Chem & BioDraw

Chem & BioDraw 11.0 enables scientists, science students, and scientific authors to draw chemical reactions and structures. It is designed to be interactive and easy to use while still providing results that meet the most demanding publication standards.

Starting Chem& BioDraw

You can start the ChemDraw application in the two ways:

The First

· From the desktop, double-click the Chem&BioDraw application icon .

· Click the Chem&BioDraw application and click Open from the File menu.

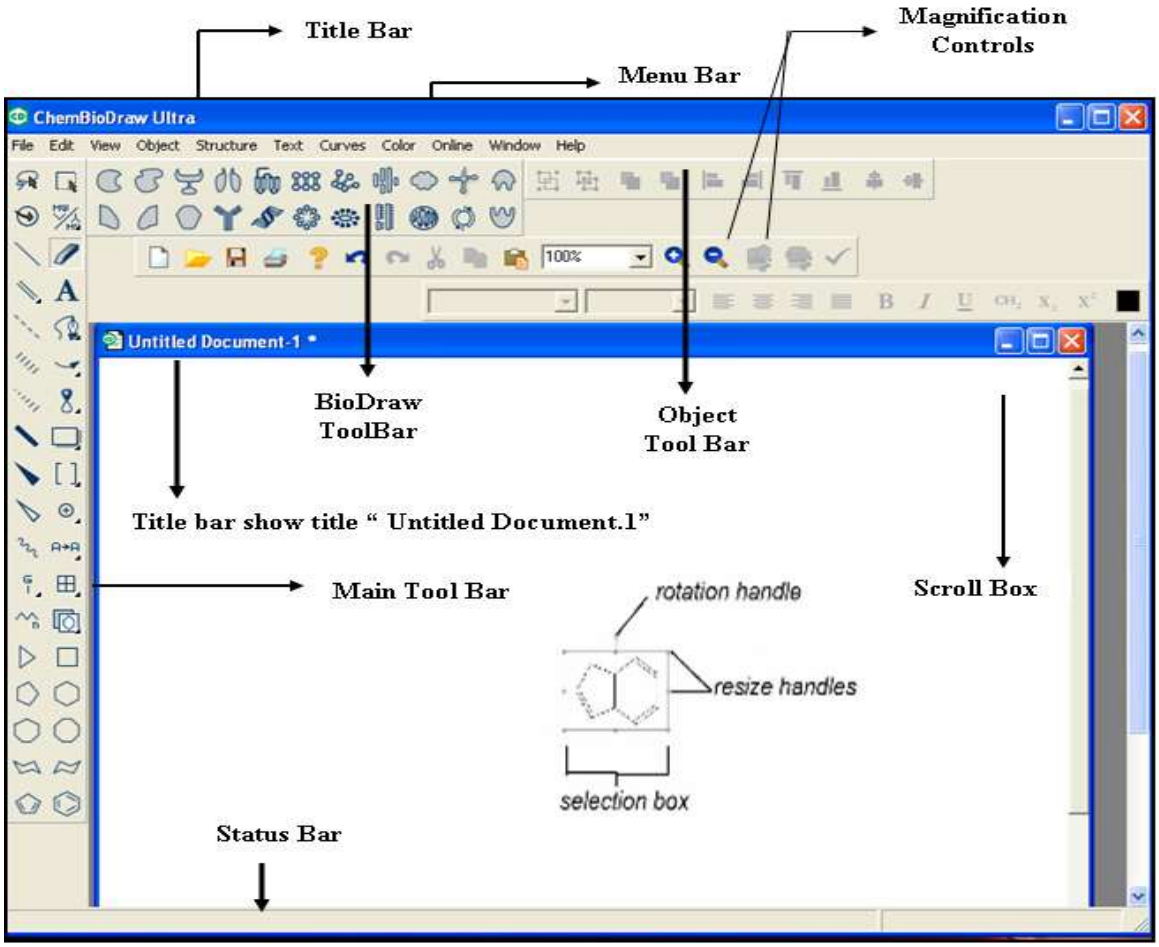
The Second

· From the Start menu ⟶ All Program ⟶ choose Chem&BioDraw.

Chem&BioDraw opens and a new document is created.

Getting Started

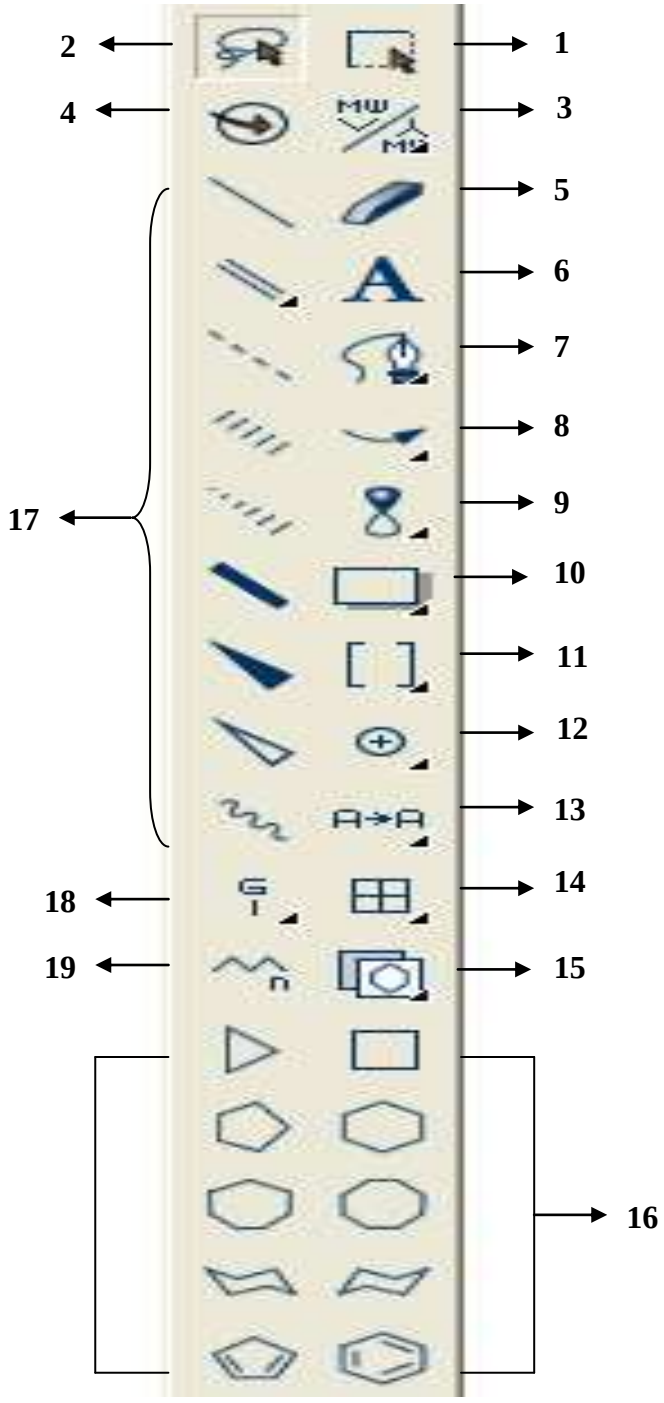
This section describes the Chem & Bio Draw 11.0 graphic user interface (GUI). It explains the various parts of the screen and how to create, open, and save documents. Although the Macintosh and Windows versions of the GUI differ slightly, they are quite similar.



Main Tool Bar

Drawing tools

ChemDraw has 9 types of bond drawing tools in the palette down the left hand side, as shown below. Holding the mouse down on some of the other tools (the ones with the little black triangles) gives you access to lots of options.



	Tool Name	Description
1	Marquee Tool	Used to select objects by dragging diagonally across them. Objects that are selected can be further manipulated using menu commands.
2	Lasso Tool	Used to select objects by dragging around them. Objects that are selected can be further manipulated using menu commands
3	Fragmentation toolbar	The Fragmentation toolbar includes three tools: •**Fragmentation tool**. Splits molecules across specific bonds. •**Dissociation tool**. Breaks bonds and draws a reaction. •**Retrosynthesis tool**. Breaks bonds and draws a reaction
4	Structure Perspective	Rotate a selected object in three dimensions.
5	Eraser Tool	Used to delete objects.
6	Text Tool	Used to create atom labels and captions
7	Curve tools	Draw freehand shapes such as custom arrows and orbitals.
8	Arrow Tool	Used to draw arrows. Arrows of different types can be selected from the Arrow Tools palette .
9	Orbital Tool	Used for drawing orbitals. Orbitals of different types can be selected from the Orbital Tools palette.
10	Drawing Elements Tool	Used to draw objects common to reaction schemes, such as brackets and lines. Drawing Elements of different types can be selected from the Drawing Element Tools palette
11	Brackets toolbar	Draw brackets, parentheses, and braces. Brackets of different types can be selected from the Brackets toolbar
12	Chemical Symbols toolbar	Draw chemically significant symbols such as charges, radicals, and lone pairs. Symbols of different types can be selected from the Symbols toolbar.
13	Query Tools toolbar	Draw stereochemical flags, indicate free sites, alternative groups and correspondences between atoms in query structures. Various options can be selected from the Query toolbar.

14	Table	Draw tables with multiple cells and TLC plates with multiple lanes and adjustable solvent fronts and spots.
15	Templates toolbars	Draw structures with templates stored in template documents
16	Rings	Draw common structural components.
17	Bond	Draw bonds and set bond properties
18	Sequences Tools toolbar	This collection of four tools lets you create protein, DNA, and RNA sequences. For instructions on how to draw sequences, see Drawing sequences
19	Acyclic Chain	Draw chains of any length.

Using Documents

A document is a workspace where you create and edit structures. You can create a new document or open an existing document and edit it.

Creating a Document

You can create a new document using the default settings, or use a Style Sheet with customized settings. To create a document, go to File>New Document.

Using Styles

To create a new document using a different style style sheet or stationery pad:

1. Go to File>Open Special.
2. Choose a Style Sheet from the list.

A new document is created with the settings (and objects) stored in the Style Sheet.

Chem & Bio Draw 11.0 provides predefined Style Sheets located in the ChemDraw Items folder. For example, the ACS Document 1996 is configured to create documents that are set with the bond lengths, bond width, spacing, and fonts used in the 2-column format of all American Chemical Society journals.

For a list of the settings stored in these documents.

Opening Documents

To open a document, do one of the following:

•Go to File>Open. In the Open dialog box, select the name and location of the file and click Open or OK.

•In the File menu, choose the document from the list of previously opened documents at the bottom of the menu.

Discarding Changes

To retrieve the last saved version of a file, Go to File>Revert.

All changes made to the file since it was saved last are discarded and the previous version of the file appears.

Edit>Undo to remove an unsaved change.

Undo, Redo, and Repeat

Chem & Bio Draw 11.0 keeps track of the actions you perform. To undo, redo, or repeat your last action, select the appropriate option in the Edit menu. The number of actions that can be undone or redone is limited only by the amount of memory (RAM and virtual memory) available.

Saving Documents

To save a document in the default format:
1. Go to File>Save. The Save dialog box appears.
2. Choose a folder in which to store the file.
3. Type a file name in the File name in the Save As text box.
4. Select a file format.
5. Click Save or OK.

Aligning Objects

You can align objects vertically and horizontally along their centers or edges. To align two or more objects:
1. Select the objects with a selection tool.
2. Go to Objects>Align and select an Align command.

Fixed Bonds

Use the Info Window to display the bond length and angle as you drag the bond. You can draw any bond length or create any angle relative to the X-axis. However, it is generally more useful to draw bonds that are constrained to a fixed length and a fixed angle.
Fixed bond lengths
To draw bonds that are constrained to a fixed length:
1. Go to Objects>Fixed Lengths. A check mark appears next to the Fixed Lengths command.
2. Using the Solid Bond tool, begin drawing a structure. The bonds in the new structure appear at stand lengths.

Fixed bond angles

To draw bonds with constrained angles that are multiples of 15 degrees relative to the X-axis:
1. Go to Objects>Fixed Angles. A check mark appears next to the Fixed Angles command.
2. Select a bond tool.
3. Begin drawing a structure.

To change the default fixed values:
1. Go to File>Document Settings and click the Drawing tab.
2. Enter a value in the Fixed Length text box. Use in, cm, pt, or iu for units (default is .4167 in.).
3. Enter a value in the Chain Angle text box.
4. Click OK.

Check Structure

To check the valences of all selected atoms in a structure:
1. Select a structure, part of a structure, or caption with a selection tool.
2. Click the Check Structure command on the Structure menu.
Each label in the structure is checked. sequentially. When a label is incorrect, a message window appears. To continue checking the structure when a message appears, click

Ignore. To ignore all subsequent errors in a structure, click Ignore All. To stop checking a structure when a message appears, click Stop.

Converting Names to Structures

Insert Structure lets you type the name and convert it to its structure. For example, to insert 2-bromobenzoic acid:

1. Go to Structure>Convert Name to Structure.

The Insert Structure dialog box appears.

2. Type 2-bromobenzoic acid.

Converting Structures to name

To insert the name of a structure into your drawing:

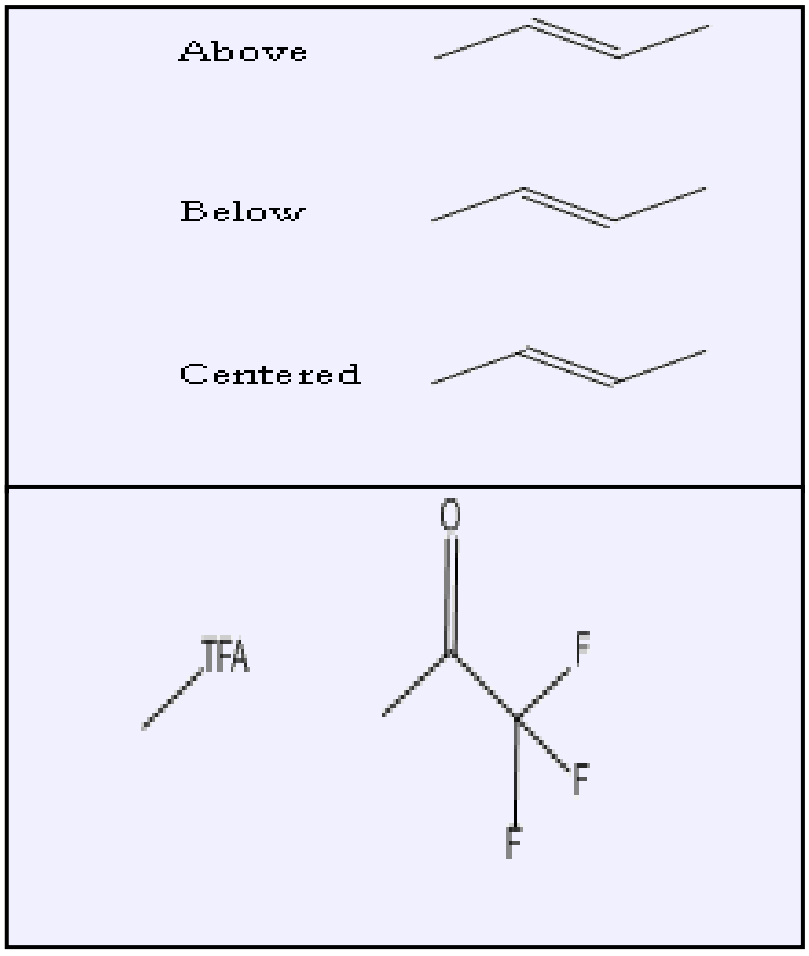
1. Select the drawing for which you want to insert a name.
2. Go to Structure>Convert Structure to Name.

The name of the structure appears as a caption under your drawing.

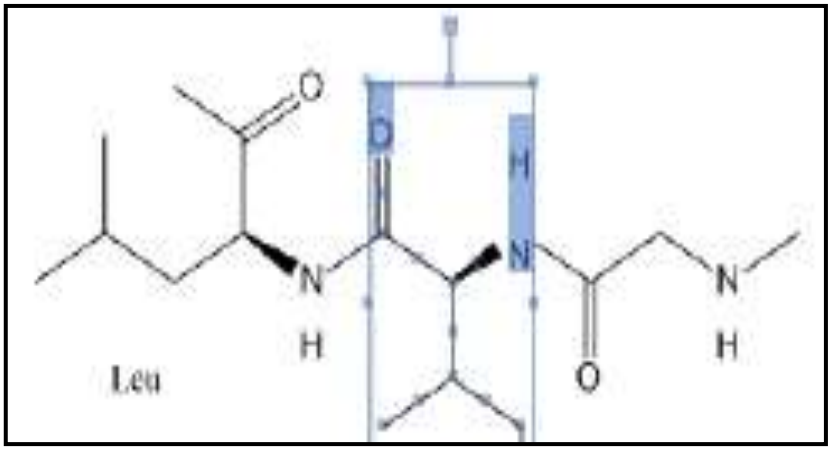
Drawing Structures

The Main Toolbar and Multiple Bonds toolbar offer a variety of options for drawing bonds. Some of the bond tools, such as double bond, are for drawing bonds of a specific type. Others, like the Any bond, are intended to represent nonspecific bonds–a single bond, double bond, or something else.

Example : to draw bonds



You can select any part form structure see the figure below



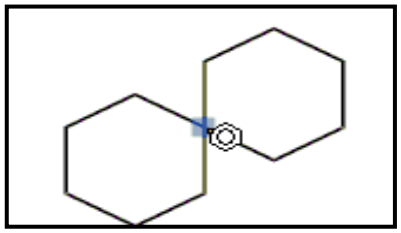
Rings

The Main Toolbar contains several ring tools that let you draw various ring sizes and types: To draw a ring:

1. Select a ring tool from the Main Toolbar.
2. Click and drag in the document window to orient the ring the way you want.

Spiro and sprout rings

If you click an atom in a ring, a spiro link is formed.



You can change this default behavior to sprout a bond instead.

1. Go to File>Preferences.
2. On the Building/Display tab, check the box next to Sprout Rings Instead of Spiro When Clicking.