CHEMDRAW ULTRA 12.0

ITEC107 - Introduction to Computing for Pharmacy

Objectives

- Basic drawing skills with ChemDraw

- Bonds, captions, hotkeys, chains, arrows

- Checking and cleaning up structures

- Chemical warnings

Basic Drawing With ChemDraw

- ChemBioDraw provides a variety of tools for drawing everything from simple chemical structures to complex reactions.

- In this section, we introduce basic techniques to help you create your structures. We also explain how to add features, such as arrows, shapes and labels to enhance structures and reactions.
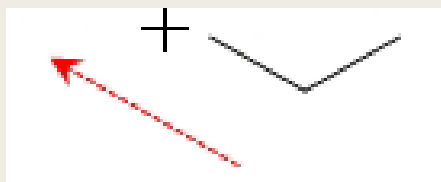
Bonds

The Main toolbar and Multiple Bonds toolbar offer numerous options for drawing bonds. Some tools are for drawing specific types of bonds, while others are for drawing structures for database queries.

- **Drawing Bonds**

- To draw the first bond of your structure, select the solid bond tool in the Main toolbar and click in the document window.

- The bond appears in the drawing window. To draw another bond attached to the first, click either end of the first bond.

- The second bond appears in the drawing window, as shown:
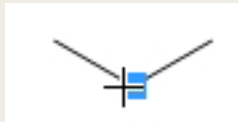
Bonds

You can draw a bond in any direction. Using a bond tool, click and drag from an existing atom or an empty area in the document window. The bond is drawn in the direction you drag the cursor.

Double Bonds

There are four ways to draw a double bond:

1. Draw a bond using the Double bond tool.

2. Draw a single bond over an existing single bond.

3. Using any bond or selection tool, point to an existing bond and type '2'.

4. Right-click any bond and select **Double**>**Plain** in the context menu.

Bonds

Double Either Bonds

Double either bonds, or crossed double bonds, indicate unspecified double bond configuration, or a mixture of configurations.

To draw a double either bond, use the double either bond tool from the Multiple Bonds toolbar, or:

1. Draw a bond using the Wavy Bond tool.

2. Click the center of the bond to create a double bond.

3. Click again to create a double either bond.

Triple Bonds

There are three ways to draw a triple bond:

■ Draw a bond using the Triple Bond tool.

■ Using the Solid, Dashed, or Bold Bond tool, drag from one end of an existing double bond to the other end.

■ Using any bond, or selection tool, point to an existing bond and type '3' on your keyboard.

Bonds

Quadruple Bonds

There are three ways to draw a quadruple bond:

1. Draw a bond using the Quadruple Bond tool.

2. Using the Solid, Dashed, or Bold Bond tool, drag from one end of an existing triple bond to the other end.

3. Using any bond or selection tool, point to an existing bond and type '4' on your keyboard.

To change a quadruple bond into a single bond:

- 1. Select any bond tool.

- 2. Drag from one end of an existing quadruple bond to the other.

Wedged Bonds

To draw a wedged bond:

1. Click one of the wedged bond tools.

2. Drag from the narrow end of the wedged bond to the wide end of the wedged bond.

Wedged bonds are drawn with a fixed orientation in a document window.

To change the orientation of the wedged bond:

- Click the bond using the wedged bond tool.

Changing Bonds

You can change bonds by:

- Changing bond types

- Changing bond alignment and orientation

- Moving atoms

- Layering bonds

Changing Bond Types

Change a single bond from one type to another using one of the following methods:

■   Select a bond tool and click an existing bond or

■   Right-click and select the new type from the context menu
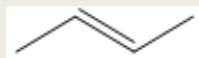
Changing Double Bonds

To change one type of double bond to another:

1. Select the Bold, Dashed, or Solid Bond tool.

2. Click a double bond.

The double bond changes to the new bond type. One of the bonds in the double bond is always a solid or dashed bond.

Aligning Double Bonds

- Double bonds can have one of three alignments relative to other bonds—above, below, and centered
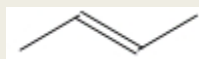

- Above

- Below

- Centered

1. Click the bond tool used to create the existing double bond.

2. To change the alignment, do one of the following:

- Click the center of the double bond.

- Right-click, point to **Bond Position** on the context menu, and choose the alignment.

Moving Atoms

To move an atom in a structure, click and drag it using a selection tool.

To move two bonded atoms in a structure, click and drag the bond between them.

To move individual atoms:

1. Click a selection tool.

2. Point to the atom you want to move. A highlight box appears over the atom.

3. <SHIFT>+drag the atom.

Fixed Bonds

■ By default, ChemBioDraw draws structures with fixed bond lengths and bond angles. The values of those lengths and angles is determined by the settings for the particular type of document.

Fixed Bonds

Drawing Fixed Length Bonds

To draw bonds constrained to a fixed length:

*1. Navigate to **Object>Fixed Lengths** and ensure a check mark appears next to **Fixed Lengths**.*

2. Draw a bond using any bond tool.

Drawing Fixed Angle Bonds

Bond angles are generally either set to the default chain angle of 120 degrees, or are constrained to angles of 15 degree increments.

To draw fixed angle bonds:

*1. Navigate to **Object>Fixed Angles** and ensure a check mark appears next to **Fixed Angles**.*

2. Draw a bond using any bond tool.

# Fixed Bonds

Changing Fixed Values

To change fixed values:

*1. Navigate to **File>Document Settings** and click the Drawing category.*

*2. Enter a value in the **Fixed Length** text field. Use in, cm, pt, or picas for units.*

*3. Enter a value in the Chains **Angle** text field.*

*4. Click **OK.***

Atoms

By default, when you draw structures with the various bond, ring, or chain tools, simple hydrocarbons are created.

You can add atom labels to the atoms using the Text tool. You can also use the Text tool to add textual captions to a document. For example, you can add the atom label "OH" to a drawing of toluene to create phenol:

1. Draw the toluene structure.

2. Using the Text tool, click the methyl carbon.

A text field appears.

3. Type OH in the text field.

4. Click outside the text field.
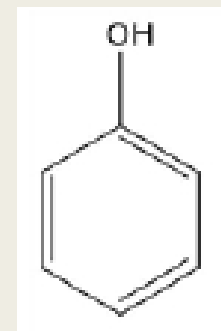
■   To edit the atom label, click in the text field with the text tool and begin typing.

Captions

You can add and edit captions to your structures using the Text tool. The following example adds the caption 'Phenol' to a phenol structure.

To add the caption 'Phenol' to a phenol structure:

1. Draw the phenol structure.

2. Using the Text tool, click below the

drawing and type "Phenol" in the text

field.

3. Click outside the text field.
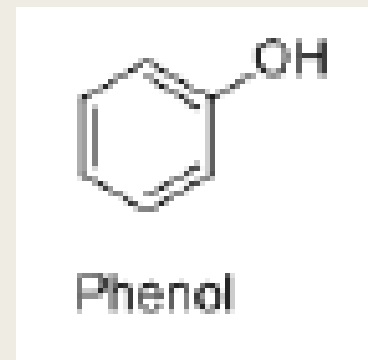
To edit the caption, click in the text field with the Text tool and begin typing

Formatting Text

Each new caption, or atom label, uses default document settings for font, size, and style of captions and atom labels.

You can change the format in 3 different ways:

1. Changing the document settings for subsequent drawings in the current document. **File > Document Settings**

2. Choosing a new format for an individual caption or label from the **Text menu (right-click on selected text)** or **Style toolbar (activate from View menu)** before you type.

3. Selecting text and applying a new format to an individual label after you type using the **Text menu** or **Style toolbar** .

Formatting Text

Character Map

- The floating character map window displays the 256 ASCII characters in any font. The default font is Symbol.

- Use the character map to add symbols to your document in various font styles. To show or hide the map, navigate to **View>Show Character Map Window**. The character map is shown below.
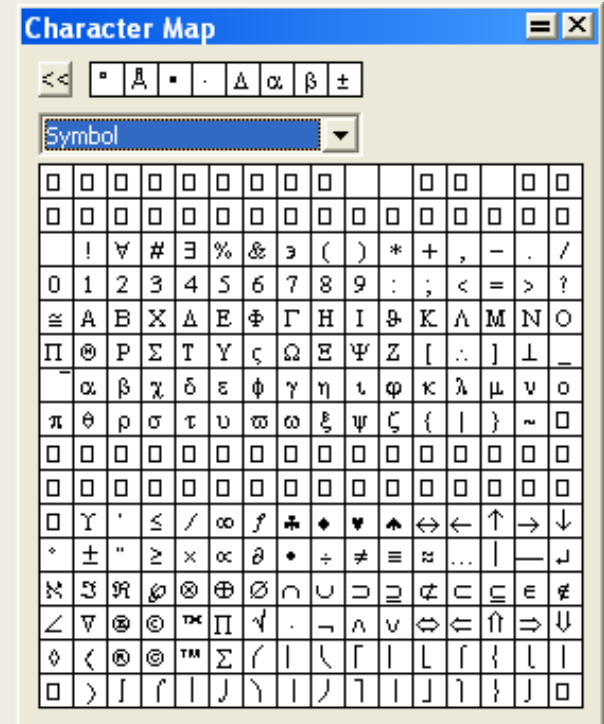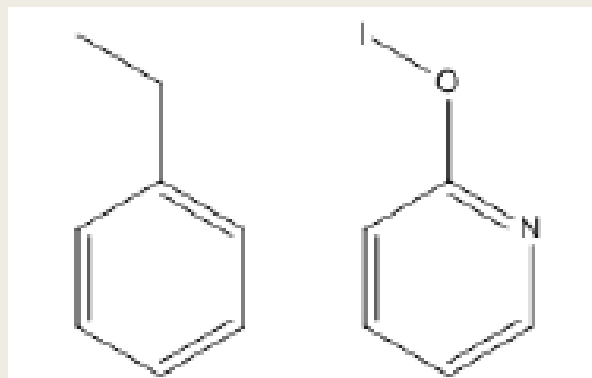
** Hotkeys **

- Hotkeys are keys on your keyboard that are linked to specific atom labels. Use ChemBioDraw hotkeys to quickly label atoms and apply atom properties.

- (The Hotkeys.xml file in the ChemDraw Items folder contains the hotkeys provided with ChemBioDraw. You can add or change hotkeys by editing this file in a text editor.)
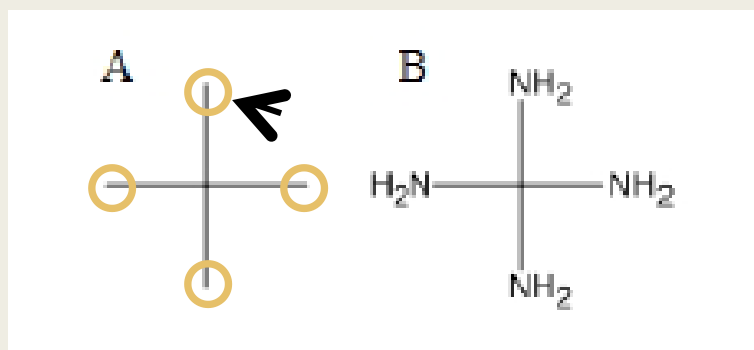
How to use Hotkeys

Using the hotkeys <n> (nitrogen), <O> (oxygen), and <I> (iodine), you can turn ethylbenzene into pyridin-2-yl hypoiodite.

Hover the cursor over the line where you want to add the label, then press the required letters.

How to use Hotkeys

You can also label several atoms at a time. For example, you can change neopentane (figure A below) into methanetetraamine (figure B):

1. Create the neopentane structure

2. Activate the selection tool

3. Use <SHIFT>+click on the tip of the carbon atoms and press <n> on the keyboard. All atom labels will be inserted.

Chains

You can draw hydrocarbon chains using the Acyclic chain tool

1. Select the Acyclic chain tool.

2. Click and drag in the document window in the direction you want the chain to grow. The number at the end of the chain indicates how many atoms you have drawn.
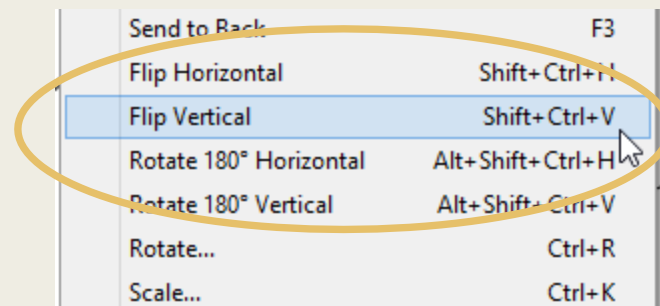
Chains

Changing Chain Direction

Press the **<Ctrl>** key while the Selection tool is activated, then click on the tips of the atom and drag to another direction.

Or select the chain and right-click.

Select the flip or rotate option.

Send to Back	F3
Flip Horizontal	Shift+Ctrl+H
Flip Vertical	Shift+Ctrl+V
Rotate 180° Horizontal	Alt+Shift+Ctrl+H
Rotate 180° Vertical	Alt+Shift+Ctrl+V
Rotate...	Ctrl+R
Scale...	Ctrl+K

Chains

Adding Chains to Structure

To add an Acyclic chain to an existing structure, click an atom in the structure. Click and drag in the direction you want to draw the chain.

Arrows

- You can use arrows to show the conversion of reactants to products and to indicate electron flow.

- Simply click on the Arrow Tools option and drag mouse until the required arrow is selected.

- Then draw the arrow shape on the page.
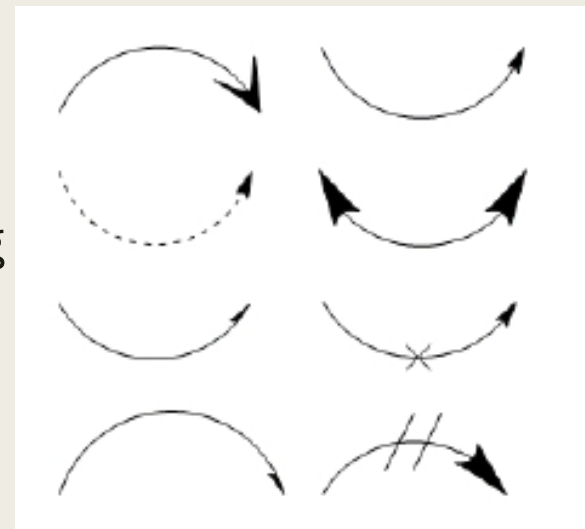
Selecting Objects

Use the Marquee tool to select objects and structures within a rectangular area.

1. Select the Marquee tool.

2. Click and drag diagonally over the structures or other object.

Selecting Entire Structures

To select an entire chemical structure, double-click a bond or atom in the structure using a selection tool.

If the chemical structure or other object is part of a group, the group is selected.

Selecting Objects

Selecting Objects by Clicking

1. Select the Lasso or Marquee tool.

2. Point to an object in a document window.

A highlight box appears over the pointed object.

3. Click the object.

The selected objects appear within the selection rectangle and the cursor changes to a hand.

Selecting Multiple Objects

When you select multiple objects, each object displays a selection box.

To add more objects to the selection, press <shift> and select the other objects.

Resizing Objects

You can resize objects by dragging the resize handle of a selected object or by scaling.

To resize a selected object proportionately:

1. Select the objects to resize. The resize handle is located in the lower right corner of the selection rectangle.

2. Point to the Resize handle. The cursor

becomes a double-headed arrow.

3. Drag the resize handle until the object

is the size you want.
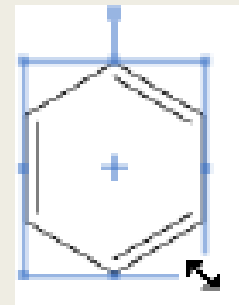
Rotating Objects

1. Select an object to rotate. For objects that can be rotated, the rotation handle appears at the top of the selection rectangle.

2. Drag the rotation handle clockwise or counterclockwise.

3. To rotate an atom label with a structure, press the <Ctrl> key while dragging the structure.
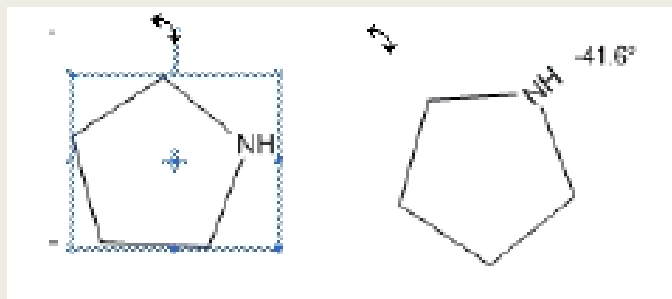
Copying Objects

1. Select one or more objects.

2. <Control>+drag the object(s) to create a copy and position it.
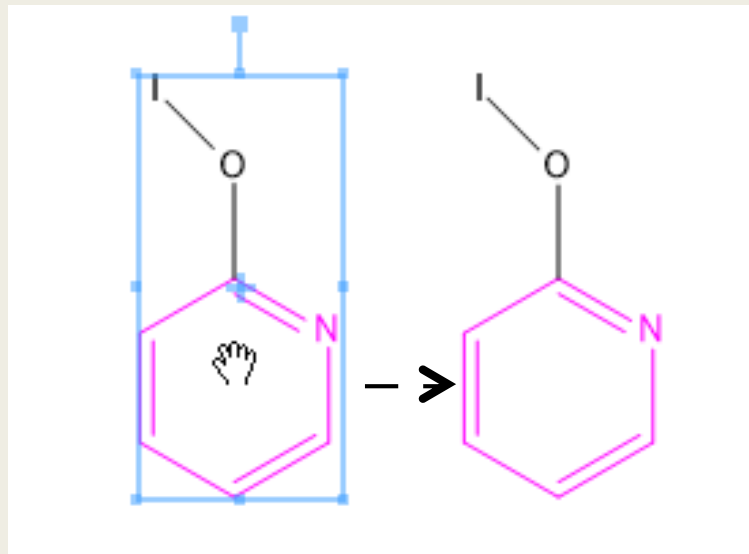
Clean Up Structure

- The **Clean Up Structure** (under **Structure** menu) command is used to neaten the appearance of molecules by regularizing bond lengths and angles.

- Graphic objects, such as arrows and aromatic circles, are not affected. You can use this command to redraw structures that you may have drawn freehand, or to neaten structures that you may have imported from another application.

Clean Up Structure

How To use Clean Up Structure:

1. Select the structure, or part of the structure, to clean up.

2. Navigate to **Structure**>**Clean Up Structure**, or type <Shift>+<Ctrl>+<K> .
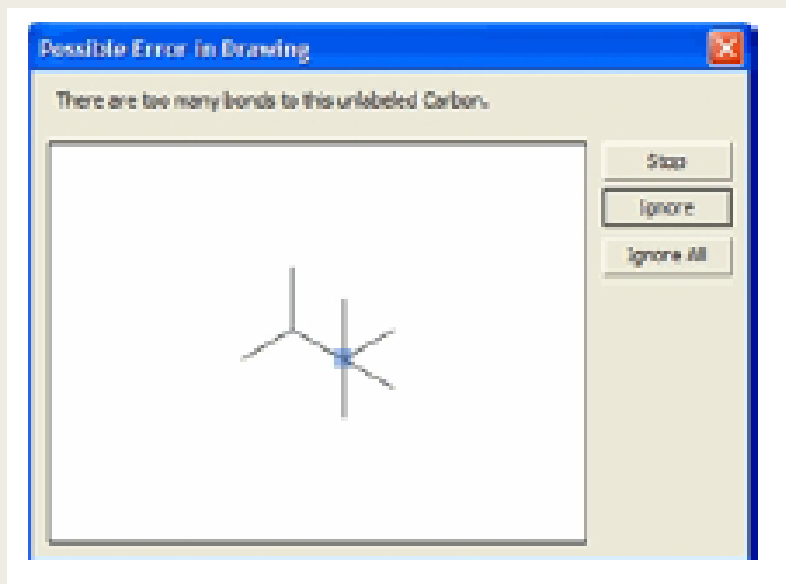
Checking Structures

You can check the chemistry of a selected structure, part of a structure, or caption (in Formula style) with the **Check Structure** command. The structure is checked using normal valences and elements, and defined nicknames.

■ To check the valences of all selected atoms in a structure:

1. Select a structure, part of a structure, or caption.

2. Navigate to **Structure**>**Check Structure**.

Checking Structures

■ If a structure is incorrect, a message window appears, for example:

3. To continue checking the structure, click **Ignore**.

4. To ignore all subsequent errors, click **Ignore All**.

5. To stop checking for errors, click **Stop**.

Chemical Warnings

ChemBioDraw checks chemical syntax as you draw. If it finds an error in your structure, a wavy red box appears around the object. The box displays on the screen only and does not print.

To view a description of the problem, perform one of the following:

- Point at the warning with the mouse to display a tool tip that describes the error.

- Right-click the warning and select **Explain This Warning**.

- Select the structure and navigate to **Structure>Check Structure**.

Chemical Warnings

Warning	Description
Valence and Charge Errors	An Object drawn has an improper valence or charge. For example, when positive and negative charges have been assigned to the same element, charges have been assigned in more than one way, or a charge has been assigned to a nickname, generic nickname, or alternative group name.
Unbalanced Parentheses	Parentheses are not matched into nested open-close pairs.
Invalid Isotopes	Generated for invalid isotopes. For example, this warning is generated for every label that has a numeric superscript immediately preceding an atomic symbol, where the superscripted number does not correspond to a recognized isotope. For example, $^{24}CH_3$.
Isolated Bonds	An unlabeled single bond is not attached to other bonds.
Atoms Near Other Bonds	An atom is close to a bond but not attached to it.
Unspecified Stereo-Chemistry	An asymmetric center is without attached wedged, hashed, dashed, or bold bonds.
Ambiguous Stereochemistry	A stereocenter where the absolute stereochemistry cannot be determined from the structure as drawn. For example, this warning would be generated for a carbon atom attached by bold bonds to four different ligands.