, press the undo button, .

The other tool is the chain draw, , which builds large chain hydrocarbons for things like fatty acids. The style of the cursor changes and counts the number of carbons in the chain as you draw.

An easy way to move a structure into a document is to highlight the structure with the lasso tool, , and then copy and paste it into a Word or PowerPoint document.

Templates

ChemSketch has a very large number of pre-drawn molecules and radicals. To get to the templates you click the template button on the toolbar, encircled in green. Select a template from the menu available either from the complete list in the dropdown menu (red box) or the partial list to the side. The screen below shows the carbonyls. The templates are a great source for more complicated molecules especially with ring structures.
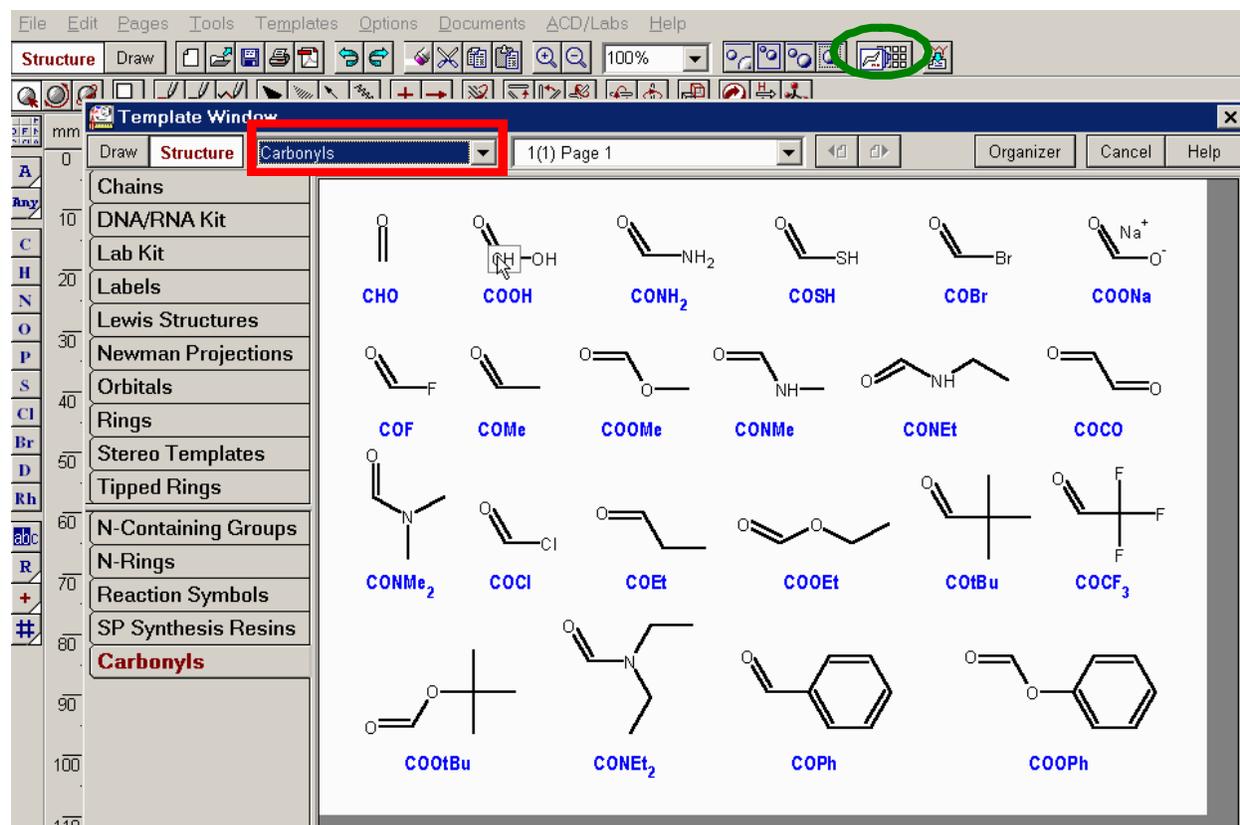

In the structure mode on the template window, if you move the cursor over the possible selections the atom that will form the bond is highlighted in the box (for some a bond will highlight). You can start building a molecule from a template.

If you need benzene, go to the aromatics template, select it and click on the screen. To add benzene onto another molecule, select a carbon atom on the benzene (left below) and click on the atom that it will be joined to. To fuse a ring onto another ring, select a bond on benzene (right below) and click on the first ring.

Benzene   Benzene

The radicals button, circled in green, on the right side of the ChemSketch screen will allow you to bring up a table of structures including cyclic compounds (alkanes, benzene). The variety of structures is shown to the right below.
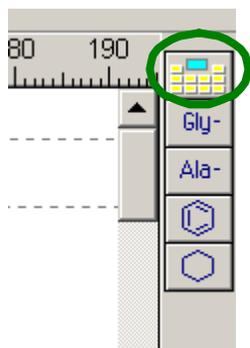

As you use this table the structures used will appear below the button on the right side of the screen so they can be used again quickly.
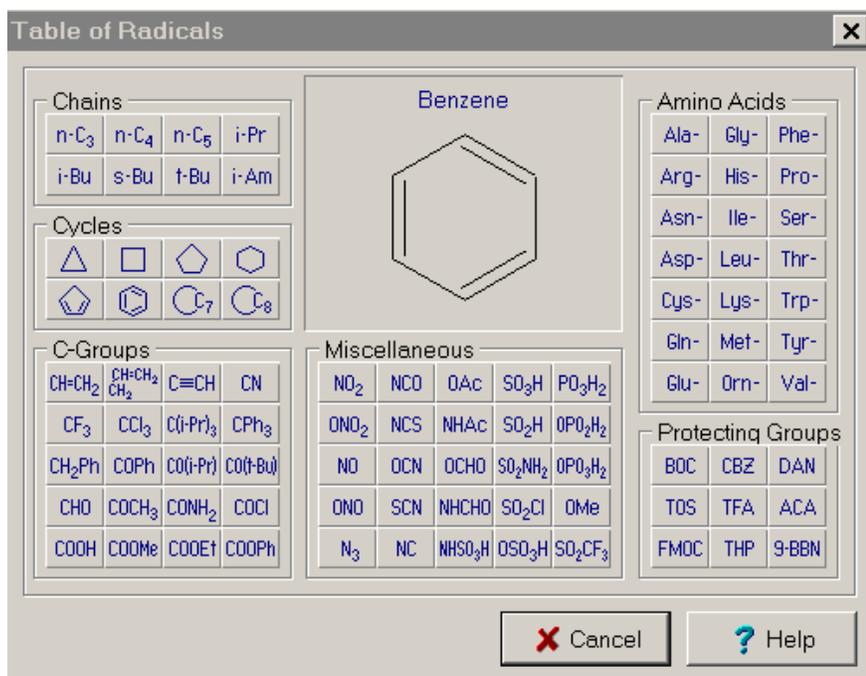
If you click on any radical and then click on a carbon in the exiting structure, the radical will be added to that carbon.
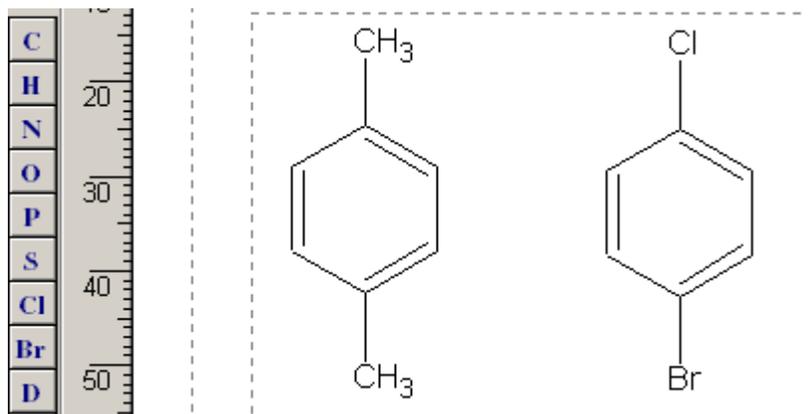
Drawing Isomers

To draw some isomers you will have to build the molecule by default, add extra bonds and carbons and then erase unwanted ones using the ⬜ button.
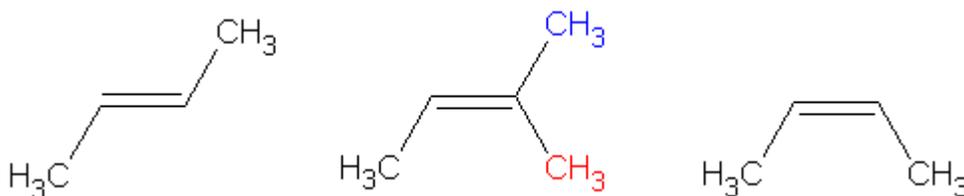
Build the four carbon chain and place the double bond for the trans isomer. Then add the red methyl group and remove the blue one to form the cis isomer.

To build 1,4-bromochlorobenzene, you will need to draw 1,4-dimethylbenzene and then replace the methyl (-CH$_3$) groups with halogens. Go to the templates, select aromatics, and get a benzene ring. Click on C on the left-side menu and then place the two methyl groups in the 1 and 4 positions. Then click on Cl and substitute for the top methyl. Click on Br and substitute for the bottom methyl group.


Building the 1,2- and 1,3- isomers is left to the reader for practice.

Naming a Molecule
ChemStekch will name a molecule using IUPAC rules. After drawing the molecule select the [icon] button. If you have multiple molecules, select one to name it. The text of the name can be edited in the "Draw" mode, using the [ab] button. Just click on this button and then the text to be edited.

Saving a File
Go to "File" on the menu bar to view the menu shown below. If you want to modify the file in the future, select "Save As…" to save it as a .sk2 file.
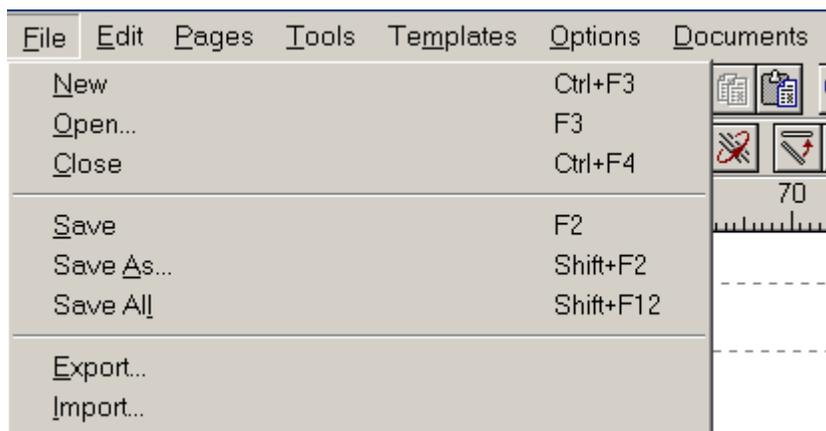

If you want to save it as a finished graphic, select "Export…" and when the Export box appears, click on the drop down menu of "Save as type:" and select gif (at the bottom of the list).

This (gif) is a good format for inserting graphics into Word, PowerPoint, or FrontPage documents. Other common image formats are available.

Files for Chime and RasMol: Before you export you need to optimize the three dimensional structure. In the structure mode, click on the ![button] button on the toolbar. This runs an energy minimization program on the molecule. ChemSketch uses a molecular mechanics algorithm to minimize interactions in the structure. When it asks to remove the hydrogen before minimization, select "NO." This will distort your two-dimensional drawing. So save it first before doing this or hit the ![button] button to undo the 3-D optimization and go back to the 2-D drawing after completing the next steps.
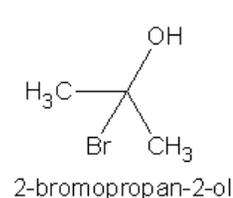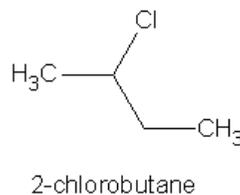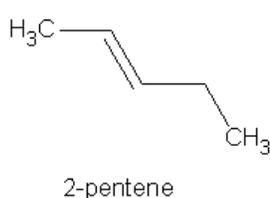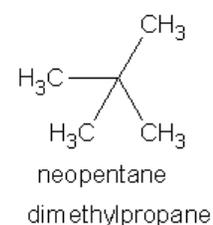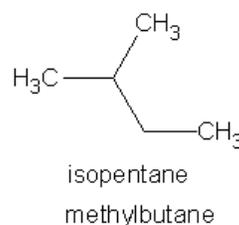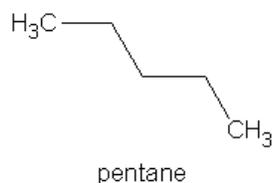
You can preview the 3-D structure in the viewer; just follow the steps shown to the right. The viewer works like Chime or RasMol (except in different atom colors); click and hold on the molecule and move the mouse to rotate. The buttons on the toolbar allow you to change the display (or a right click will toggle through display modes) and make measurements. Just close the viewer to return to ChemSketch.
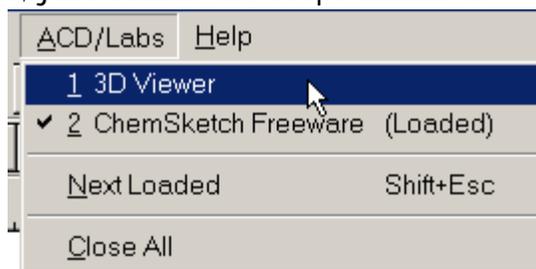
To save a 3-D structure, you select the MDL Molefiles (.mol) format from the "Save as type:" list and the file can be read by Chime and RasMol. This format can also be imported (opened) into Spartan '04 for further work.

Drawing Practice
Here are some practice molecules to try drawing. The upper name (of a pair) on each is the one given by ChemSketch.

pentane

isopentane
methylbutane

neopentane
dimethylpropane

2-pentene
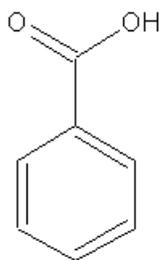
2-chlorobutane

2-bromopropan-2-ol

Draw cyclopentane, a five carbon ring structure. How many hydrogens are on this molecule?

Try to draw the functional groups given in the table below.

parent			
H₃C—CH₂ / CH₃	H₃C—CH₂ / OH click end C with O alcohol		H₃C—CH₂ / SH thiol click O with S
	H₃C—O / CH₃ click center C with O ether		

parent

H₃C—CH₂
      |
      CH₃

H₃C—CH₂   click end C with O   *alcohol*
      |
      OH

H₃C—CH₂   *thiol*
      |
      SH
   click O with S

H₃C—O   click center C with O   *ether*
      |
      CH₃

CH₃ (red)
 |
H₃C—HC
 |
CH₃ (green)

OH
 |
H₃C—HC
 |
CH₃ (green)

ketone   O
            ‖
H₃C—C
     |
     CH₃ (green)

aldehyde   O
             ‖
H₃C—C
     |
     H

click red C with O and then click on C-O bond   click green C with H

OH
 |
H₃C—HC
 |
OH

acid   OH
           |
H₃C—C
      ‖
      O

click both red and green C's with O then click lower C-O bond

CH₃ (red)
 |
H₃C—HC
 |
CH₂ (red)
 |
H₃C

OH
 |
H₃C—HC
 |
O
 |
H₃C

ester   O
           ‖
H₃C—C
      |
      O (red)
      |
      H₃C

amide   O
           ‖
H₃C—C
      |
      NH
      |
      H₃C

replace red C's with O's   click C-O bond   click red O with N

H₃C—CH₃

H₃C—NH₂   *primary amine*
click N once on red C

H₃C—NH
      |
      NH₂ (green)
click N twice on red C

H₃C—NH
      |
      CH₃   *secondary amine*
replace green N with C

NH₂ (green)
 |
H₃C—N
      |
      NH₂ (green)
click N thrice on red C

CH₃
 |
H₃C—N
      |
      CH₃   *tertiary amine*
replace green N's with C's

H₃C—CH₂
      |
      CH₂-CH₃ (red)

H₃C—S
      |
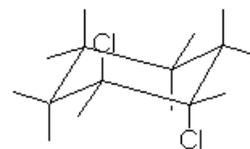   S—CH₃   *disulfide*
click on red C's with S

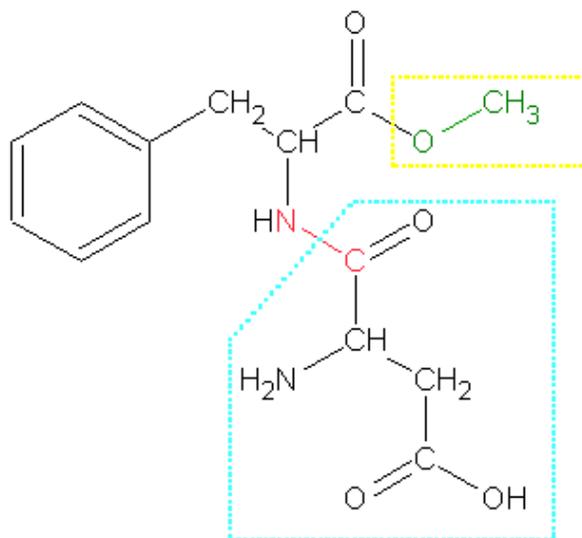Now try some examples that use the templates.

benzoic acid
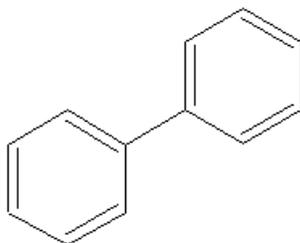
1,1'-biphenyl

1,2-dichlorocyclohexane

chlorines are trans

Try drawing aspartame which is a combination of the two amino acids bound at the amide linkage (red C-N bond) – aspartic acid (in the bluish box) and phenylalanine with a methyl ester added (yellow box).

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For further information, especially advanced drawing options, see the *ChemSketch User's Guide* at:

http://www.acdlabs.com/download/docs/chemsk.pdf

Get ChemSketch at: http://www.acdlabs.com/download.

We thank ACD Labs for making ChemSketch available as freeware.