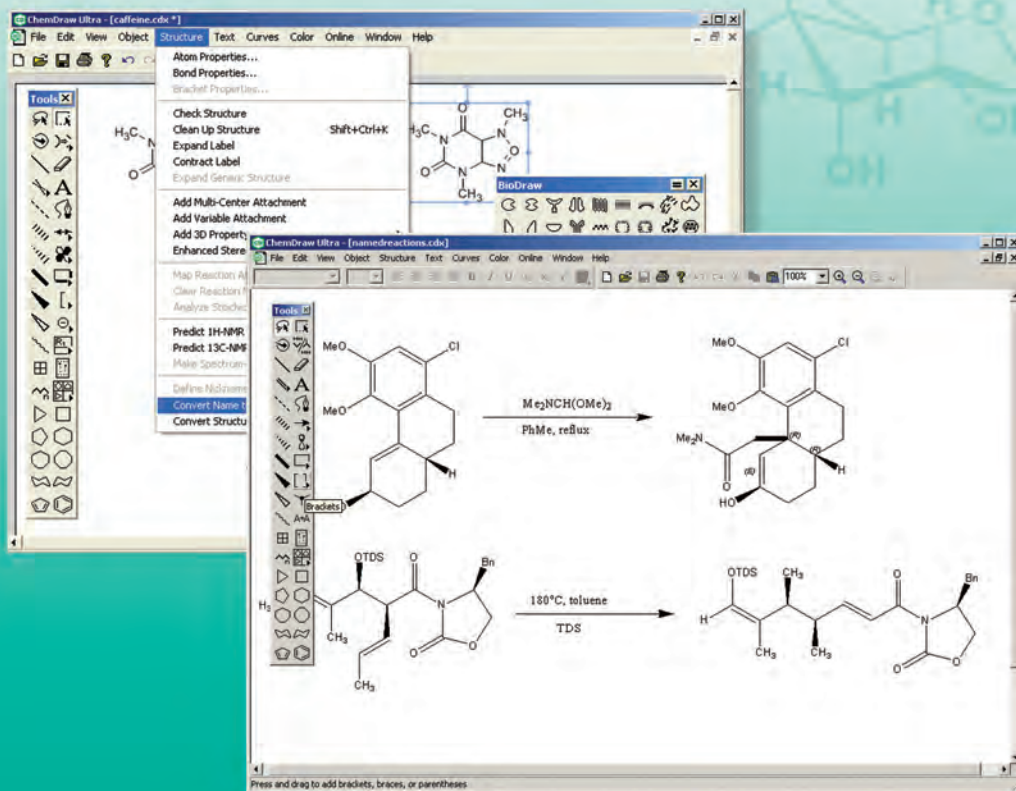




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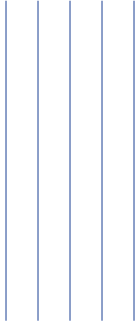
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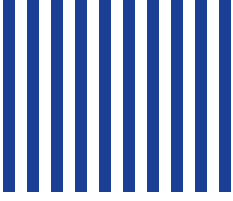
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### **Q: That makes sense, but what do I get out of purchasing my own software?**

**A:** When you purchase authorized copies of software programs, you receive user guides and tutorials, quick reference cards, the opportunity to purchase upgrades, and technical support from the software publishers. For most software programs, you can read about user benefits in the registration brochure or upgrade flyer in the product box.

### **Q: What exactly does the law say about copying software?**

**A:** The law says that anyone who purchases a copy of software has the right to load that copy onto a single computer and to make another copy “for archival purposes only” or, in limited circumstances, for “purposes only of maintenance or repair.” It is illegal to use that software on more than one computer or to make or distribute copies of that software for any other purpose unless specific permission has been obtained from the copyright owner. If you pirate software, you may face not only a civil suit for damages and other relief, but criminal liability as well, including fines and jail terms of up to one year

### **Q: So I'm never allowed to copy software for any other reason?**

**A:** That's correct. Other than copying the software you purchase onto a single computer and making another copy “for archival purposes only” or “purposes only of maintenance or repair,” the copyright law prohibits you from making additional copies of the software for any other reason unless you obtain the permission of the software company.

### **Q: At my company, we pass disks around all the time. We all assume that this must be okay since it was the company that purchased the software in the first place.**

**A:** Many employees don't realize that corporations are bound by the copyright laws, just like everyone else. Such conduct exposes the company (and possibly the persons involved) to liability for copyright infringement. Consequently, more and more corporations concerned about their liability have written policies against such “softlifting”. Employees may face disciplinary action if they make extra copies of the company's software for use at home or on additional computers within the office. A good rule to remember is that there must be one authorized copy of a software product for every computer upon which it is run

### **Q: Can I take a piece of software owned by my company and install it on my personal computer at home if instructed by my supervisor?**

**A:** A good rule of thumb to follow is one software package per computer, unless the terms of the license agreement allow for multiple use of the program. But some software publishers' licenses allow for “remote” or “home” use of their software. If you travel or telecommute, you may be permitted to copy your software onto a second machine for use when you are not at your office computer. Check the license carefully to see if you are allowed to do this.

### **Q: What should I do if become aware of a company that is not compliant with the copyright law or its software licenses?**

**A:** Cases of retail, corporate and Internet piracy or non-compliance with software licenses can be reported on the Internet at <http://www.siiia.net/piracy/report.asp> or by calling the Anti-Piracy Hotline: (800) 388-7478.

**Q: Do the same rules apply to bulletin boards and user groups? I always thought that the reason they got together was to share software.**

A: Yes. Bulletin boards and user groups are bound by the copyright law just as individuals and corporations. However, to the extent they offer shareware or public domain software, this is a perfectly acceptable practice. Similarly, some software companies offer bulletin boards and user groups special demonstration versions of their products, which in some instances may be copied. In any event, it is the responsibility of the bulletin board operator or user group to respect copyright law and to ensure that it is not used as a vehicle for unauthorized copying or distribution.

**Q: I'll bet most of the people who copy software don't even know that they're breaking the law.**

A: Because the software industry is relatively new, and because copying software is so easy, many people are either unaware of the laws governing software use or choose to ignore them. It is the responsibility of each and every software user to understand and adhere to copyright law. Ignorance of the law is no excuse. If you are part of an organization, see what you can do to initiate a policy statement that everyone respects. Also, suggest that your management consider conducting a software audit. Finally, as an individual, help spread the word that users should be "software legal."

**Q: What are the penalties for copyright infringement?**

A: The Copyright Act allows a copyright owner to recover monetary damages measured either by: (1) its actual damages plus any additional profits of the infringer attributable to the infringement, or (2) statutory damages, of up to \$150,000 for each copyrighted work infringed. The copyright owner also has the right to permanently enjoin an infringer from engaging in further infringing activities and may be awarded costs and attorneys' fees. The law also permits destruction or other reasonable disposition of all infringing copies and devices by which infringing copies have been made or used in violation of the copyright owner's exclusive rights. In cases of willful infringement, criminal penalties may also be assessed against the infringer.

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	Chem & Bio 3D		■	
	Chem & Bio Finder		■	
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	ChemACX, ChemMSDX			■
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	ChemINDEX, NCI & AIDS, ChemRXN			■
	Ashgate Drugs, Traditional Chinese Medicines			■
	ChemSynth, ChemReact68			■
	Medicinal Chemistry			■
Tips	Structure Drawing Tips	■		
	Searching Tips	■	■	■
	Importing SD Files		■	

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# Introduction

This User's Manual provides information on three CambridgeSoft products: ChemDraw, BioDraw, and ChemDraw/Excel.

## About ChemDraw

ChemDraw<sup>®</sup> is a desktop application that enables professional scientists, science students, and scientific authors to communicate chemical structures. It is designed to work according to conventions that we have found to be most intuitive for such users. Our goal has been to make ChemDraw as easy to use as possible while providing superior drawing quality.

ChemDraw is integrated with the following CambridgeSoft products:

- ChemFinder
- Chem3D
- ChemDraw/Excel
- ChemOffice 2006

## About BioDraw

BioDraw<sup>®</sup> is a desktop application for drawing and presenting biological pathways. Common pathway elements (membranes, DNA, enzymes, receptors, etc.) are built in, and other elements may be imported. The pathways you create with BioDraw can be exported for use in presentations, grant proposals, and publications.

## About ChemDraw/Excel

The ChemDraw/Excel<sup>®</sup> add-in is an extension of Microsoft<sup>®</sup> Excel<sup>®</sup> for Windows. ChemDraw/Excel enables you to:

- Add chemical structures and other data from ChemDraw or a ChemFinder database to an Excel spreadsheet.
- Search using the same search features as ChemFinder.
- Perform calculations on chemical structures.

See the ChemOffice manual for information on other CambridgeSoft add-ins for Excel.

## About This Manual

This User's Manual contains information for the ChemDraw application for Windows and Macintosh. It assumes that you are familiar with the basics of your Windows operating system. If you are not, please refer to your system manual before using the applications. Some of the material describes tasks that must be performed in conjunction with other integrated CambridgeSoft products. The material on the Addins describes tasks that must be performed in conjunction with Microsoft Excel. If you are not familiar with this product, please consult the relevant User's Manual for more detailed information.

The chapters in this guide are organized by task. They are intended to help you familiarize yourself with the ChemDraw applications and start using them as quickly and efficiently as possible.

New users should read the **Introducing ChemDraw** chapter to get an overview of the product GUI and how to use it. They may then continue with Chapter 2 **Tutorials**, which demonstrate most of the features of the application. Perform the tutorials in the order they are presented.

Chapter 3 covers the basic structure drawing techniques: bonds, atom labels, selecting and moving objects.

Chapter 4 continues the discussion of structures with more advanced techniques: drawing reactions, joining and grouping structures, formatting and repeating labels, constrained bonds, and more.

Chapter 5 discusses the special ChemDraw features that allow you to create query structures for searching databases.

Chapter 6 discusses ChemDraw's chemistry features: chemical analysis and properties, stereochemistry, and the new Stoichiometry Grid.

Chapter 7 discusses ChemDraw's naming algorithms, Struct=Name and Name=Struct.

Chapter 8 discusses ChemNMR.

Chapter 9 describes the Drawing Objects you can add to your ChemDraw structures to produce drawings for publication or presentations.

Chapter 10 continues the topic of publication/presentation with a detailed discussion of page layout.

Chapter 11 discusses sharing information, both importing other chemical and graphical formats and exporting to chemical software, spreadsheet, or publication software.

Chapter 12 discusses BioDraw.

Chapter 13 discusses ChemDraw/Excel.

The appendices discuss using the CambridgeSoft website, ChemDraw customization, details of ChemDraw's chemistry features, file formats, document setting, and troubleshooting.

## What's New in ChemDraw 10.0

Enhancements to ChemDraw 10.0 include:

- [New Lasso](#)
- [New Arrows](#) (see also "Tutorial 2: Drawing an Intermediate" on page 31)
- [Adjustable Drawing Objects](#)
- [Terminal Carbon Labels](#)

- **Pro** [Relative Stereochemistry](#)
- **Ultra** [Improvements to Struct=Name](#)
- **Ultra** [BioDraw](#)
- **Ultra** [Stoichiometry Grid](#)
- **Pro** [Improved ISIS compatibility](#)
- [Improved Table tool behavior](#)
- [InChI™ support](#)

Enhancements to PlugIns and ActiveX include:

- [More Browser Support](#)

## Conventions

The following notations are used throughout this user's guide:

**Ultra** The Ultra symbol indicates that a feature is available in the Ultra version only.

**Pro** The Pro symbol indicates that a feature is available in both the Pro and Ultra versions.

Features that are available in the Standard version are not indicated by a symbol.

*NOTE: Notes such as this are used to highlight important information.*

*TIP: Tips supply useful, "nice to know", information supplemental to the main text.*

---

### CAUTION

*Indicates important information that, if ignored, might lead to data loss or other serious problems.*

---

When a shortcut key sequence is given, the Windows OS sequence is listed first, with the Macintosh OS sequence following, for example: "Use the command: Shift+Control+G or Shift+Command+G to ungroup objects."



A special font is used to indicate labels or commands in the GUI, for example: “Click the **Help Contents**. command on the Help menu.” The exact text you will see in the GUI is used in these references.

## Additional Information

Additional sources of ChemDraw information are:

- The Quick Reference Cards.
- The Help system
- CambridgeSoft Web Pages.  
<http://www.cambridgesoft.com/>

## Quick Reference Card

The ChemDraw Quick Reference Cards are located in the back of the manual. The cards provide summaries of ChemDraw Desktop Application commands and features. Because many of the instructions require knowledge of the interface elements, use the Quick Reference card as you perform the tutorials in Chapter 2: “Tutorials”.

## Help System

ChemDraw provides the following types of Help:

- **ChemDraw Help**. An HTML reference guide.
- **Context-sensitive Help** (Windows). Help topics related to user interface objects. To access Context sensitive Help type **Shift+F1**.
- **ToolTips**. Short descriptions of user interface objects displayed by pointing.
- **Status Bar**. The lower left corner of the GUI displays useful information as you work.

## CambridgeSoft Web Pages

The following table contains the addresses of ChemDraw-related web pages.

Table 1: ChemDraw-related web pages

For information about ...	Access ...
Technical Support	<a href="http://www.cambridge-soft.com/services">http://www.cambridge-soft.com/services</a>
ChemDraw Plugin	<a href="http://www.cambridge-soft.com/services/documentation/chemdrawplugin/">http://www.cambridge-soft.com/services/documentation/chemdrawplugin/</a>
Chem3D ActiveX control	<a href="http://www.cambridge-soft.com/services/documentation/chem3dcontrol/">http://www.cambridge-soft.com/services/documentation/chem3dcontrol/</a>
Software Developer's kit	<a href="http://sdk.cambridge-soft.com/">http://sdk.cambridge-soft.com/</a>
Purchasing CambridgeSoft products and chemicals	<a href="http://chemstore.cambridge-soft.com/">http://chemstore.cambridge-soft.com/</a>

## Installation and System Requirements

Before installation, see the “ReadMeFirst” and any other ReadMe documents on the installation CD-ROM.

### Microsoft® Windows® Requirements

- Windows 2000 or XP.
- Microsoft® Office add-ins require Office 2000, 2003, or XP.

- Screen resolution must be 800 x 600 or higher.

ChemDraw plugins/ActiveX<sup>®</sup> controls support Microsoft IE 6.x, Netscape<sup>®</sup> 7.x and 8.x, Mozilla 1.x, and Firefox 1.x.

The Chem3D ActiveX control supports Microsoft IE 6.x, Netscape<sup>®</sup> 7.x and 8.0, Mozilla 1.x, and Firefox 1.x.

*NOTE: Windows XP Service Pack 2 includes security features that automatically block active content. This means that by default, Internet Explorer blocks ChemDraw and Chem3D ActiveX controls. To activate them, you must choose the option to “allow blocked content” from the bar appearing under the address bar notifying you that the security settings have blocked some of the content of the page. IE does not remember this information, so you must repeat the*

*activation each time you access the page.*

*If you visit a site frequently, you can add it to the list of trusted sites in IE’s security settings.*

## **Macintosh<sup>®</sup> Requirements**

- Mac<sup>®</sup> OS X 10.2.2-10.2.8, 10.3.x, or 10.4
- Screen resolution must be 800 x 600 or higher.

ChemDraw Plugin supports Safari 1.4 or higher, Mozilla 1.7.5 or higher, Firefox 1.x, and Netscape 7.0.x

## **Site License Network Installation Instructions**

If you have purchased a site license, please see the following web site for network installation instructions:

<http://www.cambridgesoft.com/services/sl/>

# Chapter 1: Introducing Chem & Bio Draw

## Overview

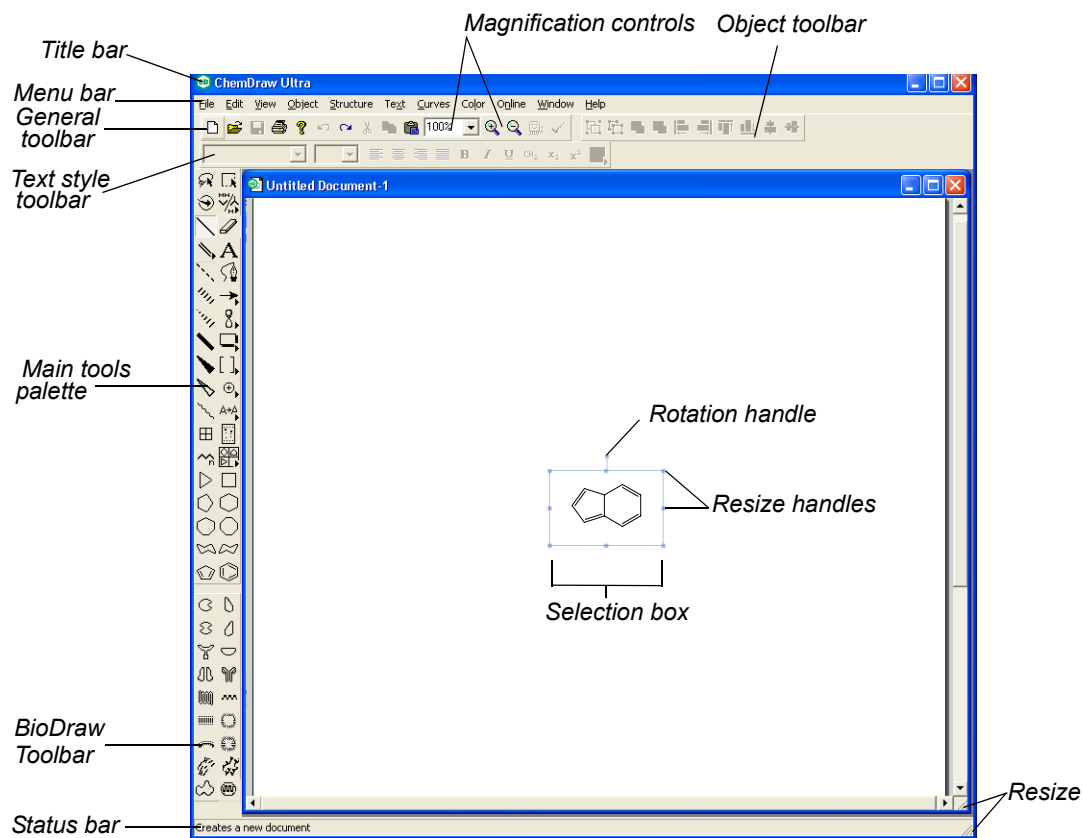
This section introduces the new user to the ChemDraw GUI. It covers the following topics:

- Identifying the parts of the ChemDraw interface.
- Creating, opening, and saving documents.

Figure 1.1: ChemDraw Windows Ultra GUI

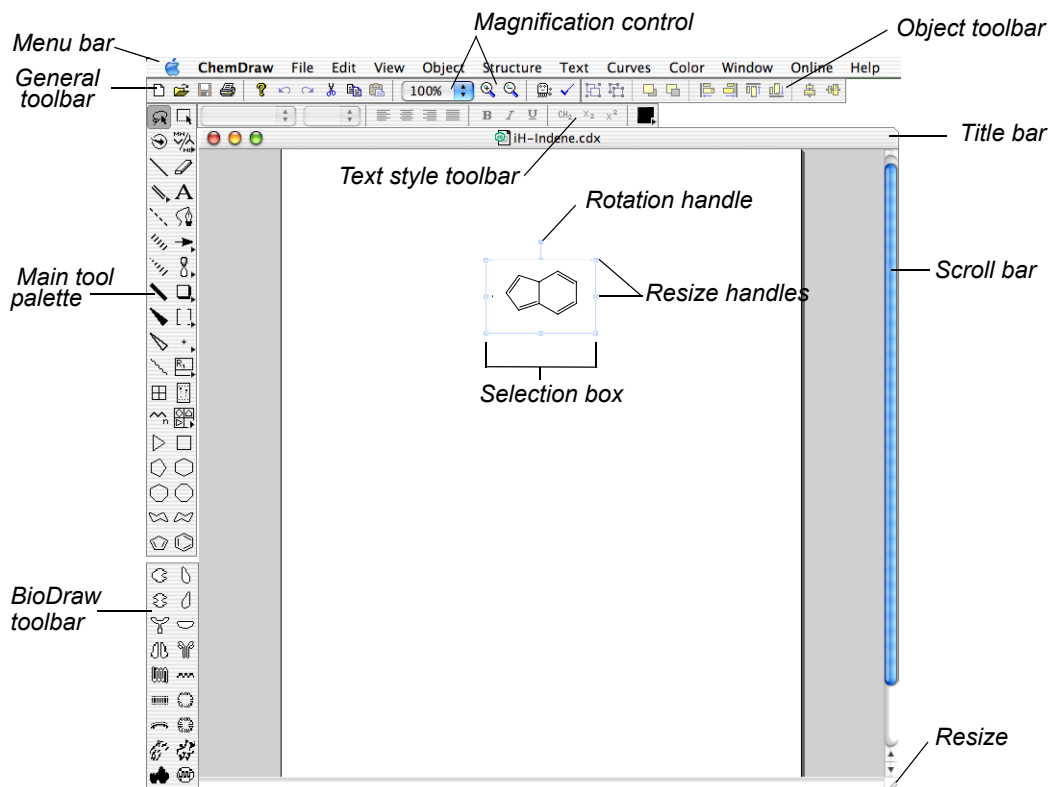
## The ChemDraw Graphical User Interface

Although the Macintosh and Windows versions of the ChemDraw graphical user interface (GUI) differ slightly, the essential GUI consists of the same elements. The Windows version of ChemDraw is shown in *Figure 1.1*.



The Mac GUI is shown in *Figure 1.2*.

Figure 1.2: ChemDraw Mac Ultra GUI



## The Main Tools Palette

different for the different versions of ChemDraw.

Use the main tools palette to create and manipulate drawings. The appearance of the toolbar is slightly

The toolbar for ChemDraw Ultra is shown in Figure 1.3.

Figure 1.3: Main Tools Palette

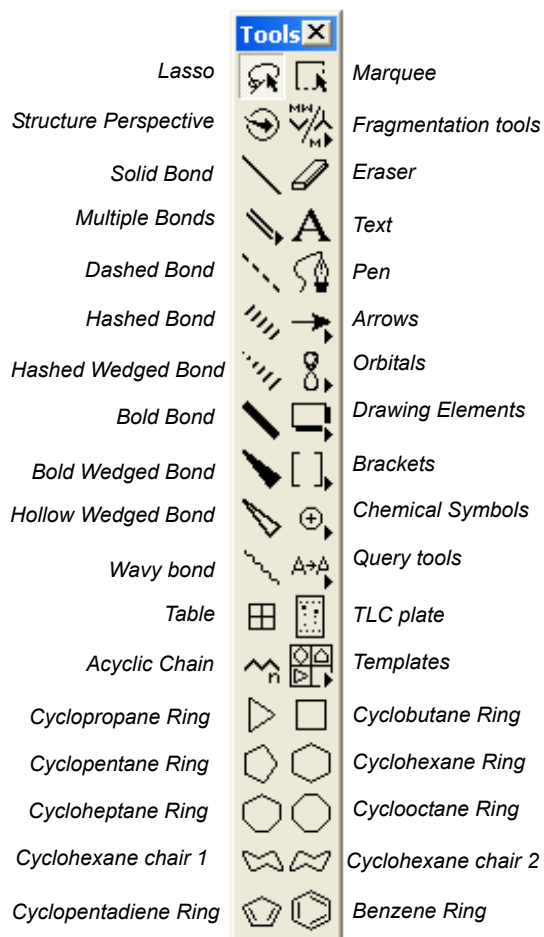


Table 2 describes the functions of the tools for all versions. Some of the tools have multiple options that can be selected from a tool palette.

Table 2: Main Tools Palette

Tool	Use to...
Selection	<b>Lasso.</b> Select objects by dragging around them.
	<b>Marquee.</b> Select objects by dragging diagonally across them.
	Selected objects can be further manipulated using menu commands.
Structure Perspective	Rotate a selected object in three dimensions.
Fragmentation toolbar	<b>Fragmentation tool.</b> Splits molecules across specific bonds.
	<b>Dissociation tool.</b> Breaks bonds and draws a reaction.
	<b>Retrosynthesis tool.</b> Breaks bonds and draws a reaction.
Bond	Draw bonds and set bond properties.
Eraser	Delete objects. Click on an object to delete; drag to delete multiple objects. If you click a multiple bond, it will reduce the bond order. If you double-click any part of a structure, it deletes the entire structure
Multiple Bond toolbar	Draw multiple bonds and set bond properties. Bonds of different types can be selected from the Multiple Bonds tool palette.

Table 2: Main Tools Palette

Tool	Use to...
Text	Create atom labels and captions.
Pen	Draw freehand shapes such as custom arrows and orbitals.
Arrows toolbar	Draw arrows. Arrows of different types can be selected from the Arrows toolbar.
Orbitals toolbar	Draw orbitals. Orbitals of different types can be selected from the Orbitals toolbar.
Drawing Elements toolbar	Draw annotations that lack chemical significance, such as boxes and lines. Drawing Elements of different types can be selected from the Drawing Elements toolbar.  Includes the Arc tools. <b>Pro</b>
Brackets toolbar	Draw brackets, parentheses, and braces. Brackets of different types can be selected from the Brackets tool palette.
Chemical Symbols toolbar	Draw chemically significant symbols such as charges, radicals, and lone pairs. Symbols of different types can be selected from the Symbols tool palette.

Table 2: Main Tools Palette

Tool	Use to...
Arcs toolbar	Draw arcs. Arcs of different degrees can be selected from the Arcs tool palette.  The Arcs tool is a separate tool only on ChemDraw Standard.
Acyclic Chain	Draw chains of any length.
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 tool palette.
Templates toolbars	Draw structures with templates stored in template documents. Templates can be selected from the Templates toolbars.
Rings	Draw common structural components.
Table	Draw tables with multiple rows and columns.
TLC Plate <b>Pro</b>	Draw TLC plates with multiple lanes and adjustable solvent front and spots.

## Tearing Off Palettes

Some tools have toolbars extending from them, indicated by an arrow at the bottom right of the tool button.

Figure 1.4: Tearing off the symbols palette

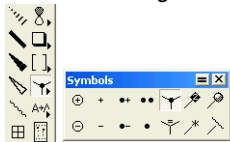


You can “tear off” these toolbars and place them anywhere in the ChemDraw screen. You cannot dock torn off toolbars.

To tear off a toolbar:

- Click the arrow on the lower right of the tool.
- Holding the mouse button down, point to the title bar and release the mouse button.

Figure 1.5: Symbols as a floating toolbar



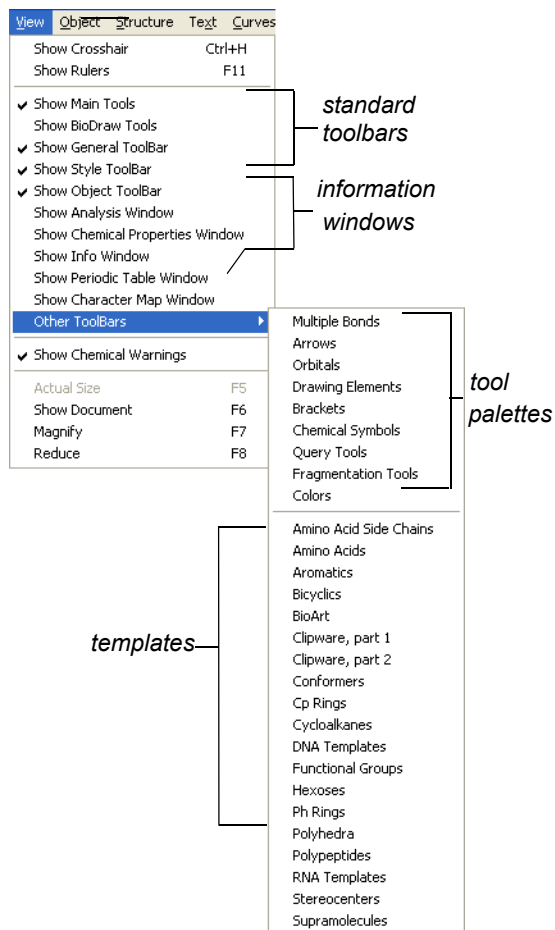
You can drag the toolbar by its title bar to reposition it.

You can also show or hide a toolbar by selecting it from the Other Toolbars submenu on the View menu.

## Optional Toolbars

ChemDraw provides a number of optional toolbars and information windows to facilitate production of ChemDraw documents. These toolbars are accessed from the View menu. They are divided into three basic groups: Standard Toolbars and Show Windows, Tool Palettes, and Templates

Figure 1.6: Optional toolbars on the View menu



## Showing and Hiding Toolbars

To show or hide a toolbar:

- select a toolbar from the View menu.

A check mark appears next to the item when the toolbar is displayed.

## Docking and Undocking Toolbars

The standard toolbars, can be docked or undocked. Docked toolbars can attach to any edge of the ChemDraw window. Undocked toolbars can float anywhere in the on your monitor screen.

To dock a toolbar do one of the following

- Drag the toolbar to the edge of the ChemDraw screen where you want it to dock.
- Double-click the toolbar background. This will dock the toolbar in the default position. (All toolbars default to the top of the ChemDraw window, except for the Tools toolbar which defaults to the left side.)

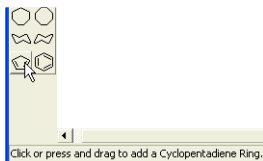
To undock a toolbar do one of the following:

- Drag the toolbar into the position you want
- Double-click the toolbar.

## The Status Bar or Message Area (Windows)

The status bar or message area displays information about the menu or toolbar you are using.

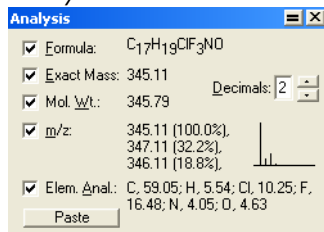
Figure 1.7: Status bar




## The Analysis Window

The Analysis window displays the chemical analysis of the selected structure. If nothing is selected, the values shown are for the entire document.

Figure 1.8: Analysis window



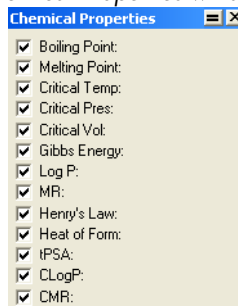
See “Viewing Analysis Information” on page 111 for information on the Analysis window.


The Paste button inserts all selected items into the document. The button  shrinks the window to just the title bar.

## Pro The Chemical Properties Window

The Chemical Properties window displays properties of the selected structure. When no structure is selected, properties will be displayed only if there is one (and only one) structure in the document.

Figure 1.9: Chemical Properties window



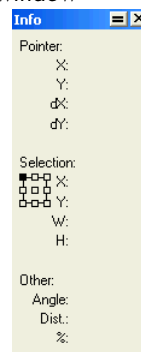
The Paste button inserts all selected items into the document. The button  shrinks the window to just the title bar, while leaving it active.

*NOTE: CLogP and CMR values are displayed only in ChemDraw Ultra.*

## The Info Window

The Info window shows size/positioning information about what's going on in ChemDraw.

Figure 1.10: Info window





The fields are shown in *Table 3*.

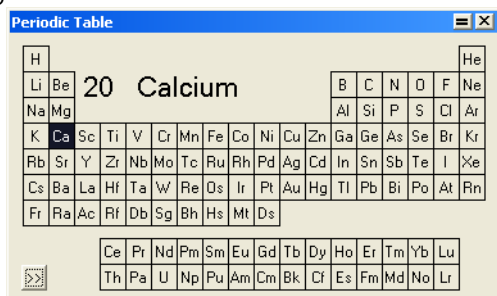
Table 3: Info window fields


Field	Shows...
<b>Pointer:</b>	
X/Y	current mouse coordinates
<b>Pointer:</b>	
dX/dY	change in X and Y coordinates of a moved selection
<b>Selection:</b>	
X/Y	position of a selection
W/H	width/height of a selection
Angle:	angle of a bond; rotation of a selection
Dist:	length of a bond; distance a selection has been moved
%	% of original size when resizing a selection

## Periodic Table

The Periodic Table window displays a floating periodic table. It can be used both for reference and to insert elements into structures. To show or hide the Periodic Table, select/deselect it in the View menu.

Figure 1.11: Periodic Table:



Click an element symbol to highlight the element and activate the Text tool. Drag across the table to highlight each element in turn. Click the  button to show or hide the detailed information.

After selecting an element, click in the document to add an atom label consisting of that element and the appropriate number of hydrogens. Labeling behavior is shown in *Table 4*.

Table 4: Labeling with the Periodic Table

### click on... to...

an existing unlabeled atom	label the atom
an existing labeled atom	cycle the hydrogen count (if it matches the selected element) or change the label
an empty space	create a new atom

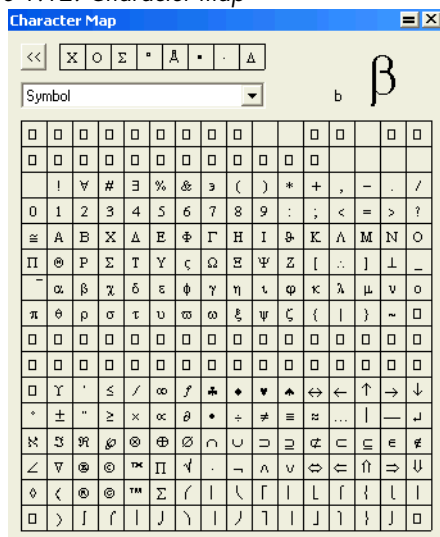
Double-clicking on an existing atom will open it for editing without changing the label.

*NOTE: Some element names conflict with ChemDraw Hotkeys, and may not be interpreted correctly by Chemical Warnings or Check Structure. For more information and troubleshooting see "Defining Nicknames" on page 82.*

## Character Map

The floating Character Map window displays the 256 ASCII characters in any font. The default font is Symbol. Use it to add symbols or styled fonts to labels.<sup>6</sup>


Figure 1.12: Character map



The character map is active only when a text box is open for editing. It will appear grayed-out at all other times. With a text box open, mouse over the character map to view a larger version of the characters in the top right corner of the window. Click any character in the table to enter that character in the text box. The selected font (shown in the character map window) is applied to that character only. It does not change the active font in the text box.

*NOTE: You can cancel a selection by dragging to some other character before releasing.*

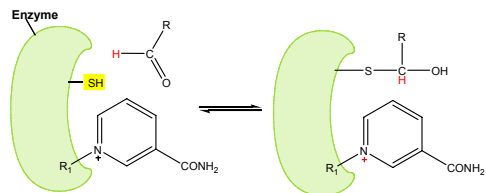
The 8 most recently used characters are displayed at the top of the window. These characters retain their font and are not affected by changes to the window. A single character may appear more than once in this section if the versions use different fonts.

Click the back button to toggle between the 8 most recently used characters and the entire character map. 

## BioDraw

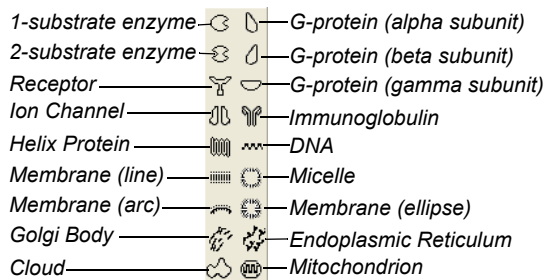
ChemDraw Ultra now incorporates BioDraw tools, allowing you to include drawings of metabolic pathways in ChemDraw files.

Figure 1.13: Partial depiction of the mechanism of action of glyceraldehyde 3-phosphate dehydrogenase<sup>1</sup>



The BioDraw tools palette is activated from the View menu. The toolbar contains special drawing tools such as enzymes and receptors. Standard shapes, such as circles or ellipses, can be added from the Drawing Elements tool palette. You can also use the Pen tool to create custom shapes.

Figure 1.14: BioDraw Toolbar



As with the Drawing Elements, you can change the color of an object with the Color menu, and the line and fill properties with the Curves menu. You can also rotate, or change the size, after selecting it. You create a BioDraw object by either clicking or dragging on the page where you want it to appear. Clicking gives you the default size and shape, dragging allows you not only to enlarge the object, but to distort it as well by dragging differently on the x

1. H. Lodish, et. al., **Molecular Cell Biology**, Scientific American Books, New York, NY, 1995, p. 743.

and y axes. Linear objects elongate in the direction they are dragged. The membrane and protein tools (DNA and Helix) add more subunits as they are dragged; proteins display the subunit count.

## Customizable Objects

Some of the BioDraw objects can be customized after being created. The table below describes the customization options.

Table 5: Customizable BioDraw Objects

Tool	Customization Options
1-Substrate Enzyme	size of the enzyme opening
Receptor	width
Helix Protein	height, width of the strands, width of the cylinders, spacing
DNA	height, width of the strands, offset of the second strand, spacing
Membrane (line)	size of subunit
Membrane (arc)	length, arc, size of subunit
Membrane (ellipse)	size of subunit
Micelle	size of subunit
Golgi part (long)	length, width, curvature

## Other Toolbars

The **Other Toolbars** command on the View menu gives a list of toolbars that can be opened from the

main Tools Palette and a list of structure and clip art templates that users may find useful.

Table 6: Structure and Clipart Templates

BioArt	Clipware 1	Clipware 2
Amino Acids	Aromatics	Bicyclics
Conformers	Cp Rings	Nanotubes
Amino Acid side chains	DNA templates	RNA templates
Functional groups	Hexoses	Supramolecules
Ph Rings	Polyhedra	Stereocenters

## Using Documents

Documents are the ChemDraw workspace where you create and manipulate structures. You can create a new document or open an existing document and edit it.

### Creating a Document

You can create a new, blank document using the ChemDraw default settings, or use a Style Sheet or Stationery Pad with customized settings.

### Creating a New Document

To create a document:

Click the **New Document** command on the File menu.

### Creating a Document Using a Style Sheet or Stationery Pad

To create a new document using a different Style Sheet or Stationery Pad:

1. Click the **Open Special** command on the File menu.
2. Choose a Style Sheet or Stationery Pad from the list.

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

ChemDraw provides pre-defined Style Sheets or Stationery Pads 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, see Appendix B: “Document Settings”. For more information on publication guidelines, see

<http://www.cambridgesoft.com/services/downloads/stylesheets.cfm>

*NOTE: Predefined Style Sheets or Stationery Pads may restrict your options in unexpected ways. For example, not all Save As... format options are available in all Style Sheets or Stationery Pads. For general use, you should stay with the default Style Sheet or Stationery Pad.*

## Opening a Document

To open a document:

From the File menu, do one of the following:

- Choose **Open**, and in the Open dialog box, select the name and location of the file and click **Open** or **OK**.
- Choose the document from the list of previously opened documents at the bottom of the menu.

## Discarding Recent Changes to a Document

To retrieve the last saved version of a file, click the **Revert** command on the File menu.

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

*NOTE: You can use the Undo command in the Edit menu to remove each individual action since the last save.*

## Saving Documents

To save a ChemDraw document in the default ChemDraw CDX file format:

1. Click the **Save** command on the File menu.  
The Save dialog box appears. The appearance of the dialog box depends on the platform you are using.
2. Choose a folder in which to store the file.
3. Type a file name in the File name (Windows) or Save As (Macintosh) text box. You may type up to 255 characters for a file name, including spaces. For example: “my first structure in ChemDraw”.
4. Click **Save** or **OK** to create the file.

The title of the document window changes to the name of the saved file. The file name is added to the bottom of the File menu.

---

### CAUTION

*ChemDraw uses the CDX file format to store chemical information accurately with a structure drawing. Other file formats may be capable of storing a picture of your drawing, but they might lose chemically relevant information about the structure. For example, if you save a ChemDraw drawing in the EPS file format, you will store only a picture of the structure without storing the chemical significance of the connections between atoms and bonds.*

---

## Saving a Document in a Different File Format

To save a ChemDraw document in another file format:

1. Click the **Save As** command on the File menu.  
The Save As dialog box appears.
2. Select a folder in which to save the document.
3. Type a file name in the in the **File name** or **Save As** box.
4. Select a file format from the **File Format** or **Save as Format** list.

*NOTE: When you select some formats, the Options button becomes active. Click it to open a dialog box for setting options specific to these formats. For more information about these options, see Chapter 11: “Sharing Information”.*

5. Click **Save** or **OK**.

If you type a name that already exists in the same directory, the existing document is replaced. If you do not want to replace the original ChemDraw document, use a different name. For information about other file formats, see Chapter 11: “Sharing Information”.

## Reversing and Repeating Actions

ChemDraw keeps track of the actions you perform. You can reverse actions one at a time by

choosing the Undo command then restore them with the Redo command. The number of actions that can be undone or redone is limited only by the amount of memory (RAM and virtual memory) available for use by ChemDraw. When you save your document the Undo queue is reset and starts over.

## Repeating Actions

If an action is repeatable, the name of the action appears next to the Repeat command on the Edit Menu.

To repeat an action:

Click the **Repeat** command on the Edit menu.

The last action performed is repeated.

## The Window Menu

The Window menu lists all open ChemDraw and Template documents. The document you choose from the Window menu becomes the active window.



# Chapter 2: Tutorials

## Overview

The tutorials are designed to teach you the fundamental drawing techniques available in ChemDraw. In addition to the major theme (“Reaction Schemes”, “Perspective Drawings”) each tutorial introduces new techniques, or variations of techniques learned in previous tutorials. We therefore suggest that you do the tutorials in order.

Before you begin, you may want to review “Conventions” on page 10 to familiarize yourself with the terminology used in the tutorials. You may also want to use your Quick Reference Card while you perform the tutorials.

ChemDraw automatically checks for correct chemical syntax as you draw. If ChemDraw finds a potential problem, a red box is displayed around the erroneous object. The red box is displayed on screen only and does not print.

To disable the automatic warning on a specific object:

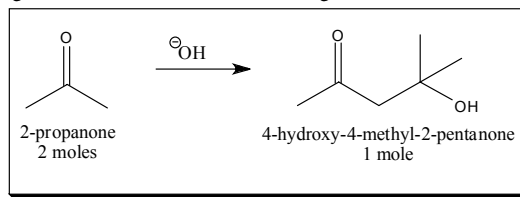
- Right-click the object and deselect the **Display Warnings** command on the context menu.

*NOTE: Some of the following tutorials make use of HotKeys. They assume the default configuration, i.e. that none of the HotKey assignments have been changed.*

## Tutorial 1: Reaction Schemes

In this tutorial, you will draw the following (simplified) reaction scheme:

Figure 2.15: Tutorial 1: Drawing a reaction scheme

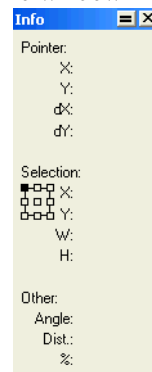


Create a ChemDraw Document:

1. Start ChemDraw.
2. Click the **Save As** command on the File menu.
3. Type `tut1.cdx` in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.
6. Click the **Show General Toolbar** command on the View menu.
7. Click the **Show Info Window** command on the View menu.

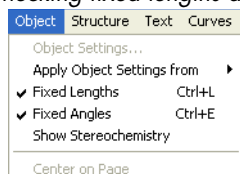
The Info window appears and displays drawing parameters as you draw.

Figure 2.16: The Info window




8. Click the Object menu and make sure there is a check mark next to the **Fixed Lengths** and **Fixed Angles** commands. If either command is not checked, select it.

Figure 2.17: Checking fixed lengths and angles



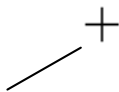
NOTE: Applying fixed lengths and fixed angles enables you to create structures with consistent bond lengths and angles. The fixed length dimension is set in the *Drawing Settings* tab of the Document settings dialog box. The fixed angle dimension increments angles by 15 degrees.

Create a bond:

1. Select the Solid Bond tool .
2. Position the pointer (+) anywhere in the document window and click.

The bond is extended to its fixed length at a 30-degree angle.

Figure 2.18: Adding the first bond



Add a second bond:

1. Point to the right atom of the bond.
2. Click the atom to add a bond.

Figure 2.19: Attaching a bond to an existing bond



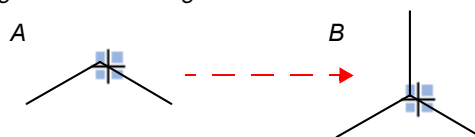
A second bond is drawn, forming a 120-degree angle between the bonds.

NOTE: The angle used when clicking to add bonds is controlled by the Chain Angle setting in the *Drawing Settings* tab of the Document settings dialog box. If this bond angle cannot be established, the next smaller and logical bond angle is used.

Add a third bond to the same atom:

1. Continue pointing to the atom shown in Figure 2.20 A.
2. Click the atom to add a bond.

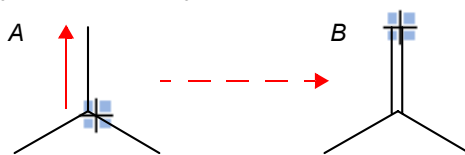
Figure 2.20: Adding a third bond.



Change the single bond into a double bond:

1. Point to the atom shown in Figure 2.21 A and hold the mouse button down.
2. Drag as shown below over the existing single bond. Release the mouse button.

Figure 2.21: Adding a double bond



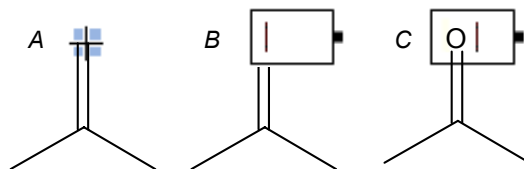
Add labels to the structure:

1. Point to the atom shown in Figure 2.22 A, and double-click.

A text box appears on the atom position to allow you to create an atom label. See “Creating Text” on page 56 for an explanation of the difference between atom labels and captions.

2. Type an uppercase O in the text box that appears.

Figure 2.22: Adding an atom label



3. Close the text box by doing one of the following:

- Use the Esc key.
- Click another tool.

Next, you duplicate a structure and create another structure from the duplicate.

Duplicate the structure:




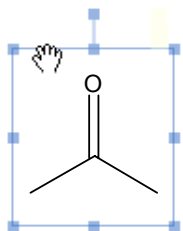
1. Click the Lasso tool  .  
The last structure drawn is automatically selected.
2. Point over the Selection Rectangle.

Figure 2.23: Selecting a structure



3. Press and hold the **Ctrl** or **option** key.

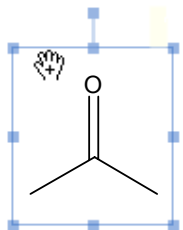
---

*TIP: Just a reminder that instructions of this type give the PC function first, followed by the equivalent Mac function.*

---

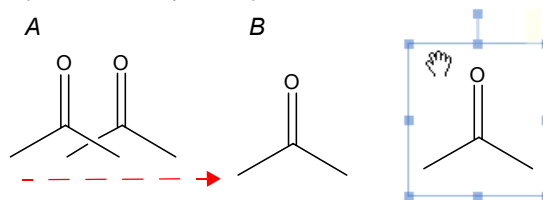
The hand pointer with a plus sign indicates that you are in the duplication mode of a selection tool.

Figure 2.24: The duplication hand icon



4. Drag the Selection Rectangle to the right.  
As you begin drag, a copy of the structure appears and the selection box is not visible. The original structure remains in its position. Release the mouse button when the copy is clear of the original.

Figure 2.25: Duplicating a structure



NOTE: When you create a copy as shown above you can drag it anywhere in the document window. If you want the copy to remain aligned with the original, hold **Shift** while dragging.

Modify the duplicated structure:


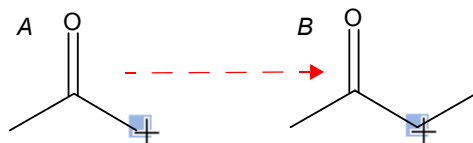
1. Click the Solid Bond tool  .
2. Point, in the copied structure, to the atom shown in Figure 2.26 A and click.

Figure 2.26: Adding more bonds



Add several bonds to a single atom:

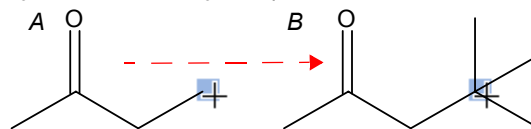
1. Point to the atom shown in Figure 2.27 A.
2. Click the atom three times, allowing a pause between each click.

---

NOTE: If you click too fast, the click is interpreted either as a double-click, which opens a text box or a triple-click, which duplicates your last atom label.

---

Figure 2.27: Adding multiple bonds to an atom

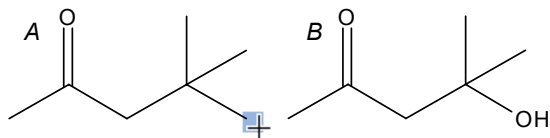


Create another atom label, this time using HotKeys. HotKeys are keys on your keyboard that are linked to specific atom labels. For more information about HotKeys, see “Labeling Atoms with HotKeys” on page 60.

1. Point to the atom shown in Figure 2.28 A.

2. Type O or o.

Figure 2.28: Adding an atom label with a HotKey



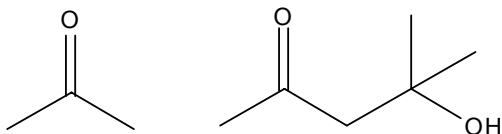
When you use HotKeys that represent a single element, the correct number of hydrogen atoms is added to the label.

Align the structures:


1. Select both structures with the Lasso or Marquee.
2. Point to **Align** on the Object menu, and click the **T/B centers** command.

You structures should appear as shown in Figure 2.29.

Figure 2.29: Tutorial intermediate status: two structures



In the following steps, you use a different method for selecting structures and separate the structures to make room for an arrow.

1. Click the Marquee tool .

---

*NOTE: Alternatively, you can select the Lasso tool and hold **Alt** or **option** to use the Marquee tool.*

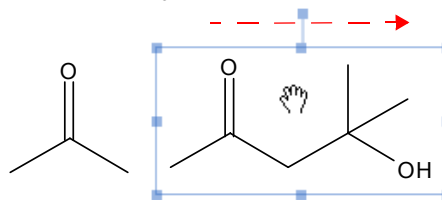
---

The last object drawn is selected.


Drag the selection to make room for an arrow:

- Press **Shift** to maintain the alignment of the structure and drag the Selection Rectangle to the right.

Figure 2.30: Moving a structure



Add arrows to the reaction scheme.

1. Click the Arrow tool  to display the Arrow palette.

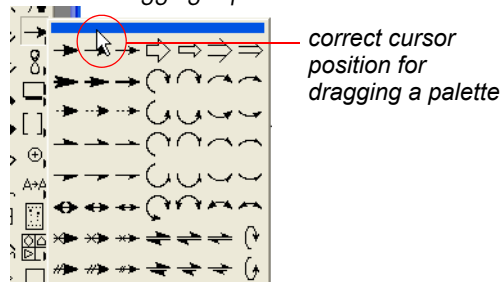
---

*NOTE: The triangle in the lower right corner of the Arrow icon indicates it contains a palette.*

---

2. Holding the mouse button down, move the mouse to the palette title bar, then release the mouse button.

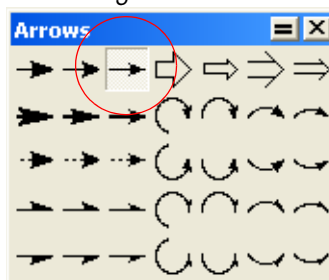
Figure 2.31: Dragging a palette



The palette becomes a floating tool bar. Drag the palette to the location you want.

3. Click the third arrow from the left in the top row.

Figure 2.32: Selecting an arrow



- After the arrow is selected, close the Arrows palette.

---

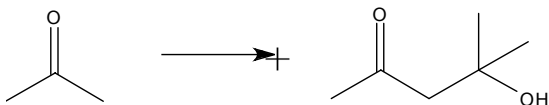
*NOTE: The arrow you choose from the palette becomes the default arrow type. To change the arrow type, display the arrow palette and select the arrow type you want.*

---

Draw the arrow you selected:

- Point after the first structure and drag the arrow toward the second structure.

Figure 2.33: Adding an arrow to a drawing

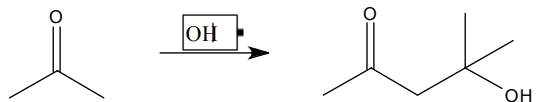


Use the Text tool to add line formula or other captions for representing reagents and reactions.

Insert text in the drawing:

- Click the Text tool **A**.
- Point above the arrow. A text insertion point appears. When you have positioned the text pointer where you want it, click to create a text box.
- Type OH.

Figure 2.34: Adding a caption




---

*TIP: If you want to realign the caption, use a selection tool to drag the caption.*

---

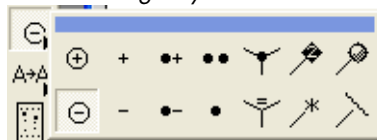
If **Show Chemical Warnings** is turned on (the default) a red box will appear around the OH label as soon as you change tools or open another text box indicating an error. Ignore this for now.

Add a charge symbol using the specialized symbols available in the Chemical Symbols tool palette:

- Click the Chemical Symbol tool

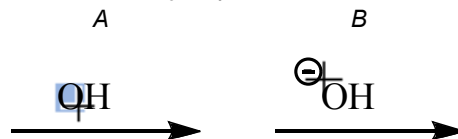
- Holding the mouse button down, select the circled **negative charge symbol**, as shown in Figure 2.35.

Figure 2.35: Selecting a symbol



- Point to the center of the OH label. Moving the cursor slightly right or left will cause either the O or the H to be selected.
- With the O selected, drag the charge symbol around the atom to the desired position.

Figure 2.36: Adding a symbol



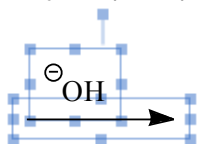
Objects added from the Chemical Symbols palette are associated chemically with the structure they are closest to. Note that the red valence error warning disappeared when you added the minus charge. To show this, try dragging the minus sign around to the other oxygen atoms in the drawing. What happens? Don't forget to put it back when you've finished experimenting.

Some objects, such as arrows, are not associated automatically. You can manually group objects using the Group command. You can then select the grouped objects to manipulate or move them together.

To group objects:

- Click the Marquee tool.
- Do one of the following:
  - Draw a box around the arrow, caption and symbol to select them.
  - Click the arrow, then hold the shift key down while you click the OH caption and the charge symbol.

Figure 2.37: Selecting multiple objects



The Shift key allows you to add objects to a selection without deselecting other objects.

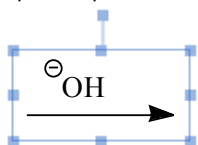
---

*NOTE: If you click a selected object while holding Shift, that object is deselected.*

---

3. Click the **Group** command on the Object menu.

Figure 2.38: Grouped objects



---

*NOTE: You can still select individual objects within a group by clicking them.*

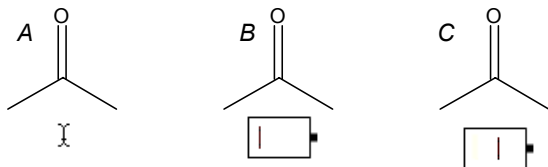
---

Use the Text tool to create a caption containing the name and amount of reactant, and center the caption under the structure.

1. Click the Text tool **A**.
2. Point below the first structure.
3. Click to create a text box. The default cursor is flush left.
4. Click the **Centered** command on the Text menu.

The cursor moves to the center of the text box.

Figure 2.39: Centering text in the textbox

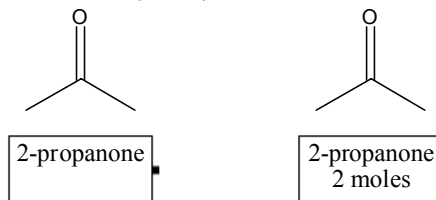


Type the caption:

1. Type 2-propanone.

2. Press the **Enter** or **Return** key to insert a new line.
3. Type 2 moles.

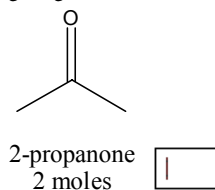
Figure 2.40: Adding a caption with two lines



Create an aligned caption for the other structure.

1. Press the **Tab** key to create another Text box that is aligned adjacent to the first.

Figure 2.41: Aligning a second textbox



---

*NOTE: You can use the Tab key in the caption mode of the text tool to create multiple aligned captions with the same font, font size, style, and justification as the previous caption.*

---

2. Type 4-hydroxy-4-methyl-2-pentanone, press the **Enter** or **Return** key, and type 1 mole.

If your captions are not aligned properly beneath the structures you can move them using a selection tool.

1. Click a Selection tool (Lasso or Marquee).

The text box is automatically selected because it is the last object drawn.

*NOTE: The object that is automatically selected is set in the Preferences dialog box.*

2. Press the Left or Right Arrow key to center the caption beneath its structure. This method maintains the alignment created by the Tab key.

To complete the drawing, add a shadowed box around the scheme:


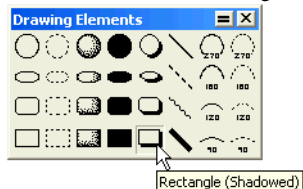
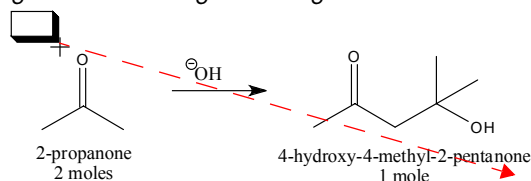
1. Click the Drawing Elements tool .
2. Select the shadowed box from the palette of drawing elements.

Figure 2.42: Shadowed box drawing element



3. Point to the upper left corner of the reaction scheme. Hold the down the mouse button and drag diagonally downward to the right to draw the box.

Figure 2.43: Adding a drawing element



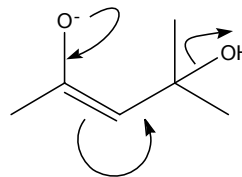
Save and close the document:

1. Click the **Save** command on the File menu.  
Your document is saved.
2. Click the **Close** command on the File menu.

## Tutorial 2: Drawing an Intermediate

In this tutorial you will draw the following intermediate structure starting from a ring and add arrows with customized shapes using the Pen tool.

Figure 2.44: Tutorial 2: Intermediate structure with arrows



Create a new ChemDraw Document:

1. Click the **New Document** command on the File menu.
2. Click the **Save As** command on the File menu.
3. Type `tut2.cdx` in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.

Draw a ring:



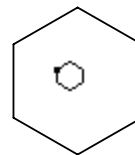
1. Click the Cyclohexane Ring tool .
2. Point in the document window. The Cyclohexane cursor  appears.
3. Click to add a ring.

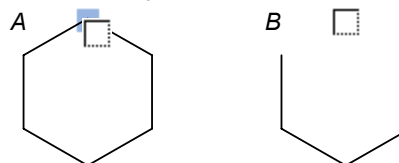
Figure 2.45: Using the cyclohexane ring tool



Delete an atom and its bonds from the ring:

1. Click the Eraser tool .
2. Point to the atom shown in Figure 2.46 A.
3. Click the atom.


Figure 2.46: Erasing an atom



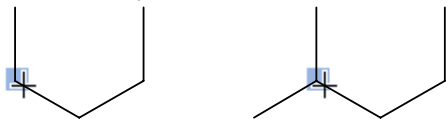
NOTE: You can delete a bond individually by pointing at the center of the bond and clicking.

You can also drag the eraser to make multiple deletions.

Add a bond:

1. Click the Solid Bond tool .
2. Point to the atom shown in *Figure 2.47*.
3. Click to add a bond.

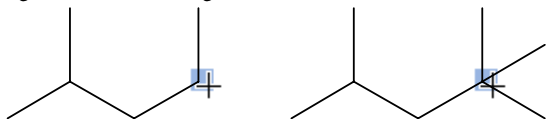
*Figure 2.47: Adding a bond*



Add second and third bonds:

1. Point to the atom shown in *Figure 2.48*, and click twice (slowly) to add two more bonds.

*Figure 2.48: Adding two bonds to an atom*

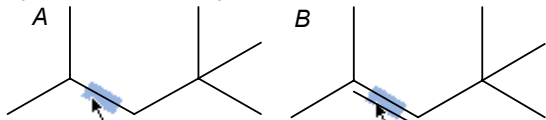


Create a double bond. This is a different method than the one used in the first tutorial:

1. Point to the bond shown in *Figure 2.49* and click.

The double bond will initially form to the inside. Click twice more to move it to the outside, as shown in *Figure 2.49 B*.

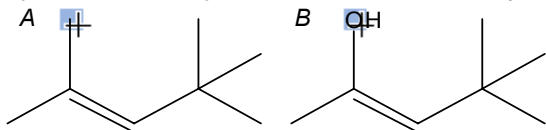
*Figure 2.49: Creating a double bond.*



Add an atom label. This step will expand on your HotKeys knowledge from Tutorial 1.

1. Point to the atom to label shown in *Figure 2.50* and type the letter o.

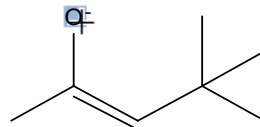
*Figure 2.50: Adding an atom label with a HotKey:*



2. Without moving the cursor, type a “-” (minus).

The OH label changes to O<sup>-</sup>.

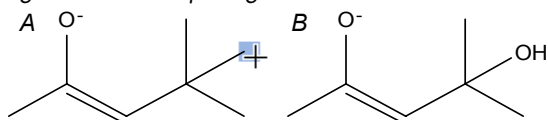
*Figure 2.51: Changing OH to O<sup>-</sup> with a HotKey*



Complete the intermediate structure by adding another OH:

1. Point to the atom shown in *Figure 2.52 A*.
2. Do one of the following:
  - Type the letter o.
  - Double-click the atom to open a text box, and type OH.

*Figure 2.52: Completing the intermediate structure*

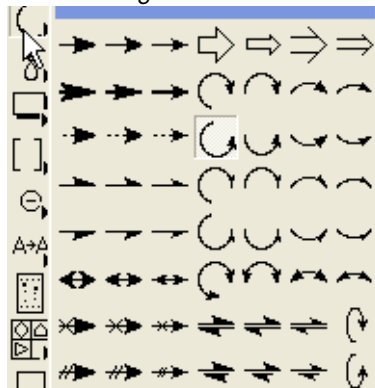


Next you will add arrows to indicate electron flow. The first arrow will demonstrate the new adjustable Arrows tool. The others will be created with the Pen tool.

Add an arrow with the arrows tool:

1. Choose an upward curved arrow from the Arrows palette.

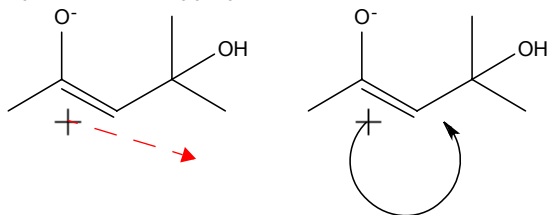
*Figure 2.53: Selecting an arrow*



2. Point near the double bond where you want to indicate the start of electron flow.

3. Drag to the right. Don't worry about the size of the arrow right now, just make it approximate.

Figure 2.54: Dragging an arrow

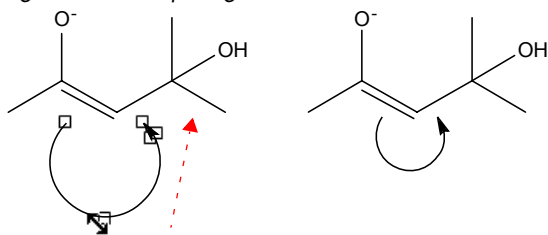


4. Point to the arrow.

Adjustment handles appear at the ends and in the middle.

5. Drag the center up to decrease the curve. You may also drag the ends or the point-width adjustment handles to adjust the arrow as necessary.

Figure 2.55: Adjusting an arrow



The remaining arrows are created with the Pen tool.

To create a customized arrow using the Pen tool.


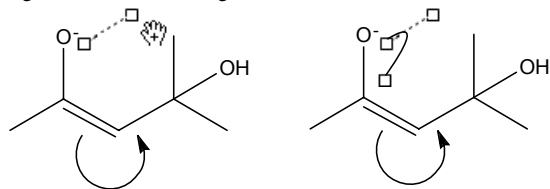
1. Select the Pen tool .
2. Starting just to the right of the O<sup>-</sup> atom label, drag upward and to the right. Release the mouse button.  
The hand with a "+" cursor indicates that you are in the editing mode of the Pen tool.
3. Position the cursor where you want the arrow-head to appear, and click.

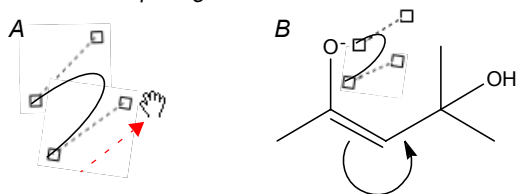
Figure 2.56: Drawing custom arrows



Refine the shape of the arrow:

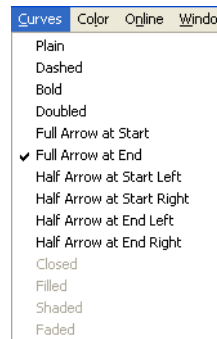
1. Point to the handle at the lower end. You should see a plain hand without the plus sign.
2. Drag up to the right, as shown in Figure 2.57 A. This creates a tangent line that adjusts the curvature.
3. Point to the end and drag it to the correct location.

Figure 2.57: Adjusting a curve



4. Add an arrow head. Click the **Full Arrow at End** command on the Curves menu.

Figure 2.58: The Curves menu



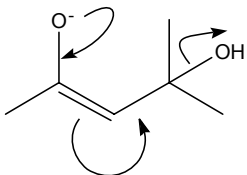
*TIP: You may select more than one option, as long as they do not conflict. For example, you may specify arrows at both start and end.*

5. Press **Esc** when you are finished.

*TIP: To edit a curve you have finished drawing, select it with a selection tool first, then click the Pen tool.*

6. Create the remaining arrow as described above to complete the intermediate as shown below.

Figure 2.59: Tutorial 2: final drawing



*NOTE: If you want to magnify the entire document so you can see arrows or other objects that are in small places, choose Magnify from the View menu.*

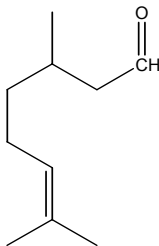
Save and close the document:

1. Click the **Save** command on the File menu.
2. Click the **Close** command on the File menu.

## Tutorial 3: Using Rings

In this tutorial you will draw more complex structures by using rings.

Figure 2.60: Tutorial 3: Using ring structures



Create a ChemDraw Document:

1. Click the **New Document** command on the File menu.
2. Click the **Save As** command on the File menu.
3. Type **tut3.cdx** in the appropriate text box.
4. Select a folder in which to save the file.

5. Click **Save**.

Create a ring:


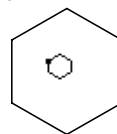
1. Click the Cyclohexane Ring tool .
2. Point in an empty area of a document window.
3. Click to add a ring.

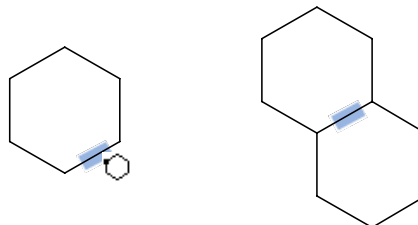
Figure 2.61: Drawing with the ring tool



Fuse a second ring to the first:

1. Point to the center of lower right bond in the ring.
2. Click to fuse another ring.

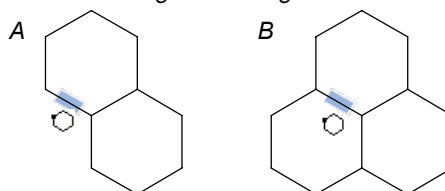
Figure 2.62: Fusing rings



Fuse a third ring:

1. Point to the bond shown in *Figure 2.63*.
2. Click to fuse another ring. Your document should contain the structure shown in *Figure 2.63 B*.

Figure 2.63: Fusing a third ring

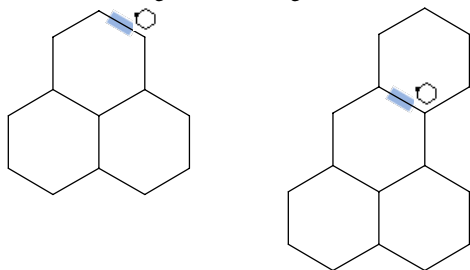


Fuse a fourth ring:


1. Point to the bond shown below.
2. Click to fuse another ring.



Figure 2.64: Adding a fourth ring



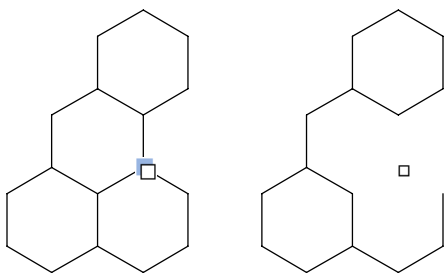
Remove atoms and their bonds from the ring using the Eraser tool:

1. Click the Eraser tool .
2. Point to the atom shown in Figure 2.65.

A highlight box appears on the atom to be removed.

3. Click to delete the atom and its bonds.

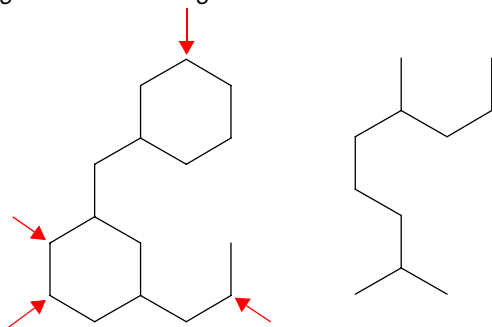
Figure 2.65: Removing atoms and bonds with the eraser tool




4. Click each of the atoms shown below to delete the bonds.

The resulting structure is shown in Figure 2.66.

Figure 2.66: Creating the final skeleton structure

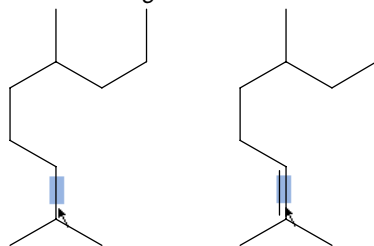


Add double bonds to the structure. In Tutorial 1 you turned a single bond into a double bond by dragging over the bond. In Tutorial 2, the method of clicking on the single bond was introduced. Here, you will learn two more methods.

1. Click the Solid Bond tool . (Actually, any bond tool will do.)
2. Point to the bond indicated in Figure 2.67.
3. Type the number 2 to change the single bond to a double bond.

*TIP: The numbers 1-4 are bond order HotKeys.*

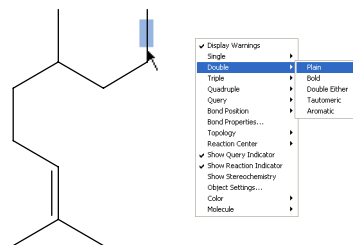
Figure 2.67: Creating a double bond with a HotKey



Add another double bond:

1. Point to the bond shown below.
2. Right-click, point to **Double** on the Bond Context menu, and choose **Plain**.

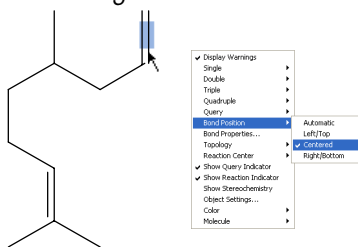
Figure 2.68: Creating a double bond from the context menu



Realign the double bond so it is centered:

1. Point to the center of the upper double bond.
2. Right-click, point to **Bond** position, and choose **Centered**.

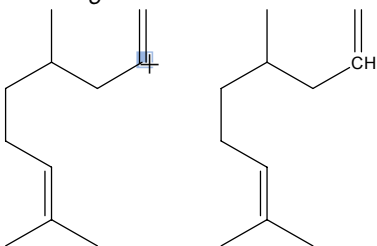
Figure 2.69: Centering a double bond



Add a carbon atom label:

1. Point to the atom shown in *Figure 2.70*.

Figure 2.70: Adding an atom label with a HotKey



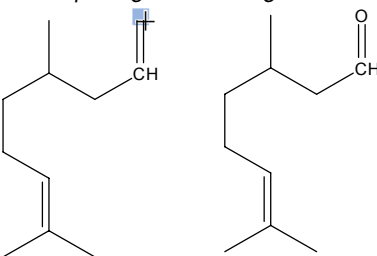
2. Type the **c** key on your keyboard. Note that the Hotkey assigned to the atom label **C** is the lower case letter. Typing an uppercase **C** will create the atom label **Cl**.

The CH atom label appears with the correct number of hydrogen atoms.

Add an oxygen atom label to complete the structure:

1. Point to the atom shown in *Figure 2.71*.
2. Type the **o** key on your keyboard. By default, both upper and lower case **O** Hotkeys are assigned to the atom label **O**.

Figure 2.71: Completing the drawing



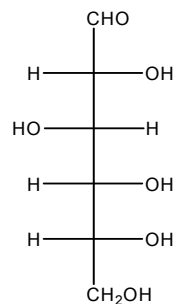
Save and close the document:

1. Click the **Save** command on the File menu.
2. Click the **Close** command on the File menu.

## Tutorial 4: Fischer Projections

This tutorial demonstrates creating a Fischer projection of glucose (shown below) by drawing a linear series of bonds. You can also create the same drawing using a template. It also demonstrates the use of standard document Style sheets (Windows) or Stationery Pads (Mac).

Figure 2.72: Tutorial 4: Fischer projections



1. Point to **Open Special** on the File menu, and choose **ACS Document 1996**.

Special Documents are Style sheets or Stationery Pads. They allow you to have pre-configured settings for different tasks.

*NOTE: In this example, the ACS template provides the required settings for structures to be published in all ACS journals:*

- *One-column layout (Page Setting)*
- *Bonds with a Fixed length of 0.2 inches (Drawing Setting)*
- *Atom Labels in 10 point Arial or Helvetica font (Text Setting)*

2. Click the **Save As** command on the File menu.
3. Type **tut4.cdx** in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.

Draw the first bond:


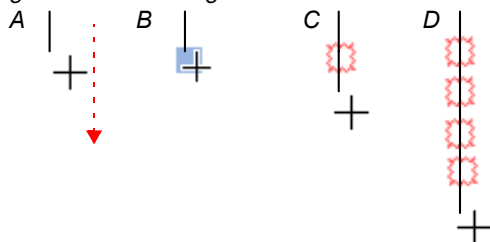
1. Click the Solid Bond tool .
2. Point in the document window. Drag downward vertically to draw the first bond.
3. Point to the lower atom, and drag downward again to draw the second bond.  
The red wavy box appears because Show Chemical Warnings flags colinear bonds. You can ignore it, or turn off warnings from the View menu.
4. Repeat step 3 three more times to draw a total of five bonds.

Figure 2.73: Drawing the backbone

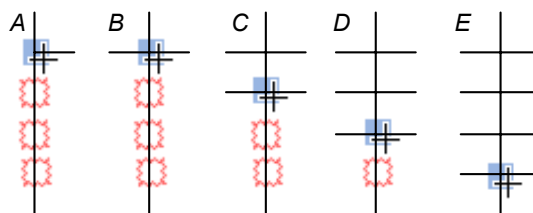


NOTE: When you drag the pointer along the length of the bonds, the pointer alternates between an arrow and a cross. The arrow indicates you are pointing over the center of a bond, and the cross indicates you are pointing to an atom.

Add horizontal bonds to the second atom in the string of bonds you created:

1. Point to C2 and click the atom to add a perpendicular bond.  
Note that the red wavy box disappears as soon as you add a bond.
2. Click again to add a horizontal bond in the opposite direction.
3. Repeat steps 1 and 2 with each successive backbone carbon until all horizontal bonds are added.

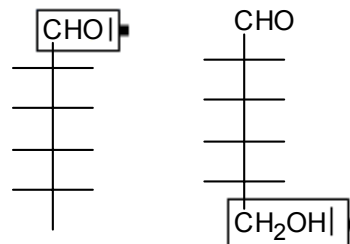
Figure 2.74: Adding horizontal bonds to the backbone



Add labels to C1 and C6:

1. Select the Text tool.
2. Click the C1 atom to create a text box, and type CHO.
3. Click the C6 atom, and type CH<sub>2</sub>OH.

Figure 2.75: Adding atom labels

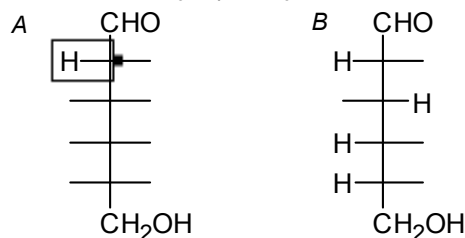


Add the repeating labels for the hydrogens and hydroxyls:

1. Click the atom shown in Figure 2.76 A and type the letter H.
2. Double-click each of the other atoms labeled as hydrogen in Figure 2.76 B.

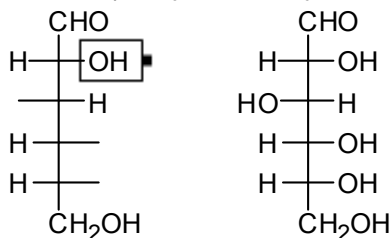
TIP: Double clicking with the text tool repeats the last label.

Figure 2.76: Adding repeating atom labels



- Click one of the remaining atoms and type **OH**.
- Double-click the remaining atoms to repeat the label.

Figure 2.77: Completing the drawing

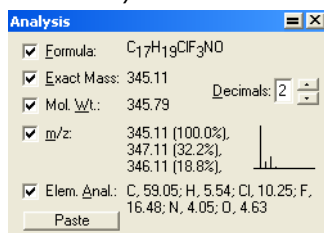


View the basic properties of the structure you drew and paste the information into your document:

- Click a selection tool to automatically select the last structure drawn. If the structure is not selected, double-click the structure.
- Click the **Analysis Window** command on the View menu.

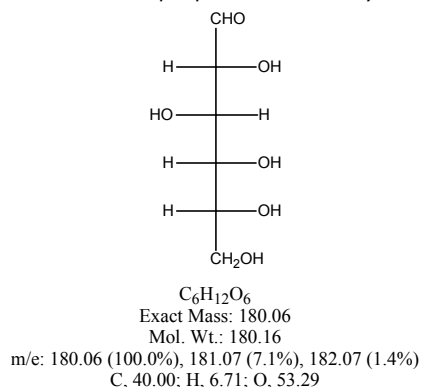
The Analysis window appears. You can drag the window to any position.

Figure 2.78: The Analysis window



- Click **Paste** to paste the information as a caption below the structure.

Figure 2.79: Fischer projection with analysis



Save and close the document:

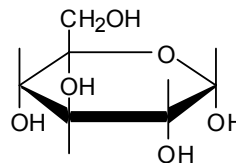
- Click the **Save** command on the File menu.
- Click the **Close** command on the File menu.

## Tutorial 5: Perspective Drawings

In this tutorial you will learn how to create a perspective drawing by creating a model of  $\alpha$ -D-glucose as a Haworth projection.

*NOTE: This tutorial was written before the Structure Perspective tool was added to the ChemDraw toolbar, to demonstrate how to create perspective drawings without such a tool. If you want to use the Structure Perspective tool for this tutorial, distort the ring before adding any bonds. Otherwise, the tutorial is the same.*

Figure 2.80: Tutorial 5: Perspective drawings



Create a new document using the ChemDraw default style:

1. Point to **Open Special** on the File menu, and choose the **New Document** command.


---

*NOTE: If you are doing the tutorials in order, ChemDraw will remember that your last drawing used the ACS style sheet, and open that as the default. Step 1 resets the default to New Document.*

---

2. Click the **Save As** command on the File menu.
3. Type **tut5.cdx** in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.

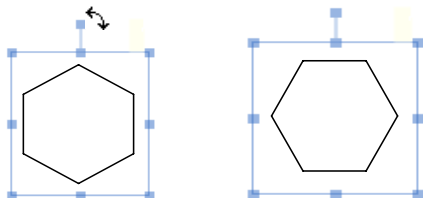
Draw a ring:

1. Click the Cyclohexane Ring tool .
2. Point in an empty area of a document window.
3. Click to add a ring.

Rotate the ring:

1. Click the **Select All** command on the Edit menu (or type **Ctrl+A**).
2. Drag the Rotation handle to the right about 30 degrees. The amount of rotation is displayed on the screen and in the Info window.

Figure 2.81: Rotating the structure



*NOTE: The cursor changes to a curved double-sided arrow to indicate the rotation mode of a selection tool is activated.*

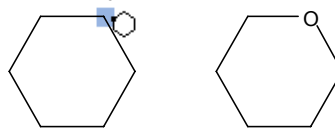
Even though Fixed Angles is on, the angle is not constrained. The Fixed Angles feature constrains angles only when they are being drawn. For example, if you created this ring by dragging instead of clicking, the angle would be constrained when Fixed Angles is on.

Change cyclohexane to tetrahydropyran:

1. Click outside the structure to deselect it.

2. Point to the atom indicated in *Figure 2.82*, and type the lower case letter **o**.

Figure 2.82: Adding an atom label with a HotKey



Add vertical bonds:


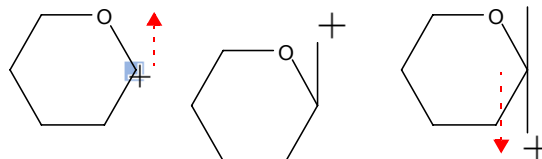
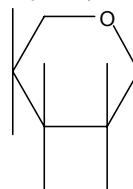
1. Click the Solid Bond tool .
2. Point to the atom shown in *Figure 2.83* and drag upward to create a bond.
3. Point to the same atom, and drag downward to create another bond.

Figure 2.83: Adding a pair of vertical bonds



4. Repeat this procedure three more times, adding the pairs of vertical bonds shown in *Figure 2.84*.

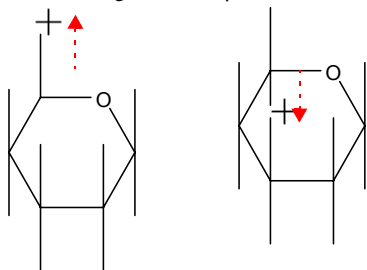
Figure 2.84: Repeating the procedure



The final pair of vertical bonds has to be drawn slightly differently:

1. Drag up from the last remaining carbon atom to form a bond.
2. Point to the atom shown below.  
For the final downward bond, you must turn Fixed Lengths off. Otherwise, the bond will be joined to the upward bond of C3.
3. Hold down the mouse button, press the **Alt** or **option** key, and drag downward from C5. Stop dragging about half the distance to the upward bond on C3.

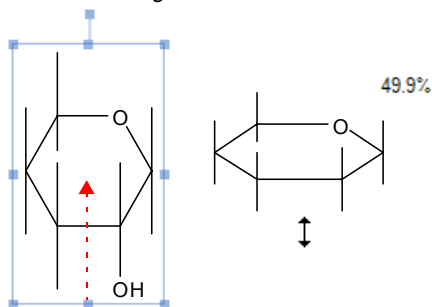
Figure 2.85: Adding the final pair of bonds



Distort the structure to change its aspect ratio to give the perspective of viewing the structure along the Z-axis.

1. Click a selection tool, and select the entire structure.
2. Drag the bottom center resize handle upwards until you have distorted the structure to about 50%, as shown on the screen or in the Info window.

Figure 2.86: Distorting the structure

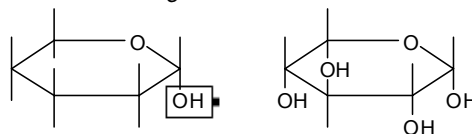


NOTE: Even though you took precautions to make one of the bonds shorter than the others, you might still have a problem with proximity after distorting the structure. If this happens, delete the upward bond on C3 and redraw it, holding the **Alt** or **option** key to cancel fixed bond length.

Next, you create OH labels. You can use the repeating bond label technique in Tutorial 4, or use HotKeys. For the HotKey method, just point and type “o”. The Text tool method is repeated here, with a slight variation.

1. Select the Solid Bond tool, point to the atom shown in Figure 2.87 A and double-click to open a text box.
2. Type OH, move the pointer to the next atom as shown, and triple-click to repeat the atom label.

Figure 2.87: Adding the OH labels



---

TIP: If you find it difficult to place the labels because of the size of the drawing, choose **Magnify** from the **View** menu.

---

---

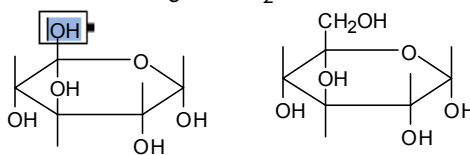
NOTE: The third OH from the right is on the bond extending up from C3, not the bond extending down from C5.

---

Add the CH<sub>2</sub>OH label:

1. Triple-click the upper atom of C5.
2. Press the **Enter** or **Return** key to open the atom label text box. Type CH<sub>2</sub> before the OH.

Figure 2.88: Adding the CH<sub>2</sub>OH label




---

NOTE: When used with a bond tool active, **Enter** or **Return** is a Hotkey that opens a text box for the last atom labeled.

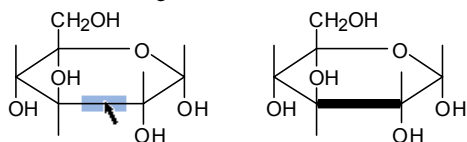
---


Change the type of the front bonds:

1. Click the Bold Bond tool .
2. Point to the center of the bond shown below.
3. Click to change to the new bond type.

The cursor changes to a bold arrow as you point at the bond.

Figure 2.89: Adding a bold bond



4. Click the Bold Wedge bond tool .
5. Click each of the ring bonds adjacent to the bold bond.

For each bond, point slightly off center in the direction that you want the wide end of the wedge to be oriented and click.

---

*TIP: If you move the pointer too far, the highlight box disappears. Choose Magnify from the View menu if you find it difficult to place the pointer.*

---

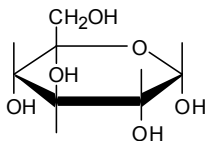
---

*NOTE: If the wedge is pointed in the wrong direction, click the bond again to flip its orientation.*

---

The resulting structure is shown in Figure 2.90.

Figure 2.90:  $\alpha$ -D-glucose, Haworth projection



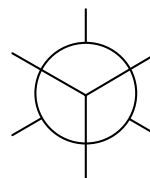
Save and close the document:

1. Click the **Save** command on the File menu.
2. Click the **Close** command on the File menu.

## Tutorial 6: Newman Projections

This tutorial demonstrates how to draw a Newman projection. You can also create the same drawing using a template.

Figure 2.91: Tutorial 7 Newman projection



Create a ChemDraw Document:

1. Click the **New Document** command on the File menu.
2. Click the **Save As** command on the File menu.
3. Type `tut6.cdx` in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.

Create the first structure:


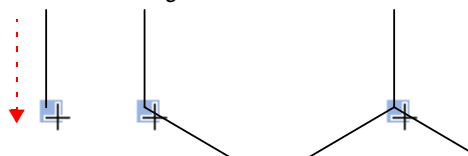
1. Click the Solid Bond tool .
2. In the document window, drag downward to create the first bond.
3. Point at the lower atom and click to add a second bond.
4. Continue pointing at the same atom and click again to add a third bond.

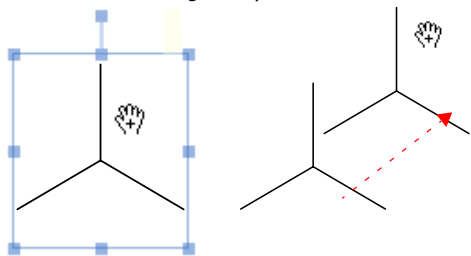
Figure 2.92: Creating the initial structure




Duplicate the structure:

1. Click a selection tool.  
The last structure you drew is automatically selected.
2. Create a duplicate by holding the **Ctrl** or **option** key while dragging the Selection rectangle upward to the right of the original.  
The selection box disappears while you are dragging.

Figure 2.93: Creating a duplicate structure



Add a bond between the duplicated structures:

1. Click the Solid Bond tool .
2. Point to the central atom of the lower fragment.
3. Drag to the central atom of the upper fragment.

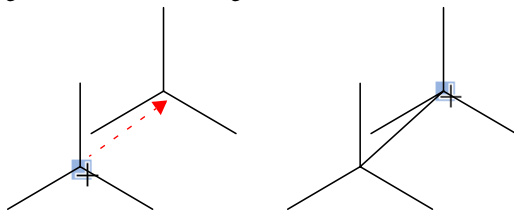
---

*NOTE: When connecting existing atoms, the Fixed Length and Fixed Angles commands are ignored.*

---

4. Release the mouse button when the highlight box over the central atom appears.

Figure 2.94: Connecting the structures



In this step, you will use the Orbital tool to draw the hollow circle that is particular to Newman Projections, rather than an orbital.


1. Click the Orbital tool, and select the unfilled s orbital. 

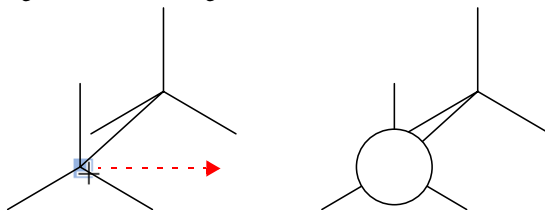
Figure 2.95: The Orbitals tool palette



2. Point to the left center carbon and drag outward.

The size of the orbital is constrained just like bonds are. The constraint is based on a percentage of the Fixed Length setting in the on the [Drawing Settings](#) tab of the Document settings dialog box.

Figure 2.96: Adding an orbital




---

*NOTE: Orbitals are not automatically grouped with the closest structure. If you want to group the orbital with the existing structure so you can move them as a unit, choose Group from the Object menu.*

---

Move part of the structure to the front to overlap the orbital:

1. Click the Marquee tool .

The orbital is selected. Click in the worksheet to deselect it.

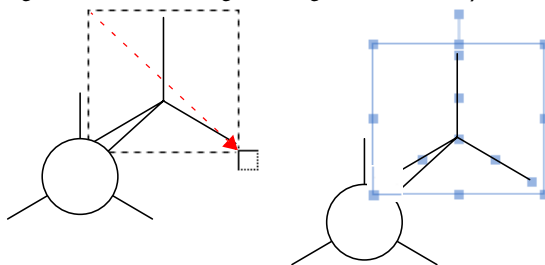
2. Point above the structure and drag around the upper fragment to select the three bonds. Do not select the bond connecting the two fragments. You can Shift+click on each bond separately, if that is easier.

---

*TIP: The new selection box makes it easy to tell which bonds are selected – selected bonds have a dot on them.*

---

Figure 2.97: Selecting the fragment to overlay



Rotate the selection:

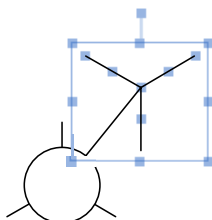


1. Double-click the rotation handle to open the Rotate dialog box.
2. Type **180** in the text box, select **degrees CW**, and click the **Rotate** button.

Figure 2.98: The Rotation dialog box



Figure 2.99: After rotation



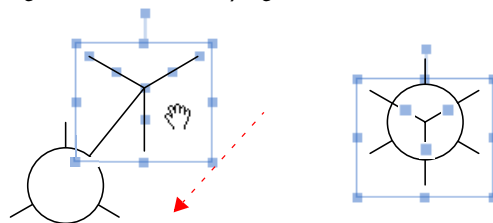
3. With the rotated bonds still selected, change the layering of the structure so that the selection is in front by clicking the **Bring to Front** command on the Object menu.

There is no visible change when you do this.

Orient the front part of the structure to create a Newman projection.

1. Point within the Selection Rectangle until the pointer changes to a hand.
2. Drag the selection until the central atom of the selection is centered within the orbital.

Figure 2.100: Overlaying the structure



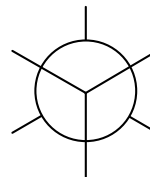

---

*NOTE: If chemical warnings are turned on, you will see a red warning box when you overlay the structure, because the center atoms are "on top of" each other.*

---

3. Release the mouse button and click outside the Selection Rectangle to deselect the structure.

Figure 2.101: Completed Newman projection



Save and close the document:

1. Click the **Save** command on the File menu.
2. Click the **Close** command on the File menu.

## Tutorial 7: Showing Stereochemistry

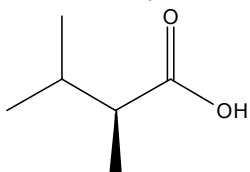
This tutorial demonstrates using Stereochemistry markers and the flip command.

Create a new document.

1. Click the **New Document** command on the File menu.
2. Click the **Save As** command on the File menu.
3. Type **tut7.cdx** in the appropriate text box.
4. Select a folder in which to save the file.
5. Click **Save**.

Draw the following structure:

Figure 2.102: S-(2,3)-dimethylbutanoic acid




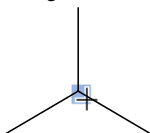
1. Click the Solid Bond tool .
2. The first three steps are identical to the previous tutorial: create an isobutane structure.

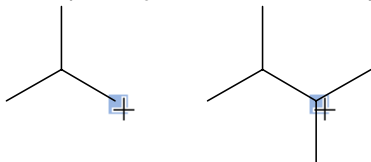
Figure 2.103: Beginning the structure



3. Point to the atom shown in Figure 2.104 and type the number 9.

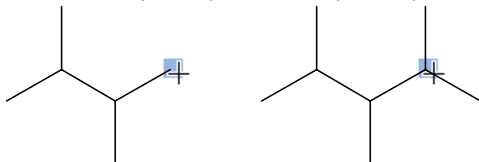
When used with a bond tool, the number 9 is a HotKey for sprouting two bonds. The number 8 sprouts three bonds.

Figure 2.104: Sprouting bonds with a HotKey



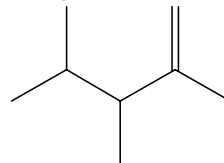
4. Point to the bond shown in Figure 2.105, and type 9 again to sprout two more bonds.

Figure 2.105: Repeating the bond sprouting



5. The upper bond on the right has to be made into a double bond. If you've gone through all the tutorials, you've learned four different ways of doing that. Use your preferred method.

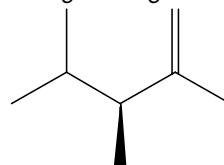
Figure 2.106: adding a double bond



Now, the lower bond has to be changed to a solid wedge bond. In tutorial 5 you were introduced to the wedge bond tool. You can also use a HotKey.

6. Point to the bond shown in Figure 2.107 and do one of the following:
  - Select the Wedge Bond tool, and click the bond.
  - Point to the bond and type the letter **w**.

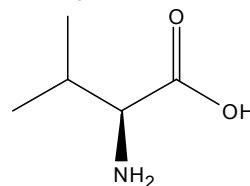
Figure 2.107: Adding a wedge bond



Add atom labels.

1. Double-click the atom shown below, and type **NH2** in the text box that appears. Press the **Esc** key when you finish.
2. Add the O and OH with the text box or the HotKey **o**.

Figure 2.108: Adding the atom labels

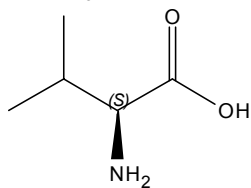


Display the stereochemical markers.

1. Select the entire structure with the Lasso or Marquee.
2. Click the **Show Stereochemistry** command on the Object menu.

The S marker appears.

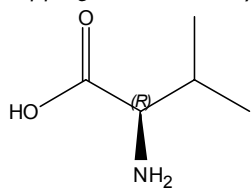
Figure 2.109: Showing stereochemistry



3. Select the structure and click the **Flip Horizontal** command on the Object menu.

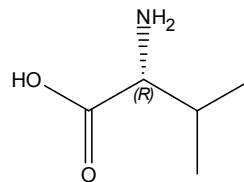
The R marker appears.

Figure 2.110: Flipping stereochemistry



4. With the structure selected, click the **Rotate 180° Vertical** command on the Object menu.

Figure 2.111: Vertical rotation



The Wedged bond becomes hashed and the (R) stereochemistry is preserved.

Save and close the document:

1. Click the **Save** command on the File menu.
2. Click the **Close** command on the File menu.







# Chapter 3: Drawing Chemical Structures

## Overview

This section describes the use of bond and ring tools used to create chemical structures.

ChemDraw provides the following tools for drawing chemical structures:

- Bond tools 
- Ring tools 
- An acyclic chain tool 
- Text tool 

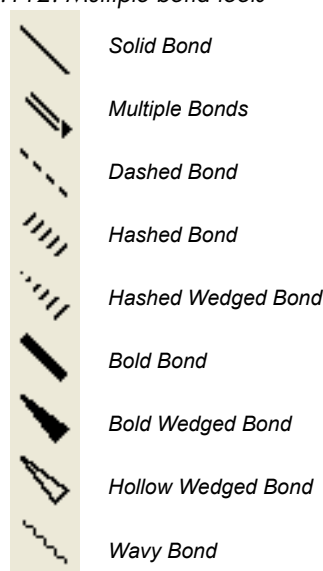
These are the basic building tools for creating and labeling structures. In addition to these basic building tools, ChemDraw gives you two selection tools, a Marquee to select large contiguous areas and a Lasso for difficult shapes, and an Eraser tool. The remaining tools are for more advanced features, described in other sections of this manual.

Especially useful when making multiple changes to structures, ChemDraw's automatic error detection flags errors that you might otherwise overlook. See "Automatic Warnings" on page 55 for more information.

## Drawing Bonds

The Main Tools palette contains the bond tools shown below:

Figure 3.112: Multiple bond tools



## Drawing Constrained Bonds

You can draw any bond length or create any angle relative to the X-axis. Use the Info Window to display the bond length and angle as you drag the bond.

However, it is generally more useful to draw bonds that are constrained to a fixed length and a fixed angle relative to the X-axis. This is the default setting.

## Drawing with Fixed Lengths

To draw bonds that are constrained to a fixed length:

1. Click the **Fixed Lengths** command on the Object menu.

A check mark appears next to the Fixed Lengths command indicating that it is selected. All bonds are constrained to the fixed length specified on the [Drawing Settings](#) tab of the dialog box.

2. Click a bond tool.
3. Drag from one end of the bond to the other.  
The Info Window displays the bond length.

## Drawing with Fixed Angles

To draw bonds with constrained angles that are multiples of 15 degrees relative to the X-axis:

1. Click the **Fixed Angles** command on the Object menu.

A check mark appears next to the Fixed Angles command indicating that it is on.

2. Click a bond tool.
3. Click in a document window.

The bond appears at a standard 120° bond angle (relative to the x-axis).

4. Using a selection tool, move the end of the bond to other angles.

The Info Window shows that the bond angle is constrained to 15-degree increments.

## Toggling Fixed Lengths and Fixed Angles

If fixed lengths or fixed angles are selected, you can temporarily deselect them. To suppress fixed lengths and fixed angles, press the **Alt** or **option** key as you drag the bond.

## Multiple Bonds

The Multiple Bond tool on the Main toolbar includes the palette shown in *Figure 3.113*.

*Figure 3.113: Multiple bond palette*



You can use the tools on the Multiple Bond palette to create the following multiple bonds:

*Table 7: Multiple bond types*

	Double
	Bold Double
	Tautomeric
	Aromatic
	Double Either
	Dative
	Triple
	Quadruple

*TIP: You can also draw multiple bonds by right-clicking over a bond and selecting the bond type from the shortcut menu or by using the bond properties dialog box, or by using HotKeys. For more information on the Bond Properties dialog box, see “Bond Properties” on page 90. For more information on HotKeys, see “Labeling Atoms with HotKeys” on page 60.*

## Double Bonds

There are three ways to draw a double bond:

- Use the Double bond tool.
- Using the Solid, Dashed, or Bold bond tool, click an existing single bond.
- Using any bond or selection tool, point to an existing bond and type the HotKey ‘2’.

## Double Either Bonds

To draw a double either bond select the double either bond tool from the Multiple Bonds palette, or:

1. Draw a bond using the Wavy Bond tool.
2. Point to the center of the bond and click to create a double bond
3. Click again to create a double either bond.

## Triple Bonds

You can draw a triple bond by drawing another single bond on top of a double bond. All bonds in a triple bond are solid bonds.

To draw a triple bond select the triple bond tool from the Multiple Bonds palette, or:

1. Click any bond tool.
2. Drag from one end of an existing double bond to the other.

## Quadruple Bonds

To draw a quadruple bond select the quadruple bond tool from the Multiple Bonds palette, or:

1. Click any bond tool.
2. Drag from one end of an existing triple bond to the other.

The triple bond changes to a quadruple bond.

To change a quadruple bond into a single bond:

1. Click any bond tool.
2. Drag from one end of an existing quadruple bond to the other.

The quadruple bond changes into a single bond corresponding to the tool used to draw over the bond.

*NOTE: You can also use the Eraser tool to reduce the bond order. For more information, see "Changing the Bond Order" on page 29.*

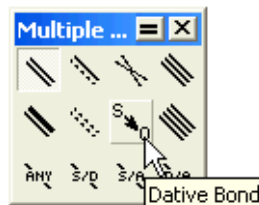
## Dative Bonds and Wedged Bonds

Dative bonds and wedged bonds are drawn with a fixed orientation in a document window.

To draw a dative bond:

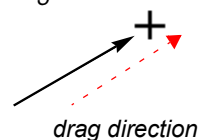
1. Click the Dative Bond tool.

Figure 3.114: Dative bond tool



2. Drag from the positive to the negative end (arrow head) of the dative bond.

Figure 3.115: Drawing a dative bond



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.

Figure 3.116: Drawing a wedged bond



To change the orientation of the dative or wedged bond, click the center of the bond using the matching bond tool.

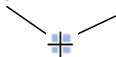
## Adding a Bond by Clicking

To add a fixed length bond:

1. Select a bond tool.
2. Click an atom.

A new bond is drawn and joined to the atom you clicked.

Figure 3.117: Adding a bond to an atom



Bonds drawn by this method are always drawn using the fixed length specified on the [Drawing Settings](#) tab of the Document settings dialog box. The angle that the deposited bond makes with its nearest neighbor is equal to the Chain Angle set on the [Drawing Settings](#) tab of the Document settings dialog box. If this angle cannot be established, a smaller angle is used.

## Adding Bonds by Dragging

To control the orientation of bonds that you draw, you can add bonds by dragging.

By using this dragging method for drawing the bond, you can control the orientation of the other end of the bond.

To add a bond by dragging:

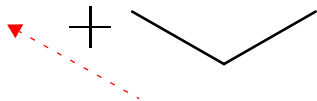
1. Click a bond tool.
2. Point to an atom.

A highlight box appears over the atom indicating where the bond will be joined.

3. Drag from the atom at which you are pointing in the direction you want the new bond to extend.

A new bond is drawn, joined to the atom where the highlight box appeared.

Figure 3.118: Adding a bond by dragging



## Drawing Rings

The Main Tools palette contains the following ring tools that enable you to draw ring sizes and types:

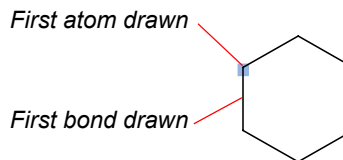
Figure 3.119: Ring tools

Cyclopropane		Cyclobutane
Cyclopentane		Cyclohexane
Cycloheptane		Cyclooctane
Cyclohexane Chair (1)		Cyclohexane Chair (2)
Cyclopentadiene		Benzene

## Drawing a Ring

To draw a ring, select a ring tool. When you point in the document window, the pointer changes to a ring tool pointer. The highlight box on the ring tool pointer indicates the atom that is drawn first. The bond directly below the highlight box is the bond that is drawn first.

Figure 3.120: Ring tool pointer



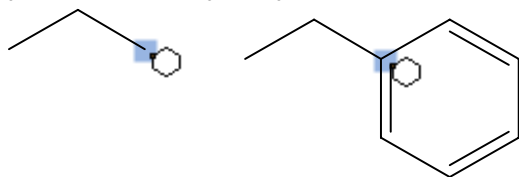
Click in the document window. A ring appears, centered around the pointer, and in the orientation shown on the ring tool icon. To draw a ring in a different orientation, drag the tool instead of clicking.

*TIP: If **Fixed Lengths** is on when you draw a ring, the length of each bond in the ring is automatically set to the fixed length. If **Fixed Angles** is on, the angle the first bond in the ring makes with the X-axis is restricted to 15-degree increments. For more information, see "Drawing Constrained Bonds" on page 20.*

If you click an atom, the ring is fused to that atom.

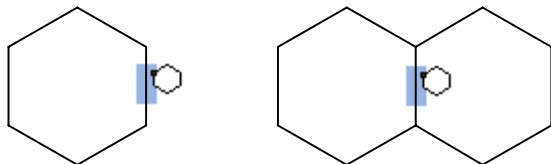


Figure 3.121: Adding a ring to an atom



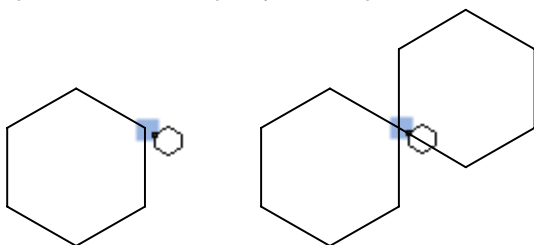
If you click a bond, the ring is fused to that bond.

Figure 3.122: Adding a ring to a bond



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

Figure 3.123: Adding a spiro linkage

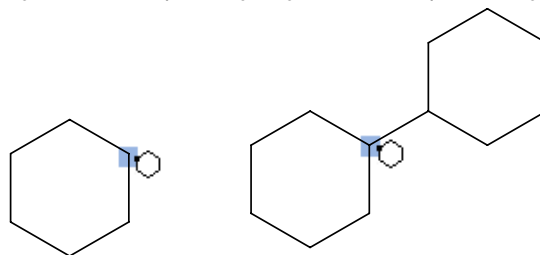


*NOTE: This behavior is controlled on the Building/ Display tab of the Preferences dialog box. See "Setting Preferences" on page 197 for more information.*

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

1. Select **Preferences** on the File (Mac: Chem-Draw) Menu.
2. On the **Building/Display** tab, check the box next to **Sprout Rings Instead of Spiro When Clicking**.

Figure 3.124: Sprouting rings instead of spiro linkage

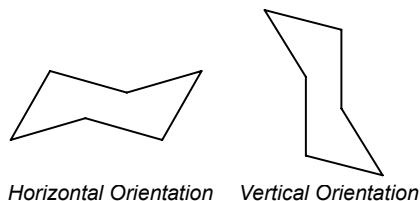


## Drawing Cyclohexane Chair Rings

You can draw Cyclohexane chair rings in two orientations: horizontal and vertical. When you draw a cyclohexane chair ring by clicking, the chair is drawn in a horizontal orientation.

To draw a cyclohexane chair ring in some other orientation, drag with the chair tool to the orientation you want.

Figure 3.125: Drawing a cyclohexane ring – dragging and clicking



## Drawing Resonance Delocalized Rings

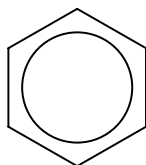
With the exception of the cyclohexane chairs, any of the ring tools can be used to draw a resonance delocalized form.

To draw a resonance delocalized ring:

1. Click a ring tool.
2. Press the **Ctrl** or **command** key and drag or click to draw the ring.

A circle appears inside the ring.

Figure 3.126: Drawing a resonance delocalized ring



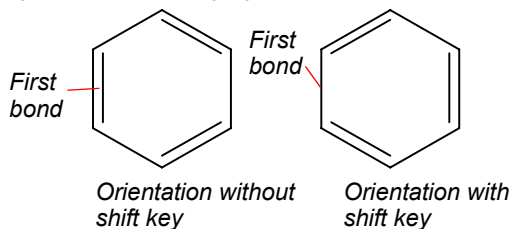
NOTE: The circle is automatically grouped with the ring when drawn. For more information on grouping objects, see “Grouping Objects” on page 112.

## Drawing Cyclopentadiene and Benzene Rings

The double bonds in the cyclopentadiene or benzene ring tools can be drawn in either of two forms.

When you draw a cyclopentadiene or benzene ring a double bond is drawn first (see Figure 22). The Cyclopentadiene and Benzene Ring tool pointers indicate this orientation. To shift the orientation so the first bond drawn is a single bond, hold down the shift key as you click or drag in the structure window.

Figure 3.127: Changing orientation with the shift key



## Drawing Acyclic Chains

Use the Acyclic Chain tool to draw long hydrocarbon chains. The behavior of the Acyclic Chain tool is affected by the fixed lengths



and fixed angles switches on the Object menu, and by the chain angle setting on the Object Settings dialog box.

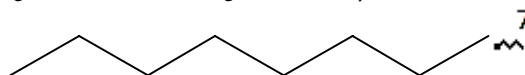
NOTE: Modifying the Chain Angle value for an existing object will have no effect on that object, but new bonds/ chains sprouted from it will sprout at the specified angle.

To draw an acyclic chain:

1. Click the Acyclic Chain tool.
2. Drag in the direction you want the chain to grow in a document window.

A number appears at the end of the chain indicating how many atoms you have drawn.

Figure 3.128: Drawing with the acyclic chain tool



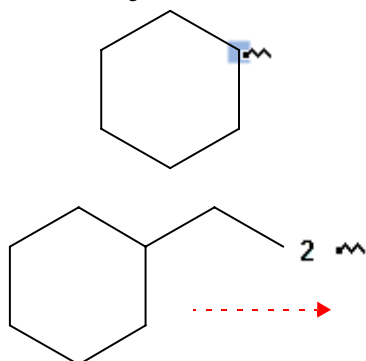
When Fixed Lengths is on, the pointer on the acyclic chain tool can be dragged to make any angle relative to the X-axis. At a constant chain length, the positions of the first bond and all subsequent odd-numbered atoms depend on the direction you drag. Before releasing the mouse button, this position can be changed by dragging in the opposite direction. When Fixed Angles is on, the angle the acyclic chain makes relative to the X-axis is constrained to 15-degree increments.

## Adding Chains

To add an acyclic chain to an existing atom:

1. Click the Acyclic Chain tool.
2. Point to the atom to which you want to attach the chain.
3. Drag in the direction you want the chain to grow.

Figure 3.129: Adding a chain to a bond

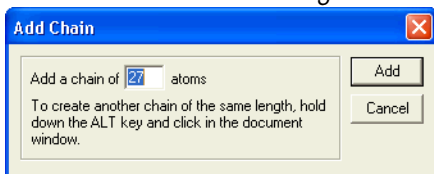


To specify a chain length:

1. Click the Acyclic Chain tool.
2. Click an existing atom or an empty area in a document window.

The Add Chain dialog box appears.

Figure 3.130: The Add Chain dialog box



3. Type the number of bonds in the chain.
4. Click **Add**.

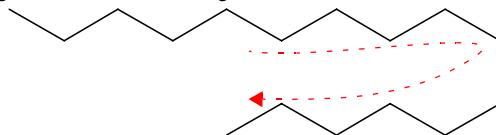
To add another chain of the same length anywhere in a document window, **Alt+click** or **option+click** an existing atom or an empty area within the document window.

## Changing Chain Direction

To change the direction of the chain as you draw, press the **Ctrl** or **command** key while drawing the chain in the direction you want.

*TIP: Make sure to release the mouse button before you release the **Ctrl** or **command** key.*

Figure 3.131: Reversing chain direction



*NOTE: If **Fixed Lengths** is off, use **Ctrl+Alt** or **command+option** to reverse chain direction. **Fixed Angles** must be on to reverse direction.*

## Editing Bonds

You can modify the appearance of chemical structures by:

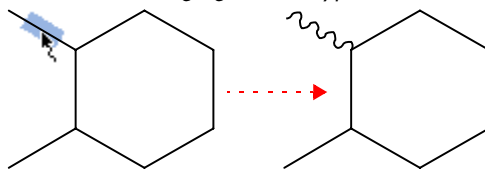
- Changing Bond Types
- [Changing bond alignment and orientation](#)
- Moving Atoms
- Layering bonds
- Changing the bond order

## Changing Bond Types

To change a single bond from one type to another:

1. Click a bond tool.
2. Point at the center of an existing bond and click.

Figure 3.132: Changing a bond type



The bond that you click changes to the new bond type.

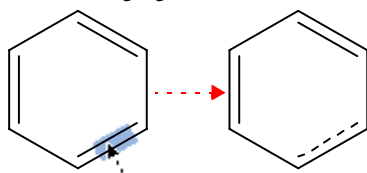
You can also change the bond type using HotKeys, see “Labeling Atoms with HotKeys” on page 60

## Changing Double Bonds

To change one type of double bond to another:

1. Click the Bold, Dashed, or Solid Bond tool.
2. Point to one of the bonds in the double bond.

Figure 3.133: Changing double bonds



3. Click the 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.

*NOTE: If you click a tautomeric bond (solid/dashed) a second time with the dashed bond tool, you create an aromatic double bond (dashed/dashed).*

## Editing Bonds With the Context Menu

You can change an existing bond by right-clicking or Control-clicking on it and selecting a different bond type from the context menu.

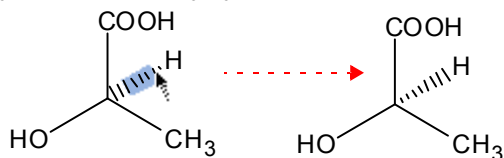
## Changing Orientation of Wedged and Dative Bonds

When you draw or change a bond to a wedged or dative bond, the orientation of the bond is chosen appropriately.

To change the orientation, click the dative or wedged bond with the tool used to create it.

The dative or wedged bond is changed to the opposite orientation.

Figure 3.134: Changing bond orientation



## Changing Alignment of Double Bonds

The bonds in a double bond can have one of three alignments relative to other bonds:

- Above
- Below
- Centered

To change the alignment of a double bond:

1. Click the bond tool used to create the existing double bond.
2. Do one of the following:
  - Click the center of the double bond.  
The alignment changes. Click the center of the double bond again to change to the next alignment.
  - Right-click or Control-click, point to **Bond Position** on the context menu, and choose the alignment.

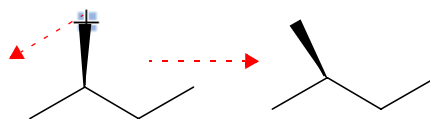
## Moving Atoms With a Bond Tool

You can use any of the bond tools to move an atom within acyclic or cyclic structures. You cannot use a ring tool.

To move an atom in a chemical structure:

1. Click a bond tool.
2. Point at the atom to move.  
A highlight box appears over the atom.
3. Shift+drag the atom.

Figure 3.135: Moving atoms



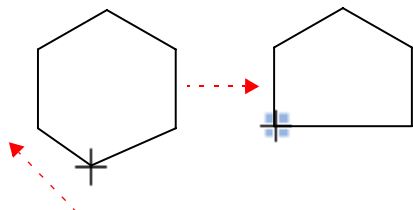
You can convert ring types by dragging one atom on top of an adjacent atom. For example, you can use this method if you want to convert a 6-membered ring into a 5-membered ring.

To convert ring types:

1. With a bond tool selected, point to an atom and Shift+Drag.

2. Release when one atom is on top of the other.  
The bond between the atoms disappears.

Figure 3.136: Changing a ring type



NOTE: You can also move atoms using a selection tool. For more information see “Moving Objects” on page 107.

## Changing Bond Crossings

When one bond crosses another, white space is used to indicate which bond is in front of the other.

To change which bond is in front:

1. Click any bond tool.
2. Double-click the bond to bring it to the front.

Figure 3.137: Changing the bond layering



You can layer bonds using the **Bring to Front** and **Send to Back** commands. For more information, see “Front to Back Ordering” on page 193. You can also change the bond crossing using HotKeys, see “Labeling Atoms with HotKeys” on page 60.

TIP: To make changing the bond layering easier, magnify the view. See “Changing Perspectives” on page 190.

## Changing the Bond Order

You can reduce or increase the order of bonds in a structure by using the Bond Properties dialog box or with the shortcut menus as follows.

To reduce the bond order:

1. Point to the bond to change and Right-click or Control-click.

2. Choose the appropriate bond type from the context menu that appears.

To use the eraser tool to reduce the bond order:

1. Select the Eraser tool.
2. Click a single, double, or triple bond.

The bond order is reduced by one.

To change the bond order using HotKeys, see “Tutorial 3: Using Rings” on page 34.

## Automatic Warnings

ChemDraw automatically checks for correct chemical syntax as you draw. If ChemDraw finds a potential problem, a wavy red box is displayed around the questionable object. The red box is displayed on screen only and does not print.

Displaying warnings is the default setting. You have two options for not displaying them:

- Turn off the automatic warnings option.

---

NOTE: This setting applies to all open documents.

---

- Suppress warnings for a specific object.

To disable the automatic display of chemical warnings, deselect the **Show Chemical Warnings** command on the View menu.

To disable the automatic error checking on a specific object, right-click the object and deselect the **Display Warnings** command on the context menu.

When Display Warnings is deselected for an object:

- Red boxes are not displayed for questionable objects.
- Problems *are* reported by the **Check Structure** command.

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

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

- Right-click on the warning and choose **Explain This Warning**.
- Select the structure, and choose **Check Structure** from the Structure menu.

For more information, see “Checking Chemistry” on page 129.

## Warning Preferences

You can choose what **Chemical Warnings** will flag in the Preferences dialog box. The option list includes:

Table 4: Chemical Warnings

Valence and Charge errors	Isolated bonds
Unbalanced parentheses	Invalid isotopes
Unspecified stereochemistry	Linear atoms
Ambiguous stereochemistry	Atoms near other bonds
Stereobond between chiral atoms	Miscellaneous warnings

To select which types of chemical warnings to display:

1. Click the **Preferences** command on the File menu.
2. Click the **Display Warnings** tab.
3. In the **Chemical Warnings** section, click the types of warnings you want to display.

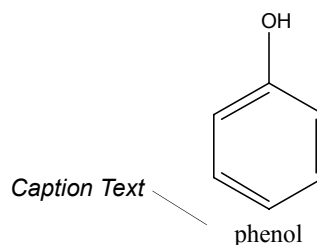
## Creating Text

Use the Text tool to create captions and atom labels. **A**

- **Caption text**—Create annotations, chemical names, chemical formulas, page titles, and information in tables. Default text formats are set in the Document Settings. See “Document

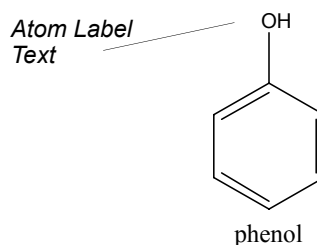
and Object Settings” on page 200 for more information. You may set different defaults for captions and labels.

Figure 3.138: Caption text



- **Atom label text**—Identify atoms and substructures by their chemical symbols and formulas.

Figure 3.139: Atom label text



To change formatting for an individual caption or label:

1. Select the text object with a selection tool.
2. Click the **Object Settings** command on the Object menu.
3. Click the **Captions** or **Atom Labels** tab, as appropriate, and change the setting.

The change affects only the selected caption or atom label only.

The behavior of atom labels is controlled by the **Automatic Atom Label Alignment** and **Automatically Rectify Hydrogens in Atom Labels** checkboxes on the **Building/Display** tab of the Preferences dialog box. The default is to have both of these preferences selected.

When Automatic Atom Labels is selected, the alignment of atom labels will adjust according to the positions of any bonds attached to the atom label.

For example, a CH<sub>3</sub> atom label entered at the *left* end of a horizontal bond would reverse itself to H<sub>3</sub>C.

When Automatically Rectify Hydrogens in Atom Labels is selected, hydrogens will be added to or removed from atom labels as necessary to preserve standard valences when bonds are added or changed.

You can use HotKeys to label atoms. For more information see “Labeling Atoms with HotKeys” on page 60.

*NOTE: ChemDraw does not install its own fonts. If you open a ChemDraw document containing fonts that are not available on your computer, they are substituted with available fonts.*

## Coloring Text

You can color captions and atom labels before or after they are typed, and as a whole or in part.

To color a caption or atom label:

1. Select the Text tool.
2. Click in the position where you want to place the text.
3. Choose a color from the Color menu.
4. Type the caption or atom label.

To color individual characters:

1. Select part of an existing caption or atom label using the Text tool.
2. Choose a color from the Color menu.

*NOTE: Macintosh: Captions that contain multiple colors change to the foreground color when rotated. However, all colors contained in the caption are printed.*


To color several captions or atom labels at once:

1. Select the captions or labels using a selection tool.

2. Choose a color from the Color menu.

## Creating Captions

To create a caption:

1. Click the Text tool .
2. Point in an empty space in a document window.

A caption text box with a flashing insertion point appears.

Figure 3.140: Caption text box



3. Type a caption.  
The text box widens as you type to accommodate the caption.
4. To create a new line, press the **Enter** or **return** key.
5. To close the text box, click outside the text box or select another tool.

## Entering Non-Roman Text

Use the Character Map for entering non-Roman text. (See “Character Map” on page 19 for details.) Any font available on the computer can be entered into a label using the Character Map.

*NOTE: Two-byte fonts such as Chinese may not work reliably with the Character Map.*

## Chemical Significance

By default, captions are considered to be chemically significant if possible. For example, if you create a caption like CH<sub>3</sub>OH, you will be able to attach bonds to it (and it will be modified appropriately) even though you intended it to be a label, not a molecule. Moreover, its values are included in the Analysis Window, which could be confusing. If you try to label structures “A”, “B”, and “C”, the “B” and “C” labels will be marked with a red box because they have “incorrect valences”. You can

change this behavior for the entire document, or for an individual label.

To change a single label:


1. Select the label with the Lasso or Marquee tool.
2. **Right+click** or **Control+click** in the selection.
3. Deselect the **Interpret Chemically** command on the context menu.

To change the behavior of labels in the entire document, deselect the **Interpret Chemically When Possible** option on the **Captions** tab of the Document Settings dialog box.

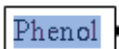
*NOTE: You can verify the chemical significance of a caption using the **Check Structure** command after selecting it with the Lasso or Marquee tool.*

## Editing a Caption

To open a caption for editing:

1. Click the Text tool .
2. Point to a caption and click to open the text box.

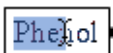
The caption text is highlighted.



3. To change all of the highlighted text within an open text box, type the new caption text over the highlighted text.



- If not all the text is highlighted and you want to select all of the caption text, click the **Select All** command on the Edit menu.
- To change part of the caption text, drag the insertion point over a part of the caption, then type in the new text.



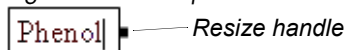
## Changing the Caption Width

To edit the width of a caption:

1. Select a caption using the Text tool.

The Caption text box appears around the caption. The right side of the text box contains a Resize handle.

Figure 3.141: Caption box resize handle



2. Drag the Resize handle.

The point at which the text wraps is adjusted as you drag the Resize handle.

**Ultra**

## Adding Analysis Data to a Caption

You can add properties from the [Analysis Window](#) to a caption created by **Struct=Name**. If auto-update is on (see “Auto Update” on page 122), the values will update as you modify the structure.

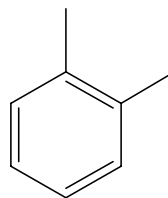
To add values to a label:

1. Point to the label.
2. Right-click, point to **Analysis** on the context menu, and choose a property from the list.

The property appears in the label displaying the current value.

*TIP: You may need to update the window before you can see the new value. If you don't see it immediately, it will appear with the next modification to the structure.*

Figure 3.142: Displaying analysis data



o-xylene  
Chemical Formula: C<sub>8</sub>H<sub>10</sub>  
Molecular Weight: 106.16

## Creating Atom Labels


The default format options of any new atom labels you create are specified in the **Atom Labels** tab of the Document Settings dialog box. You may edit



these options at any time. The settings affect the current document only.

## Labeling Atoms With the Text Tool

To place an atom label on an atom:

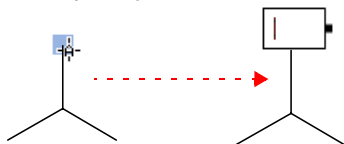
1. Click the Text tool .
2. Point to an atom.

The pointer changes when it is positioned correctly over an atom to indicate that you will create an atom label rather than a caption.

3. Click the atom.

An Atom Label text box appears over the atom.

Figure 3.143: Opening an atom label text box



4. Type an atom label.  
Numbers are automatically subscripted.
5. To close the text box, click outside the text box or select another tool.

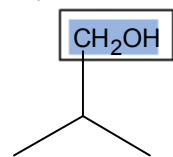
*NOTE: You can use HotKeys to label an atom instead of using the Text tool. You can also label atoms using Nicknames that are text representations of substructures. For more information, see “Labeling Atoms with HotKeys” on page 60 and “Using Nicknames” on page 81.*

## Editing Atom Labels

To edit an atom label:

1. Click an existing label using the Text tool.  
The highlighted atom label text appears within the Atom Label text box.

Figure 3.144: Editing an atom label



2. Type the new atom label text over the highlighted text.

## Deleting an Atom Label

To delete an atom label, leaving the underlying bonds unchanged, do one of the following:

- Select the Eraser tool and click the atom label.
- With a selection, bond, or ring tool selected, point to the atom label and press the spacebar, Backspace, or Delete Key.

## Labeling Atoms With a Bond or Ring Tool

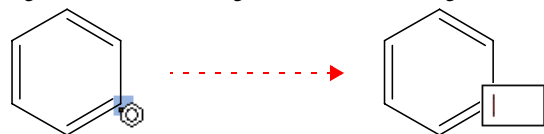
To avoid switching back and forth between tools, you can label atoms with a bond or ring tool.

To label an atom using a bond or ring tool:

1. Select a bond or ring tool.
2. Point to an atom and double-click.

An atom text label appears over the atom.

Figure 3.145: Labeling an atom with a ring tool



3. Type the text.

## Automatic Labeling of Terminal Carbons

You can set the default for document, or for a structure or group of structures, to insert terminal carbon labels.

To set the default for a document:

1. Click **Document Settings** on the File menu.

2. On the **Atom Labels** tab, check the box for **Show Labels On Terminal Carbons**.

To set the default for a structure:

1. Create a structure, or several structures.
2. Select the structure(s). Right-click, and click **Object Settings** from the context menu.  
The Object Settings dialog box appears.
3. On the **Atom Labels** tab, check the box next to **Show Labels On Terminal Carbons**.

To add or remove a single terminal carbon label, point to the label and select or deselect the **Show Terminal Carbons** command on the atom context menu.

## Hiding Implicit Hydrogens

By default, implicit hydrogen atoms are displayed. To hide implicit hydrogens:

1. Click **Document Settings** on the File menu.
2. On the **Atom Labels** tab, check the box next to **Hide Implicit Hydrogens**.

---

### CAUTION

*This feature is provided solely for those who need to produce ISIS-compatible documents. Documents produced with this setting will likely be unacceptable for publication.*

---

## Repeating an Atom Label

You can repeat an atom label using the text, bond, or ring tools.

To label several atoms with the same text using the Text tool:

1. Click the Text tool.
2. Label a single atom.
3. Double-click another atom to repeat the previous label.

To label several atoms with the same text using a bond, ring, or Acyclic Chain tool:

1. Click the tool.
2. Triple-click an atom to repeat the previous label.

## Using the Text Tool With a Selection Tool

The Text tool used in conjunction with a selection tool enables you to perform additional edits, such as simultaneously changing several captions or atom labels. For more information about selection tools, see “New Selection Box” on page 61.

You can toggle between the Text tool and a selection tool as follows:

- After using the Text tool, press **Ctrl+Alt+Tab** or **command+option+tab**.

The last-used selection tool is selected.

To switch from a selection tool to the Text tool when a caption or atom label is selected, press **Ctrl+Alt+Tab** or **command+option+tab**.

The Text tool is selected and the text box is opened for editing.

**NOTE:** **Ctrl+Alt+Tab** and **command+option+tab** will always toggle between the last selection tool used and last other tool used.

## Labeling Atoms with HotKeys

HotKeys™ is a major ChemDraw feature for rapid labeling of atoms.

*TIP:* You can access HotKey Help directly from the Help menu in ChemDraw for Windows.

There are two basic methods for using HotKeys.

To label the last atom drawn:

1. Draw a bond.
2. Immediately type a HotKey.

The last atom drawn is labeled. Each time you draw a bond, the last atom drawn is the HotKey atom.

*NOTE: HotKeys are case-sensitive. For example, the default for a carbon label is lower case 'c'. Typing an upper case 'C' will create a 'C1' label. For information on changing the defaults, see "Creating HotKeys" on page 223.*

To label an atom by pointing:

1. Using a bond, ring, or Text tool, position the pointer over an atom.

A highlight box appears over the atom.

---

*TIP: You may also use a selection tool, but you have to click the atom, not just point to it. You may use the Text tool for HotKey labeling only if there is no open text box.*

---

2. Type a HotKey.

The label is added to the atom highlighted. If the label is a single element, such as C, then the appropriate number of hydrogen atoms are added to the label. Repeatedly typing the hotkey will cycle the number of hydrogens.

*NOTE: HotKeys are "sticky", that is, typing a HotKey will always label the last atom highlighted, even if you are no longer pointing to it. This is true if even you switch tools or switch documents. You can even open another application, type in it, and return to ChemDraw. If you then type a HotKey, it will label the last atom highlighted. Only when you open a textbox is the behavior cancelled.*

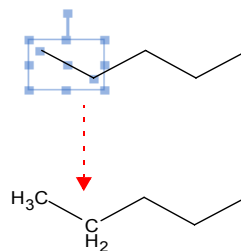
## Labeling multiple atoms

To label several atoms with the same label:

1. Select several atoms using a selection tool.
2. Type a HotKey.

The selected atoms are labeled.

Figure 3.146: Labeling several atoms at once



## Using a Selection Tool

Use the Lasso or the Marquee selection tool to select any object. You use the Lasso for freehand selection and the Marquee to select rectangular regions.

## Toggle Between Selection Tools

You can set one selection tool to behave like the other by clicking the Lasso or Marquee tool while holding the **Alt** or **option** key down.

## Toggle Between Other Tools

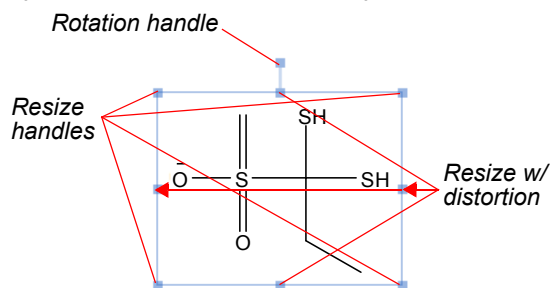
To toggle a selection tool and the last drawing tool used, press **Ctrl+Alt+Tab** or **command+option+tab**.

This command will toggle the last selection tool you have used with the last drawing tool you have used. If you haven't used either selection tool, it defaults to the Lasso tool.

## New Selection Box

ChemDraw 10 has a very obvious change in the selection tools, improving the visualization and behavior of the Lasso and Marquee. When you select a structure or object, the selection is displayed as a solid box in highlight color (blue against white background; white against blue background), with resize handles in the eight cardinal locations.

Figure 3.147: The selection rectangle



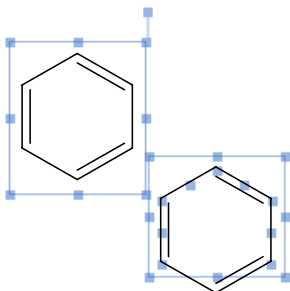
You have the following options while resizing:

- resize proportionately by dragging any corner
- resize with either X-axis or Y-axis distortion by dragging any side
- resize freely (X and Y axis distortion) by holding the **Shift** key down while dragging

The rotation handle is at the top. See “Rotating Objects” on page 65 for more information.

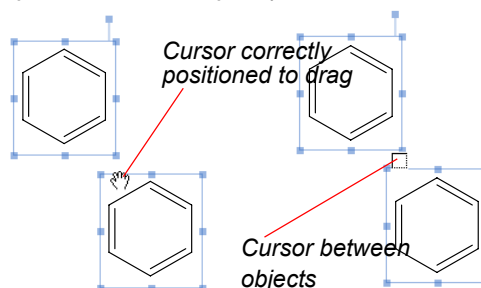
When you select multiple objects, each object displays a selection box, so that you can see exactly what is selected. For example, in *Figure 3.148* you see clearly that the lower benzene ring was only partially selected. Note that in the partially selected ring, each selected atom and bond is marked.

Figure 3.148: Partial selection



Dragging any adjustment handle changes all of the selected objects in unison. To move the selected items, position the cursor inside a selection box to display a hand, then drag. Note that spaces between objects are “dead space” where you cannot grab the selection to drag it.

Figure 3.149: Moving Objects



Attempting to drag the selection when the cursor is placed between objects will result in the objects being deselected.

The new Lasso tool also gives you more control over objects. Most drawing objects can now be rotated as well as resized.

## Selecting Objects with the Lasso Tool

Use the Lasso tool to make freehand selection of irregular areas.

To select objects using the Lasso tool:


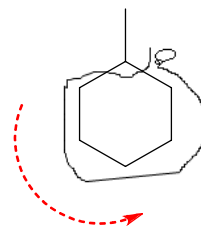
1. Select the Lasso tool .
2. Press the mouse button while the pointer is not over any object.
3. Drag around a portion of a chemical structure or other object.

Figure 3.150: Selection with the lasso



As you drag, a line appears which defines the Selection area. Bonds, structures, or other objects are selected only if they are entirely

within this area. The end points of the Lasso are automatically connected when you release the mouse button.

## Selecting Objects with the Marquee Tool

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

To select objects using the Marquee tool:


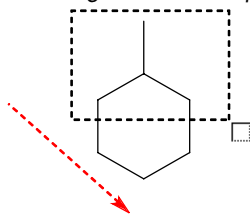
1. Select the Marquee tool .  
The pointer becomes a Marquee.
2. Drag diagonally across the chemical structures or other objects.

Figure 3.151: Selecting with the marquee



As you drag, a rectangle appears which defines the Selection area. Bonds and other objects are selected only if they are entirely within the rectangle.

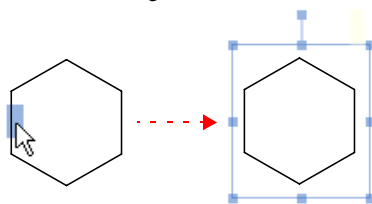
You can use the Marquee to select several objects at once if they can be surrounded by a rectangle.

## Selecting Entire Structures

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

The entire chemical structure is selected.

Figure 3.152: Selecting an entire structure



If the chemical structure or other object is part of a group, the entire group is selected. For more information, see “Grouping Objects” on page 68.

## Selecting Objects by Clicking

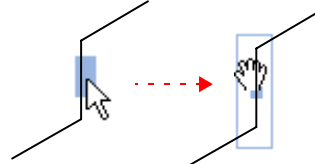
To select an object by clicking:

1. Select the Lasso or the Marquee tool.
2. Point to an object in a document window.

A highlight box appears over the selected object. If you point at a bond, the highlight box appears over the length of the bond.

3. Click the object.

Figure 3.153: Selecting by clicking



The selected objects appear within the Selection Rectangle and the cursor changes to a hand.

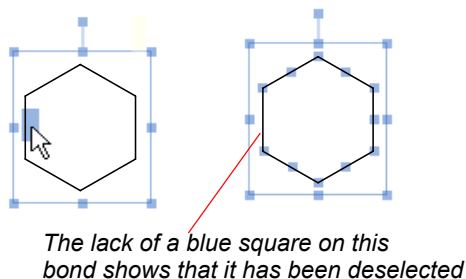
*NOTE: If the bond or other object is part of a group you can select it as an individual object. For more information, see “Grouping Objects” on page 68.*

## Removing Objects from the Selection

To remove an object from the selection, press **Shift** and select an object contained within the Selection rectangle by clicking, double-clicking, or with a selection tool.

The object is removed from the selection.

Figure 3.154: Removing selected objects



NOTE: Objects may appear within the borders of the Selection rectangle but not be selected. See the comment in Figure 3.154, above.

## Making Multiple Selections

To make multiple selections or add more objects to the selection:

- Press **Shift** and select the other objects.

You can add objects to the Selection by clicking, double-clicking, or by using the selection tools.

## Selecting and Deselecting All Objects

To select all objects within a document window, click the **Select All** command on the Edit menu.

To deselect all selected objects, do one of the following:

- Click in any empty area in a document window that is outside the Selection rectangle.
- Press **Esc**.
- Select a different tool.
- Select another object without holding down **Shift**.

The selected objects are deselected.

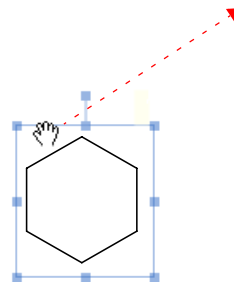
## Moving Objects

To move an object:

1. Select the object using a selection tool.
2. Point within the border of the Selection rectangle.

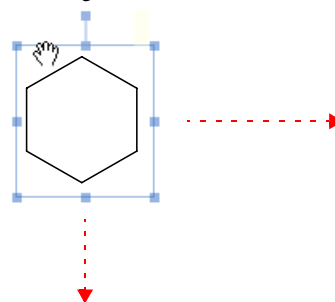
3. Drag the object to a new location.

Figure 3.155: Moving an object



To constrain the movement to the horizontal or vertical direction, **Shift+drag** the selected objects.

Figure 3.156: Constraining movement to the axes



Small incremental movements are often useful for aligning objects. To move an object a small distance:

1. Select the object.
2. Press an **arrow** key.

The selected object moves 1 point in the direction of the arrow.

To move in a larger increment, press **Alt** or **option** plus an **arrow** key.

The selected objects move 10 points in the direction of the arrow.

For more information about aligning objects, see Chapter 10: “Page Layout”.

## Moving Atoms With a Selection Tool

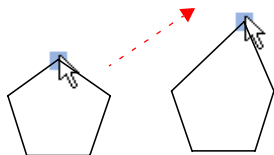
You can move the atoms within a chemical structure using a selection tool.

To move a single atom:

1. Point to an atom using a selection tool.
2. Drag the atom.

The bonds connected to the atom stretch.

Figure 3.157: Moving an atom with a selection tool



To move multiple atoms, select only the bonds that have atoms on both ends that you want to move.

The unselected bonds that are attached to the selected atoms are stretched.

*NOTE: You can also move atoms using the bond tool that was used to draw the atom. For more information, see "Moving Atoms With a Bond Tool" on page 54.*

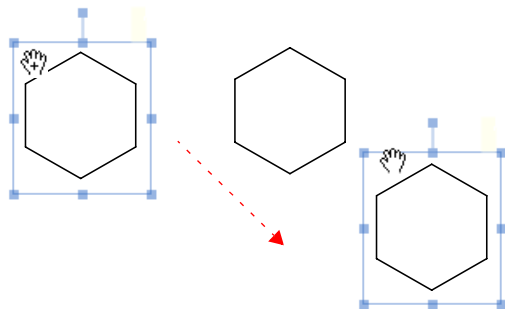
## Duplicating Objects

To duplicate objects with a selection tool:

1. Click a selection tool.
2. Select the objects.
3. **Ctrl+drag** or **option+drag** to create a copy and position it.

A "+" appears in the hand to indicate duplication, and a copy of the selected object is moved to the new position.

Figure 3.158: Duplicating objects



To duplicate the selected objects and constrain the alignment of the copy:

1. Select the objects.
2. **Ctrl+Shift+drag** or **option+shift+drag** to create a copy and position it.

Movement is restricted to the vertical or horizontal axis.

## Deleting Objects

To delete selected objects, do one of the following:

- Press the **Delete** key.
- Press the **Backspace** key.
- Click the **Clear** command on the Edit menu,

## Rotating Objects

To rotate objects:

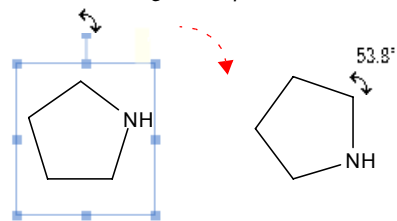
1. Select the objects to rotate using a selection tool.

The Rotation handle is located on the upper right corner of the selection rectangle

2. Drag the Rotation handle clockwise or counterclockwise.

The screen and Info window indicate the magnitude of the rotation around the center of the Selection rectangle.

Figure 3.159: Rotating an object



By default, atom labels do not rotate with the structure.

To rotate an atom label with a structure, press **Ctrl** or **command** while dragging the structure.

If a single atom is unselected when a structure is rotated, the structure rotates around the unselected atom.

To rotate the selected objects a specified number of degrees:

1. Do one of the following:
  - Click the **Rotate** command on the Object menu.
  - Double-click the rotation handle.

The Rotate Objects dialog box appears.

Figure 3.160: Rotate objects dialog box



2. Enter a number and click either **degrees CW** for a clockwise rotation or **degrees CCW** for counterclockwise rotation.

3. If you want to rotate the atom label text, click the **Rotate Atom Labels** checkbox.

4. Click the **Rotate** button.

Objects are rotated around the center of the Selection rectangle.

To repeat the same rotation on any object in the document window:

1. Immediately after performing a rotation, select the other objects to rotate.
2. Click the **Repeat Rotate** command on the Edit menu.



# Chapter 4: Advanced Drawing Techniques

## Overview

ChemDraw provides advanced drawing features that allow you to:

- Join objects
- Group objects
- Scale objects
- Create mirror images
- **Pro** Contract and expand sections of structures
- **Pro** Clean up structures
- Add bonds to specific characters in atom labels
- Create bonds whose attachment is not explicitly defined
- Add atom numbers
- View structure perspective
- Create [Mass Fragmentation](#), [Retrosynthesis](#), and [Dissociation](#) drawings
- Draw with Templates
- **Pro** Create Templates
- Label functional groups with Nicknames.

## Joining Objects

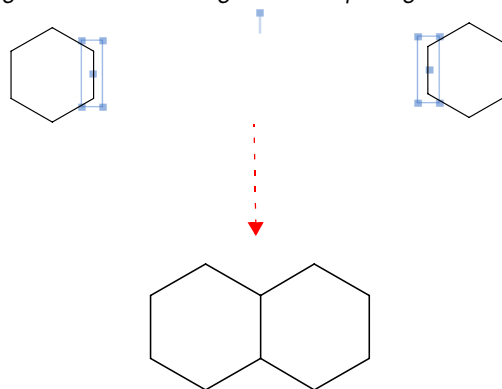
Use the **Join** command in the Object menu to fuse two chemical structures together. Once structures are joined they can be easily selected by double-clicking.

To join chemical structures along the length of a bond:

1. Select a bond or atom in one of the molecules
2. Shift+click to select the corresponding bond or atom on the second molecule that you wish to fuse.
3. Click the **Join** command on the Object menu.

The structures are joined.

Figure 4.161: Selecting bonds for joining structures

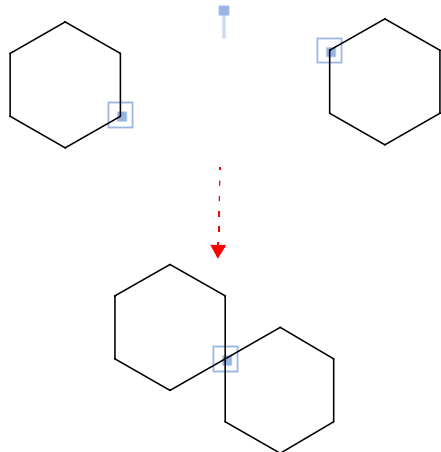


*NOTE: In some earlier versions of ChemDraw, structures had to be in close proximity before they could be joined. This is no longer the case.*

To join chemical structures at one atom to create a spiro linkage:

1. Position the two chemical structures so that the atoms you wish to fuse are more or less opposite each other.
2. Select the two atoms to be fused.
3. Click the **Join** command on the Object menu.

Figure 4.162: Creating a spiro linkage



*TIP: While you no longer have to position the chemical structures exactly, attempts to fuse atoms that are not approximately lined up will lead to incorrect results.*

*NOTE: When you join two differently colored bonds or atom labels, the color of the front object becomes the color of the resulting joined object. When you join two atoms that are labeled, the front atom label becomes the atom label of the resulting atom. For more information about front to back ordering of objects, see Chapter 10: "Page Layout".*

## Grouping Objects

You can group a number of objects drawn separately. Grouping creates an association between objects so they can be easily selected. You can select all grouped objects by double-clicking with a selection tool. Objects within a group can be selected individually and manipulated while still remaining part of the group.

If you want to group objects so that the individual objects in the group *cannot* be accessed, you can create an Integral group. When you select any object in an Integral group, the entire group is selected.

Grouping does not lock the position or orientation of objects. Grouped objects maintain their relative

positions when they are centered on the page, aligned or distributed.

Atoms and bonds making up a single chemical structure are always grouped. If you group part of a structure with other objects, the resulting group contains the entire structure. If you add atoms or bonds to a grouped structure, the new atoms and bonds are part of the group.

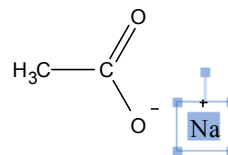
To group several objects:

1. Select the objects to group using a selection tool.
2. Click the **Group** command on the Object menu.

To select an individual object within a group, move the selection tool over an object until it is highlighted and click once.

The object is selected, not the group.

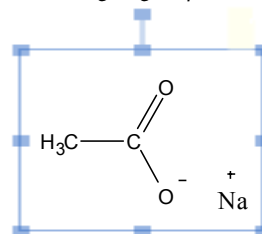
Figure 4.163: Selecting part of a group



To select grouped objects, move the selection tool over an object until it is highlighted and double click

The entire group is selected.

Figure 4.164: Selecting a group



## Ungrouping Objects

To ungroup objects that are grouped:

1. Select a group, as above.

2. Click the **Ungroup** command on the Object menu.

All the objects previously grouped become individual objects.

## Creating Integral Groups

To create a group in which individual objects cannot be accessed:

1. Select the objects to group using a selection tool.
2. Click the **Group** command on the Object menu.
3. With the group selected, right-click, point to **Group** in the context menu, and click **Integral**.

To restore an Integral group to a regular group:

1. Select the Integral group.
2. Right-click, point to **Group** in the context menu, and deselect **Integral**.

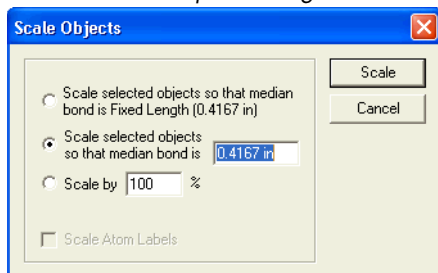
## Scaling Objects

To resize objects with the Scale command:

1. Select the objects to scale.
2. Do one of the following:
  - Click the **Scale** command on the Object menu.
  - Double-click one of the Resize handles.

The Scale Objects dialog box appears.

Figure 4.165: Scale objects dialog box



Use the first two options in the Scale Objects dialog box to scale all selected objects so that the

median selected bond has a specified length based on the following scale factor:

$$\text{scale factor} = \frac{\text{new median bond length}}{\text{current median bond length}}$$

To scale bonds so that the Fixed Length becomes the new median bond length:

1. Select the top option.

The fixed length presently on the [Drawing Settings](#) tab of the Document settings dialog box is shown in parentheses at the end of the line for this button.
2. Click the **Scale** button.

To scale the bonds to a new fixed length that you specify:

1. Select the middle option.
2. Type the new median bond length in the box to the right of the button.
3. The current median bond length for the selection is shown in the highlighted text box when the dialog box initially appears.
4. Click the **Scale** button.

To scale objects by a percentage:

1. Select the **Scale by** radio button.
2. Type the percentage in the box to the right of the button.
3. Click the **Scale** button.

This is the only available option when the selection does not contain any atoms or bonds.

## Reflecting Objects Through Planes

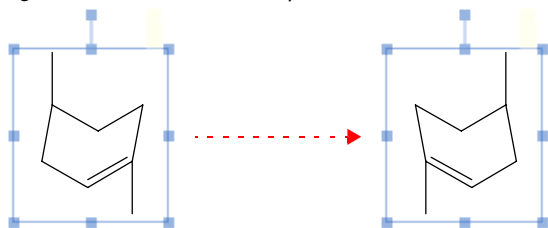
You can reflect structures through planes perpendicular to the X-axis or Y-axis using a selection tool. Used with duplicating, you can create mirror images of chemical structures for representing racemic mixtures and other stereoisomers.

## Flipping Objects

To reflect an object through a plane perpendicular to the X-axis:

1. Select the objects to reflect.
2. Click the **Flip Horizontal** command on the Object menu.

Figure 4.166: Horizontal flip

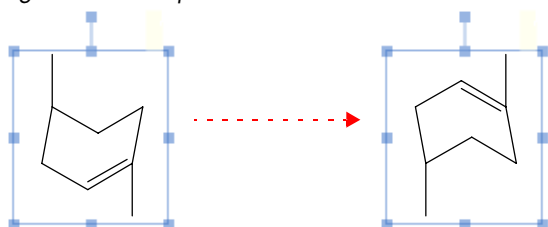


Atom labels and captions do not flip along with the object.

To reflect an object through a plane perpendicular to the Y-axis:

1. Select the objects to reflect.
2. Click the **Flip Vertical** command on the Object menu.

Figure 4.167: Flip vertical



## Creating Mirror Images

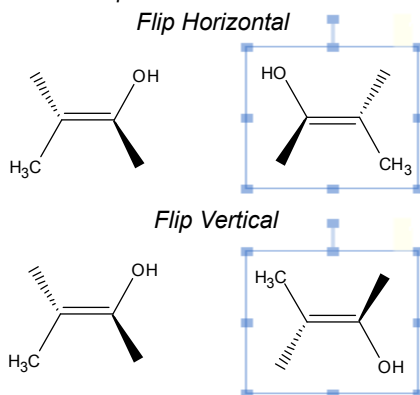
You can create mirror images from structures with defined stereochemistry by duplicating the structure and rotating it.

To create a mirror image:

1. Draw a structure with defined stereochemistry, for example, wedged bonds.
2. Select the structure and make a copy with **Ctrl+Drag** or **option+drag**.

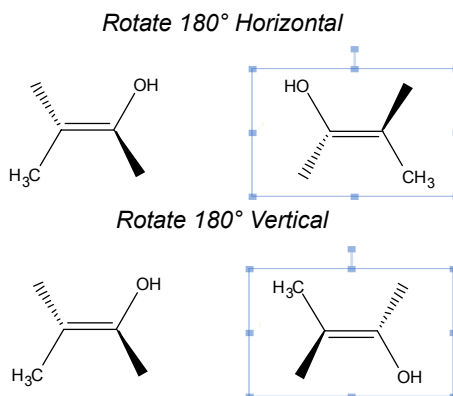
3. While the copy of the structure is still selected, choose **Flip Horizontal** or **Flip Vertical** from the Object menu.

Figure 4.168: Flip



You can also preserve the absolute stereochemistry while flipping by using the **Rotate 180°** commands on the Object menu.

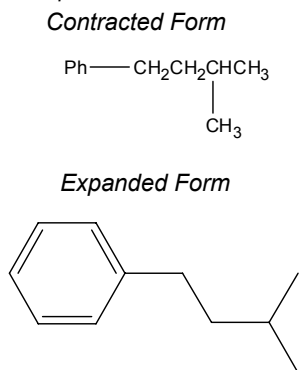
Figure 4.169: Rotate 180°



## Pro Expanding and Contracting Labels

If your structures contain defined nicknames, long atom labels, or contracted labels, ChemDraw can restore your structures to the fully expanded form.

Figure 4.170: Expanded and contracted forms



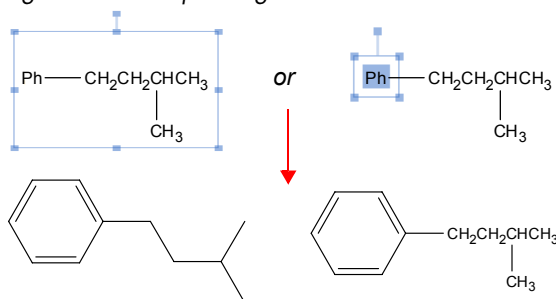
When you expand a label containing a divalent nickname, for example H-Ala-OH, the first attachment is to the character to the left of the nickname (H). The second attachment is to the character to the right of the nickname (OH).

To expand atom labels:

1. Select a selection tool.
2. Select the label to expand or double-click the structure to expand all possible labels.
3. Click the **Expand Label** command on the Structure menu.

Your structure is redrawn in its expanded form.

Figure 4.171: Expanding labels



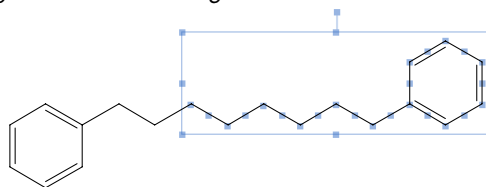
## Pro Contracting Labels

You can compress an area of a structure and replace it with a text label by using the Contract Label command. Contracted labels are similar to [Nicknames](#), but they are for one-time use only, in the current document.

To create a contracted label:

1. Select the area of the structure to contract.

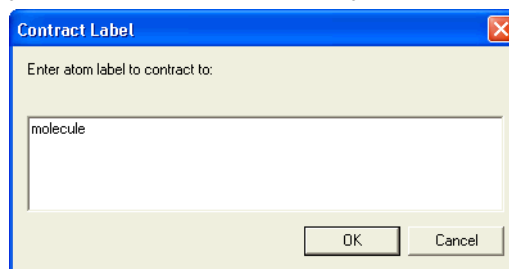
Figure 4.172: Selecting a structure to contract



2. Click the **Contract Label** command on the Structure menu.

The Contract Label dialog box appears.

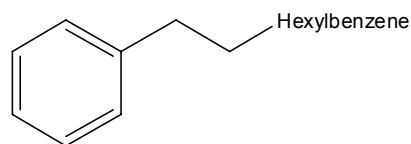
Figure 4.173: Contract label dialog box



3. Type a label for the contracted structure and click the **OK** button.

The label replaces the selected portion of the structure.

Figure 4.174: Contracted label

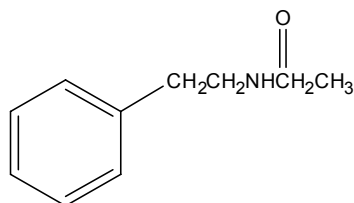
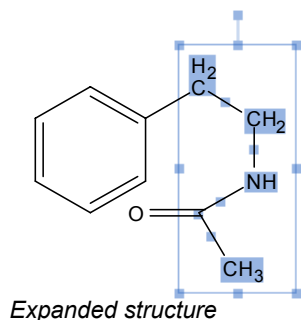


**NOTE:** If the area of the structure you contract contains errors, an error dialog box appears. Click *Ignore* to view any other errors. Click *Ignore All* to ignore all errors or *Stop* to end the contract process.

## Multi-Attached Labels

Multi-attached atom labels enable you to draw chemical structures more efficiently by allowing you to attach bonds anywhere along an atom label.

Figure 4.175: Multi-attached labels



## Adding Bonds to an Atom Label

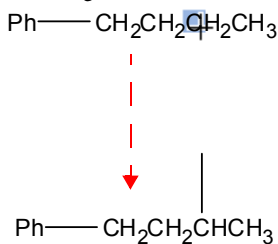
To add bonds to an atom label:

1. Draw the structure and attach any necessary atom label.
2. Select a Bond tool.
3. Position the cursor where you want to attach additional bonds.

The selected part of the atom label is highlighted.

4. Click or drag from the atom label to draw your bonds.

Figure 4.176: Adding bonds to a label



You can determine the orientation of the resulting bond by dragging. If you click to add a bond, there

are several preferential orientations for the resulting bond:

- Adding from the end of an atom label creates bonds that are preferentially horizontal.
- Adding from the middle of an atom label creates bonds that are preferentially vertical.
- Adding from the start of an atom label creates bonds that try to attain the chain angle setting on the [Drawing Settings](#) tab of the Document Settings dialog box. If that angle cannot be attained, the next best angle is used.

## Pro Structure CleanUp

The Structure CleanUp 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. Use Structure CleanUp to redraw structures that you may have drawn freehand or to neaten structures that you may have imported from another application.

Structure CleanUp may not create *the* best structure. Most structures have many “clean” forms, a problem that is particularly noticeable with straight-chain alkanes.

If you select only part of a structure when you choose Structure CleanUp, the other atoms and bonds are not affected.

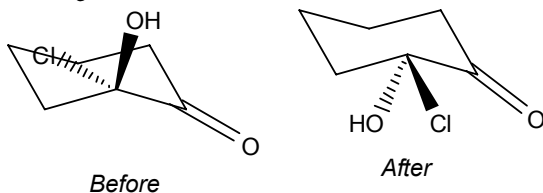
*NOTE: For some compounds, the Structure CleanUp command produces a structure that extends beyond the bounds of the page. To view the entire structure, scale the structure or increase the size of the printed page. For more information, see “Scaling Objects” on page 69 and “Page Setup” on page 151.*

General Rules for Structure CleanUp are:

- The Fixed Length setting on the [Drawing Settings](#) tab of the Document Settings dialog box determines optimum bond lengths.
- A given ring is redrawn only if all of its bonds are selected.

- Multi-attached atom labels and variable attachment points cannot be cleaned.
- Multi-center bonds cannot be cleaned.
- Structures are rotated so that as many bonds as possible are directed at a multiple of 15 degrees.
- Structure CleanUp preserves stereochemical meaning rather than the precise identity of any wedged or hashed bonds, as shown below.

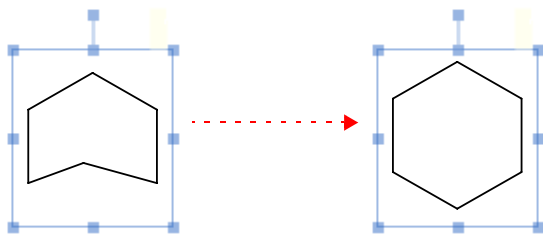
Figure 4.177: Preservation of stereochemical meaning



Using Structure CleanUp:

1. Select the structure or part of the structure you want to clean up with a selection tool.

Figure 4.178: Cleaning up a structure



2. Click the **Structure CleanUp** command on the Structure menu.

*NOTE: Structure CleanUp does not position molecules relative to other objects. Overlap may occur.*

## Multi-Center and Variable Attachments

You can draw polyhapto structures such as ferrocene ((Cp)<sub>2</sub>Fe), or an abbreviated notation for different positional isomers of a compound, using

attachment centers. The procedure is similar, and in both cases, the structure retains chemical significance.

Figure 4.179: Drawing a polyhapto structure

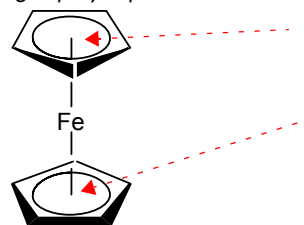
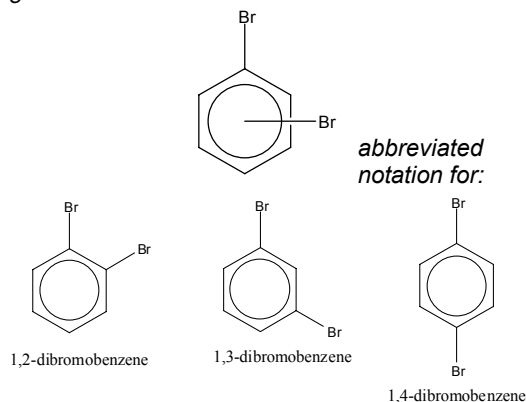


Figure 4.180: Isomers of dibromobenzene



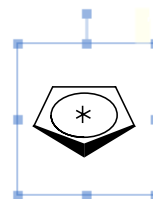
## Creating a Multi-Center Bond

To create a multi-center attachment point:

1. Select the structure whose center you want defined as a multi-center attachment point.
2. Click the **Add Multi-Center Attachment** command on the Structure menu.

An asterisk is displayed with the fragment to show that it contains a multi-center node.

Figure 4.181: Adding the multi-center attachment point

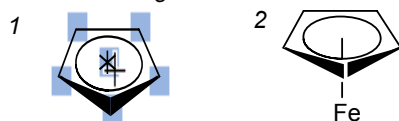


The asterisk is not visible once a bond is drawn to it. You can view the attachment point with a bond or selection tool. For more information, see “Viewing Attachment Points” on page 74.

To draw a bond to a multi-center attachment point:

1. Click the Bond tool.
2. Point to the asterisk and either click or drag to create a bond.

Figure 4.182: Adding a bond to the multi-center point



---

*TIP: Either disable or toggle Fixed Lengths to draw the bond so that it extends from the ring.*

---

## Creating a Variable Attachment Point

To create a variable attachment point:

1. Draw the structural fragment to which you want to assign a variable attachment node.
2. Select the fragment using a selection tool.
3. Click the **Add Variable Attachment** command on the Structure menu.  
An asterisk appears in the center of your fragment.
4. Point to the asterisk and drag to draw a bond.

---

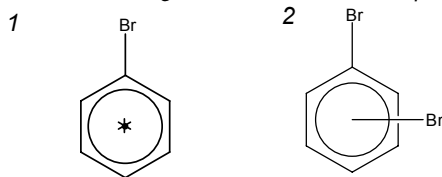
*TIP: Either disable or toggle Fixed Lengths to draw the bond so that it extends from the ring.*

---

You can treat this attachment node as you would treat the end of a normal bond.

5. Click a Bond tool.  
After you draw a bond from the attachment node, the asterisk disappears.

Figure 4.183: Using a variable attachment point



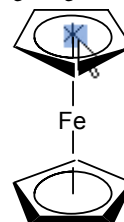
## Viewing Attachment Points

After you draw a bond from a variable or multi-center attachment point, the asterisk disappears. You can verify the node is present with a bond or a selection tool. This provides a way to check the definition of pre-existing attachment points.

To view a node with a selection tool, select the selection tool and position the cursor over to attachment point.

The attachment node is highlighted.

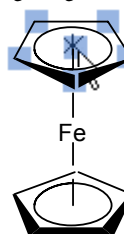
Figure 4.184: Highlighting with a selection tool



To view a node with a bond tool, select the bond tool and position the cursor over the attachment point.

The attachment node and all the atoms it represents are highlighted.

Figure 4.185: Highlighting with a bond tool





# Atom Numbering

You can add sequential numbering indicators to the atoms in a structure. ChemDraw recognizes the following types of indicators:

- Numbers (1, 2, 3, and so on)
- Text ending with a number (atom1)
- Greek letters in the Symbol font
- Letters (a, b, c, and so on)

The default indicator is numbers.

*TIP: To use text instead of numbers, number an atom then edit the number. See “Editing Atom Numbers” on page 75.*

## Showing and Hiding Atom Numbers

To add Atom Numbering to an entire structure:

1. Select the structure.
2. While pointing to the selected structure, do one of the following:
  - Right-click or control+click, point to **Atom** on the context menu, and click the **Show Atom Number** command.
  - Type the HotKey ‘ (single quote).

To number individual atoms

1. Select the atom.
2. Do one of the following:
  - Right-click (Mac: control+click), and click the **Show Atom Number** command.
  - Type the HotKey ‘ (single quote).

To hide Atom Numbering in a structure:

1. Select the structure.
2. Right-click or control+click, point to **Atom**, and deselect **Show Atom Number**.

To hide an individual atom number, do one of the following:

1. Point to or select the atom, right-click or control+click, and deselect the **Show Atom Number**.
2. Point to or select the atom number, right-click, and select **Hide Indicator**.

To remove an atom number indicator, do one of the following:

- Click the indicator with the Eraser tool.
- Point to the indicator with a Bond tool and type Backspace or Delete.

## Editing Atom Numbers

You can edit the text and style of atom number indicators.

To edit atom number text:

1. Select the Text tool.
2. Select the atom number indicator and type the changes.

*NOTE: When you type in a new indicator, you reset the counter for that structure to a new style. You may then continue numbering in that style with the standard means. For example, if you type  $\alpha$  in a text box, then point to another atom and use the context menu or HotKey, the atom will be labeled  $\beta$ . Switching to another structure resets the counter.*

To edit the atom number style, select the atom number indicator with the Text tool and use the Text menu or Text formatting toolbar.

## Positioning Atom Number Indicators

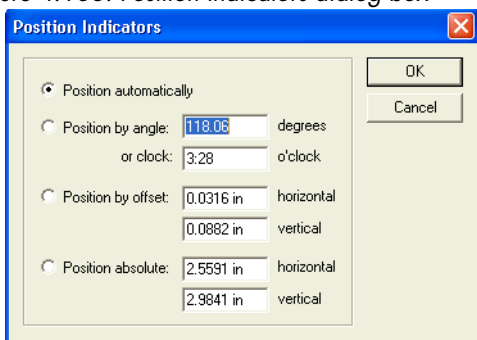
Atom number indicators are positioned automatically and move appropriately if a structure is modified. You can reposition them by dragging them to the desired position or use the Position Indicators dialog box.

To reposition an indicator:

1. Right-click the indicator to move and click the **Position** command on the context menu.

The Position Indicators dialog box appears.

Figure 4.186: Position Indicators dialog box




2. Click the appropriate position option, and enter a value.

Table 8: Positioning atom number indicators

To position ...	Type a value for Position ...
from the atom or bond center to the indicator center	by angle or by clock
from the atom or bond center to bottom left of indicator baseline	by offset—horizontal and vertical
at specified coordinates	absolute—horizontal and vertical

## Structure Perspective

You can rotate molecules or portions of molecules through three dimensions with the Trackball tool

. The Structure Perspective tool behaves similarly to the Marquee tool.

To rotate a structure:

1. Select the structure by dragging over it with the Trackball tool.

2. Place the cursor inside the marked rectangle and drag in any direction.

The structure will rotate on the X or Y axis, or a combination of X and Y.

3. Use Shift+drag to limit the rotation to the X or Y axes only.

You can also select part of a complex molecule and rotate it around a particular bond.

*NOTE: Do not try to use the Trackball to rotate objects such as orbitals or boxes. It was designed to manipulate chemical structures only.*

## Flatten Command


Although the Structure Perspective tool is not intended to be a 3D modeling tool, it does introduce z-coordinate information that is saved in CDX files. This pseudo-3D structure can be confusing when opening files that have been saved after perspective manipulation.

To remove perspective information:

1. Select a structure with the Marquee or Lasso Tool.
2. Click the **Flatten** command on the Object menu.

All z-coordinate information is removed from the structure.

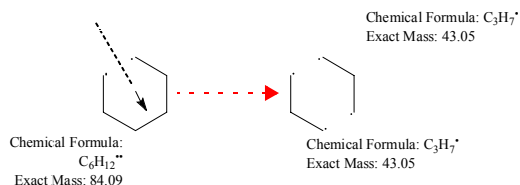
## Pro Mass Fragmentation Tool

The Mass Fragmentation tool  allows you to break existing structures across one or more bonds. This mimics the molecular fragmentation in a mass spectrometer, but does not have any predictive qualities: you must specify what bonds are to be broken.

To fragment a structure, drag the mouse across one or more bonds.

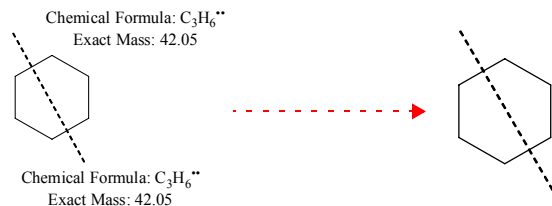
A line is drawn across the bonds that disappears when you release the mouse button. The operation is not final until the mouse is released. This means you can drag the line around holding the mouse button down to see different possibilities, and still back out without breaking any bonds. When the mouse button is released, any bonds crossed by the line are broken

Figure 4.187: Using the mass fragmentation tool



If you want the line to remain on display, hold down the **Alt** or **option** key *after* drawing the line.

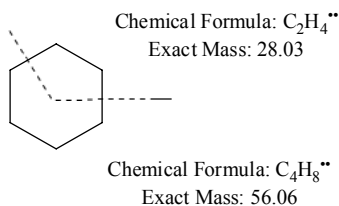
Figure 4.188: Mass fragmentation tool: displaying the line



*NOTE: The order in which you release the mouse button and the **Alt** or **option** key determines whether the line remains displayed or not. Releasing the mouse button first leaves the line displayed.*

The **Alt** or **option** key also allows you to “turn corners” and cut more than one bond.

Figure 4.189: Mass fragmentation tool: turning corners



When the line crosses a bond, the formula and exact mass for the fragments on either side of the bond are displayed as if the bond were homolytically broken. That is, a single bond turns into a monoradical on each fragment; a double bond turns into a pair of diradicals. If more than one bond is crossed, all fragments on each side of the line are considered together. If the only bond crossed is a ring bond, a single formula/mass pair is displayed.

*NOTE: It is possible to draw lines that tie themselves in knots. Use this tool with caution to avoid unrealistic fragmentation.*

You can reposition the formula and mass displays (they are text objects), or delete them altogether.

Table 9: Mass Fragmentation tool procedures

operation	behavior
drag	Breaks bond(s). The action does not take place until you release the mouse button, so you can “test alternatives”.
drag, holding down the <b>Alt</b> or <b>option</b> key	Draws a freehand line. If you release the mouse button before releasing the <b>Alt</b> or <b>option</b> key, the dashed line display remains.
drag across a bond, then press the <b>Alt</b> or <b>option</b> key.	Allows you to change direction and draw a polyline. If you release the mouse button before releasing the <b>Alt</b> or <b>option</b> key, the dashed line display remains.

## Pro Drawing Reactions



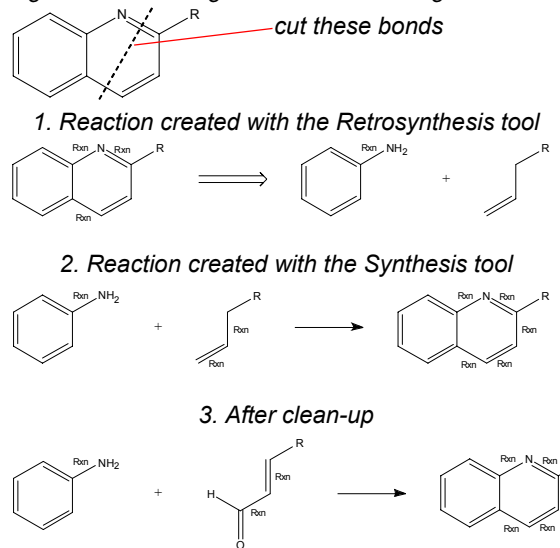
Two new tools speed the drawing of synthesis reactions. Both tools are used in a similar manner to the Mass Fragmentation tool: they are used to cut a bond or bonds in a product. The Synthesis tool  draws the resulting fragments as a standard reaction. The Retrosynthesis tool  draws the reaction with the product on the left and a broad arrow pointing to the reactants, as is customary in retrosynthetic analyses. In most cases, you will have to clean up the reaction by adding or deleting atoms or bonds.

Figure 4.190 shows how to use the tools for a demonstration of the Beyer Method for quinolines, with the simple clean up.

Figure 4.190: Using the reaction drawing tools



These tools are found in the Fragmentation tools section of the Main tools palette.

## Drawing with Templates

Template documents are collections of structures organized by structural type or functionality. A

structure in a Template document is named a template. Use an existing template instead of drawing the structure to shorten the time required to create documents.

The Template documents distributed with ChemDraw are stored in the ChemDraw Items folder in the same folder as the ChemDraw application.

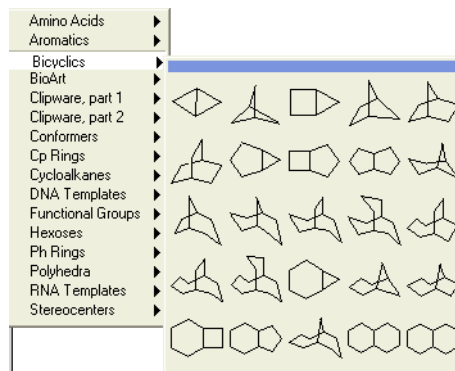
**NOTE: Pro** In ChemDraw Pro, you can define your own commonly used structures as templates. Any Template documents in the ChemDraw Folder are listed in the Windows menu (Macintosh) or Open Special on the File menu (Windows).

## The Templates Tool

The Templates tool contains a palette from which you can select different types of structures or objects. The Templates tool has two levels:

- The first level displays the available Template documents.
- The second level displays the templates within each Template document.


Figure 4.191: Using the template tool



**NOTE: Pro** In ChemDraw Pro the pop-up menu is segmented if any Template documents are open for editing. The upper segment contains Template documents that are currently open for editing.

## Choosing a Template

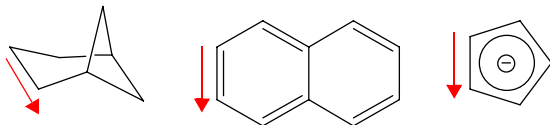
To choose a template from the Template palette:

1. Hold down the mouse button over the **Templates** tool . A menu listing the Template documents appears.
2. Point to a Template document name. A palette containing the available templates appears.
3. Choose a template from the palette.

## Using Templates

When you draw with templates, the first bond drawn determines the position of the template in a document window. All remaining bonds are drawn counterclockwise. The most nearly vertical bond on the far-left atom is drawn first, from top to bottom. If there are two equivalent bonds, the atoms that are at a lower position are used to draw the first bond.

Figure 4.192: Drawing direction of template structures



Templates are automatically scaled to the document settings of the current document in the active window. For more information, see “Autoscaling” on page 165.

After a template is drawn in a document window, the structures or objects can be manipulated by standard drawing and editing methods.

## Drawing a Template

To draw a template, click in a document window.

The template is drawn centered around the pointer in the orientation that it appears in the Templates palette.

## Fusing a Template With an Existing Structure

To draw a template and fuse it with an existing structure, click an existing bond in a document window.


To deposit a template and create a spiro-linkage with an existing structure, click an existing atom in a document window.

To draw a template in a document window and control the size and orientation, drag from the beginning of the first bond in the template to the end of the first bond.

When you drag upwards the bulk of the template is drawn to the left, and when you drag downwards the bulk of the template is drawn to the right. Templates must contain at least one bond in order to be drawn by the dragging method.

## Drawing with the Same Template

To draw another template of the same type:

1. Click the **Templates** tool .
2. Draw the template in a document window.

## **Pro** Creating Templates and Template Documents

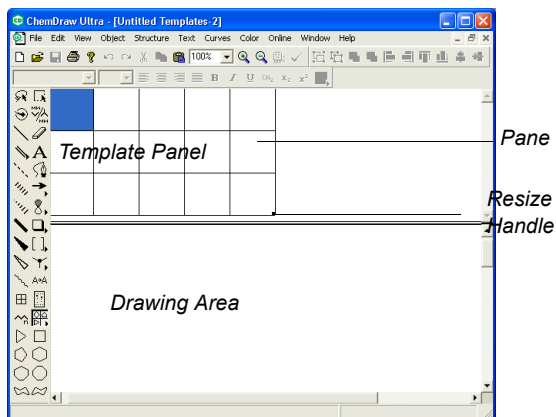
In ChemDraw Pro you can create new templates and add them to existing Template documents or create new Template documents.

To create a new Template document, open the File menu, point to **Open Special**, and choose **New Templates**.

A new and untitled Template window appears. The Template window is similar to a document window, but is divided in half by a moveable, horizontal line.

- **Template panel**—Top half of the window consists of individual panes where newly created templates appear.
- **Drawing area**—Bottom half of the window where you can draw new templates.

Figure 4.193: Template panel and drawing areas



The templates you define are not limited to atoms and bonds. Templates can contain any ChemDraw objects such as captions, boxes, arcs, orbitals, arrows, reaction mechanism symbols, and curves. The ChemDraw objects in Template documents can be colored. However, the colors do not appear in the Templates tool palette. You can paste pictures from other applications into a Template pane. Pasted objects are scaled to the current Template document settings. For more information, see “Autoscaling” on page 165.

### **Pro** Creating Templates

To create a new template:

1. Point to **Open Special** on the File menu, and choose the **New Templates** command.
2. Select a Template pane by clicking it.
3. Draw a structure or object in the drawing area of the Template window.

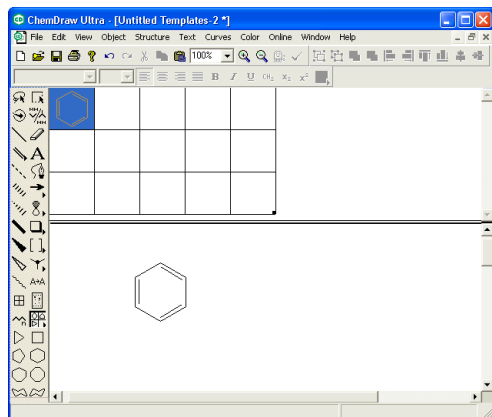
The structure appears in the Template pane as you draw. The tools in the Tools palette are used to draw a template in the drawing area of

the Template window exactly as they are used to draw structures in the drawing area of a document window.


To select a different Template pane, click another Template pane.

When you select a Template pane, the contents of the pane appear in the drawing area.

Figure 4.194: Adding a drawing to a panel



As you define templates they become available for use in your document without having to save the Template document.

To view the newly-defined Template, point at the Templates tool  and hold down the mouse button.

The name of the new Template document appears in the menu.

---

*TIP: If you haven't saved it yet, the name will be "Untitled Template".*

---

### Orientation of Templates

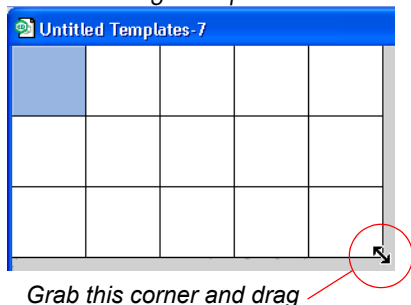
To make the templates that you create as easy to draw with as possible, it is recommended that you orient your structures so that the bond that establishes the position of the template, for example, the bond used for fusing is left and vertical. The most

vertical left bond is drawn first. For examples, see “Using Templates” on page 79.

## Resizing Template Panes

To resize the Template panes in the Template panel, drag the lower right corner of the Template panel.

Figure 4.195: Resizing a template



*TIP: If you have the Info window open, the height and width are displayed.*

## Template Panels

To increase the size of the Template panel, drag the Template dividing line.

To add a row of panes to the Template panel:

1. Select a Template pane.
2. Click either the **Add Row Before** or the **Add Row After** command on the Edit menu.

The new row is added before or after the Template pane you selected.

To add a column to the Template panel:

1. Select a Template pane.
2. Click either the **Add Column Before** or the **Add Column After** command on the Edit menu.

The new column is added to the right or left of the Template pane you selected.

To delete a row of Template panes from the Template panel:

1. Select a Template pane in the row you want to delete.

2. Click the **Delete Row** command on the Edit menu.

To delete a column of Template panes from the Template panel:

1. Select a Template pane in the column you want to delete.
2. Click the **Delete Column** command on the Edit menu.

The column is removed and all other columns are moved to the left.

## Saving Template Documents

To save a Template document and have it available in the Template pop-up menu and the Window menu:

1. Click the **Save As** command on the File menu. The Save As dialog box appears.

---

*TIP: Saving a Template document in the ChemDraw Items folder makes it accessible in the Open Special submenu and in the Templates tools palette.*

---

2. Type a name for the Template document and click the **OK** or **Save** button.

## Using Nicknames

Nicknames allow you to create short names for functional groups to use as an atom label or part of a label. When an atom is labeled with a Nickname, the chemical significance of the expanded structure is retained.

Commonly used Nicknames, such as **Me**, **Et**, and **Ph** are provided with ChemDraw in the **ChemDraw Nicknames** file located in your ChemDraw Items folder. You can edit this list using tools in ChemDraw. You should not attempt to edit this file directly.

You can assign HotKeys to Nicknames. For example, in the Nicknames and HotKeys provided with ChemDraw, the Hotkey, “4” labels an atom with

“Ph” which is a Nickname representing a phenyl group. For more information, see “Labeling Atoms with HotKeys” on page 60.

You can use Generic Nicknames when drawing query structures. For more information, see “Generic Nicknames” on page 97.

## Applying Nicknames

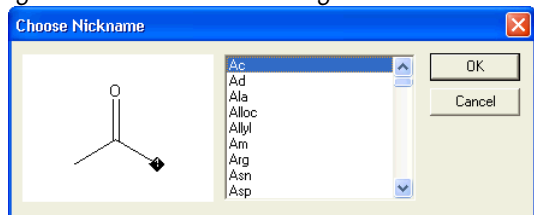
You may select a Nickname from the Nicknames dialog box or type it in manually. In either case, ChemDraw recognizes it as being chemically significant.

To select a Nickname to apply to an atom using a Hotkey:

1. Point to an atom.
2. Press the Hotkey “=” (equal sign).

The Choose Nickname dialog box appears.

Figure 4.196: Nickname dialog box



3. Select a Nickname from the list.

---

*TIP: You can jump to the approximately correct place in the Nickname list by typing the first letter of the Nickname.*

---

4. Click the **OK** button.

To enter a Nickname as an atom label:

1. Double-click an atom with a bond tool or click an atom with the Text tool.

An atom label text box appears.

2. Type a Nickname label such as **Et** or **Tos**.

*NOTE: Nicknames are tokens and do not flip orientation when applied to the left side of a structure when using Automatic Justification. For example, in the absence of a defined*

*Nickname, the label “OTHP” appears as “PHTO” when applied to the left side of a structure. However, since the Nickname “THP” is defined, the label appears as “THPO”. For more information, see “Aligning Text” on page 207.*

## Pro Defining Nicknames

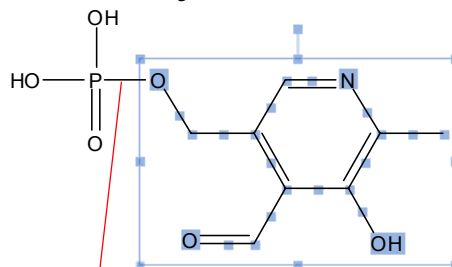
You can define Nicknames with one or two attachment points. The attachment points must be single bonds.

To define a new Nickname:

1. Create a structure containing the functional group you want to define as a Nickname.
2. Select the functional group.

You must indicate the connection point for the functional group by selecting the new fragment *without the bond* connected to the attachment point.

Figure 4.197: Adding a nickname



pyridoxal 5-phosphate

*don't include this bond*

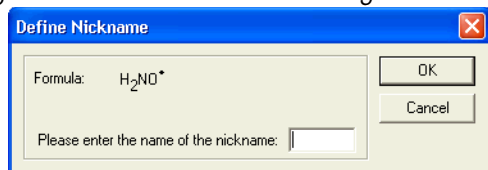
*NOTE: If stereochemistry is indicated in a structure that you are defining as a Nickname, the stereochemistry is retained.*

3. Click the **Define Nickname** command on the Structure menu.

The number of connection points is shown by radicals in the Formula. You can have only one or two connection points in a nickname.



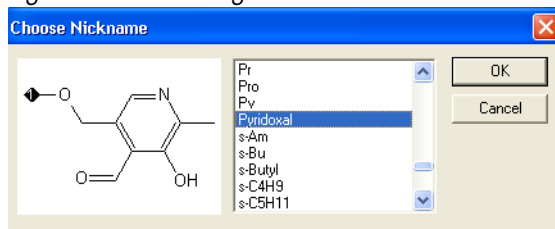
Figure 4.198: Define nickname dialog box



4. Type a short name for the Nickname.
5. Click the **OK** button.

The Nickname is defined.

Figure 4.199: Viewing the new nickname



If you use a Nickname that is the same as an element name, a message indicates that the element is replaced with the Nickname. For example, using **Ac** for an acetyl group replaces the element Actinium. The Check Structure command recognizes the label as an acetyl group rather than Actinium. ChemDraw provides the following default Nickname/Element conflicts:

Table 10: Nickname-element conflicts

Symbol	Nickname	Element
Ac	Acetyl	Actinium
Am	Amyl	Americium
Np	<i>para</i> -Nitro-phenyl	Neptunium
Pr	Propyl	Praeseodymium

To remove the overriding Nicknames, choose **List Nicknames** from the File menu and delete the overriding Nickname definition.

## Deleting Nicknames

To delete a Nickname:

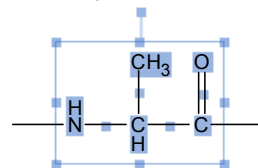
1. Click the **List Nicknames** command on the File menu.
2. Select the Nickname that you want to delete from the list.
3. Click the **Delete** button.

The Nickname is removed from the list.

## Defining Peptides with Nicknames

The definition in the figure below was used for the amino acid alanine. The unselected bond at each end of the structure indicates the connection points—Nitrogen on the left and Carbon on the right.

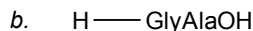
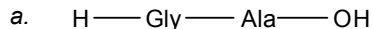
Figure 4.200: Creating an amino acid nickname



You can draw a peptide chain by:

- Stringing Nicknames together,
- Stringing Nicknames together in an atom label as long as there is a bond attached. or
- Stringing Nicknames together and not including bonds.

Figure 4.201: Creating peptides with nicknames



## Troubleshooting Nicknames

If the Define Nicknames command is disabled, check for the following:

- A connection point is not present
- More than 2 connection points are defined

- The connection point is not a single bond

In *Figure 4.202a*, the entire functional group was selected. Because there is no atom that indicates a connection point, you cannot define a Nickname.

When the sulfonamide group is attached to an unselected bond, you can define a Nickname.

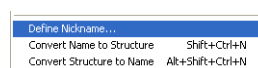
In *Figure 4.202b*, there is more than one attachment point on a single atom in a nickname.

*Figure 4.202c* attempts to define more than two selection points.

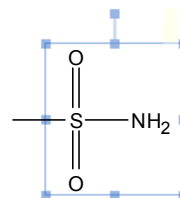
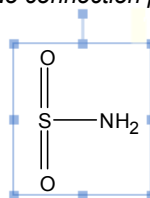
**Figure 4.202: Troubleshooting nicknames**

**Incorrect**

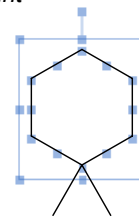
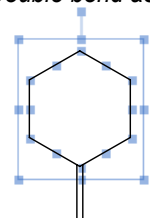
**Correct**



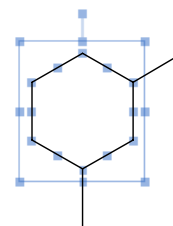
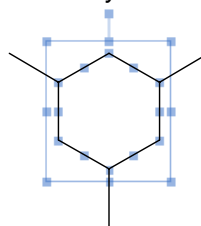
**a. No connection point**



**b. Double bond as connection point**



**c. Too many connection points**



# Chapter 5: Query Structures

## What Are Query Structures?

Using a query structure to specify properties for atoms and bonds provides an efficient way to search chemical databases such as ChemFinder, DARC, RS<sup>3</sup>, or ISIS/Base. You can use a query structure to narrow or broaden your search.

For example, creating a query structure indicating a bond as either double or single might broaden your search. Indicating atom properties where a particular atom must have a charge of +3 might narrow your search.

Because ChemDraw is not a chemical database application, the interpretation of query structures involves other programs. Not all databases support the same query properties. If you use a query structure containing properties not understood by a given database, one of the following may happen:

- An error message appears
- The unsupported properties are ignored

To use query structures for searching you may do either of the following:

- Paste the query structure into a database search window and initiate a search.
- Save the structure in an appropriate file format and open the file in the database application.

For more information on query properties see “Query Properties” on page 236, or consult the documentation for your chemical database.

*NOTE: ChemOffice 2006 does not prevent or warn you if you try to assign conflicting or nonsensical properties. For example, you can require that one of the atoms in benzene is not part of any ring, which is inherently impossible. The results of such a search depend on the query system used, but usually no matches are found.*

## Atom Properties

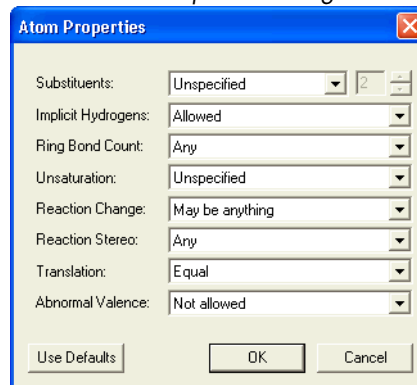
To assign properties to selected atoms in a structure:

1. Do one of the following:

Select a single atom by clicking it with a selection tool.

- Select multiple atoms by Shift+clicking the atoms.
2. Then do one of the following:
    - Right-click, select the property you want, and click the appropriate option.
    - Click the **Atom Properties** command on the Structure menu. The Atom Properties dialog box appears.
    - Press the Hotkey “I”. The Atom Properties dialog box appears.

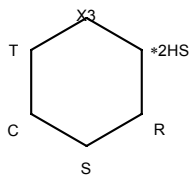
Figure 5.203: Atom Properties dialog box



In the Atom Properties dialog box, select the properties to associate with the selected atom(s). Click the **OK** button.

Query indicators appear next to atoms that have associated atom properties.

Figure 5.204: Displaying query indicators



The character that appears depends on which query properties have been assigned. If more than one property is assigned, more than one character appears adjacent to the atom. For more information, see “Query Indicators” on page 96.

Table 11: Atom properties indicators

Indicator	Query Property
*	<b>Substituents:</b> Free Sites (followed by the number of free sites)
U	<b>Substituents:</b> Up to (followed by the maximum number of substituents)
X	<b>Substituents:</b> Exactly (followed by the number of substituents)
H	<b>Implicit Hydrogens</b>
R	<b>Ring Bond Count</b>
S	<b>Unsaturation</b>
C	<b>Reaction Change</b>
T	<b>Reaction Stereo</b>
L	<b>Translation</b>

Table 11: Atom properties indicators

Indicator	Query Property
I	<b>Isotopic Abundance</b>
(none)	<b>Abnormal Valence</b>

## Viewing Atom Property Values

Except for the three Substituents query properties, the characters indicate that a given property is applied, but not the value of that property.

To find the value of a query property setting:

1. Select the atom.
2. Do one of the following:
  - Right-click, point to an atom, and point to the appropriate property.
  - Click the **Properties** command on the Structure menu and view the settings on the **Atom Properties** tab.

## Removing Atom Properties

To remove all atom properties from an atom:

1. Select the atom.
2. Click the **Properties** command on the Structure menu.
3. Click **Use Defaults**.

The atom properties are removed and the characters no longer appear.

To remove specific atom properties:

1. Select the atom.
2. Do one of the following:
  - Right-click, point to an atom, point to the property you want, and choose the appropriate option.
3. Click the **Properties** command on the Structure menu and click the atom property to remove.

## Atom Property Options

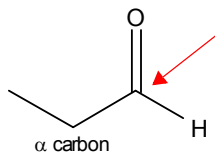
The following topics describe the atom properties you can associate with an atom.

### Substituents

The three Substituents properties specify the number of substituents that may be bonded to the selected atoms. In ChemDraw, a substituent is defined as a non-hydrogen atom connected by a bond of any order.

For example, in the figure below, the carbonyl carbon, indicated by the arrow, has a substituent count of two: the alpha carbon and the aldehyde oxygen. The double bond to the aldehyde oxygen counts as only one substituent and hydrogen atoms never count as substituents.

Figure 5.205: Substituent count



The substituent count atom property allows you to specify the number of bonds to an atom in the target structure. This includes bonds already drawn in the query structure.

Table 12: Substituent options

Option	Search Result
Unspecified	<i>Default.</i> Search is determined by the target database. Some databases (including ISIS) find compounds with any substitution at this atom and some databases (including DARC) find only compounds with substitution exactly as drawn.

Table 12: Substituent options

Option	Search Result
Free Sites	Finds compounds in which the selected atoms may contain a range of substituents up to the number specified plus the number of bonds as drawn. A value of zero finds a substituent count as drawn. You can also use the Free Sites symbol in the Chemical Symbols palette to apply free sites. For more information, see “The Chemical Symbols Tools Palette” on page 134.
Up to	Finds compounds in which the selected atoms may contain a range of substituents up to the number specified.
Exactly	Finds compounds in which the selected atoms contain the exact number of substituents as specified, up to 15 substituents.

### Implicit Hydrogens

The Implicit Hydrogens property specifies whether additional, implicit hydrogen atoms may be attached to the selected atoms. If implicit hydrogen

atoms are not allowed, all valences to that atom must be filled by bonds to non-hydrogen atoms.

Table 13: Implicit hydrogen options

Option	Search Result
Allowed	<i>Default.</i> Finds compounds regardless of whether hydrogen atoms are attached to the selected atoms.
Not allowed	Finds compounds with no additional hydrogen atoms attached to the selected atoms.

## Ring Bond Count

The Ring Bond Count specifies the number of bonds attached to an atom that are part of rings of any size. For simple cases, this also specifies the maximum number of rings in which an atom can reside.

Table 14: Ring bond count options

Option	Search Result
Any	<i>Default.</i> Finds compounds in which the selected atoms can be a member of any type of ring, or a member of no ring at all.
No ring bonds	Finds compounds in which the selected atoms are acyclic.
As drawn	Finds compounds in which the selected atoms reside in the same type and number of rings as drawn.

Table 14: Ring bond count options

Option	Search Result
Simple ring	Finds compounds in which the selected atoms is a member of only one ring (the atom has two ring bonds).
Fusion	Finds compounds in which the selected atoms lies at ring fusions (the atom has three ring bonds).
Spiro or higher	Finds compounds in which the selected atoms is a member of a spiro or higher linkage (the atom has four or more ring bonds).

## Unsaturation

The Unsaturation property specifies whether a multiple bond is attached to the selected atoms.

Table 15: Unsaturation options

Option	Search Result
Unspecified	<i>Default.</i> Finds compounds regardless of whether a multiple bond is attached to the selected atoms.
Must be absent	Finds compounds that do not have a multiple bond attached to the selected atoms.
Must be present	Finds compounds that have at least one multiple bond (double, triple or aromatic) attached to the selected atoms.

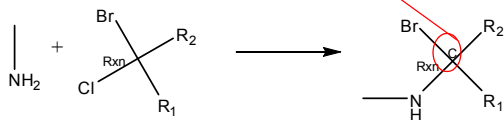
## Reaction Change

The Reaction Change property specifies whether a change occurs at selected atoms after a reaction. This property is only meaningful when searching a database containing chemical reactions. In *Chem-Finder*, only the product atom is checked. The stereo designation is ignored on reactants.

Table 16: Reaction change options

Option	Search Result
May be anything	<i>Default.</i> Finds all reactions regardless of any change to selected atoms after a reaction.
Must be as specified	Finds all reactions that are changed at the selected atoms exactly as specified by the reaction center property in the Atom Properties dialog box.

Figure 5.206: Indicating reaction change  
Reaction change indicator



## Reaction Stereo

The Reaction Stereo property specifies that the selected atoms are stereo-centers in a reaction. This property is only meaningful when searching a database containing chemical reactions.

Figure 5.207: Indicating reaction stereo  
Reaction stereo indicator

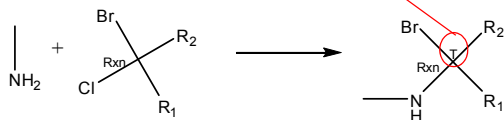


Table 17: Reaction stereo options

Option	Search Result
Any	<i>Default.</i> Finds all compounds regardless of the stereochemistry at the selected atoms.
Inversion	Finds compounds in which the selected atoms have an inverted stereo configuration after a reaction.
Retention	Finds compounds whose selected atoms have an unchanged stereo configuration after a reaction.

## Translation

The Translation property specifies what is required to match in the structure query and possible database hits in a Markush DARC query.

Table 18: Translation options

Option	Definition
Equal	<i>Default.</i> Matches specific to specific or generic to generic terms.
Broad	Translates specific query atoms to corresponding superatoms in the database.
Narrow	Translates query superatoms to corresponding specific atoms or groups in the database.
Any	Translates generic or specific terms to any term.

For more information, refer to the Markush DARC User Manual.

## Isotopic Abundance

The Isotopic Abundance property gives you the ability to distinguish between different isotopic compounds—for example between mono- and hexa-deuterobenzene—by specifying a nuclide at any location.

Table 19: Isotopic abundance options

Option	Search results
Unspecified	<i>Default</i>
Any	For ChemFinder, the same as default. Included for compatibility with other systems where the default may be different.
Natural	Indicates an isotopically unmodified nuclide.
Enriched	Indicates a mixture of isotopically substituted and isotopically unmodified nuclides.
Deficient	Indicates a depleted label, that is, the nuclide is present in less than the natural ratio.
Nonnatural	Indicates an isotopically substituted nuclide, that is, essentially all the molecules of the compound have only the indicated nuclide.

## Abnormal Valence

The Abnormal Valence property specifies whether selected atoms can have a valence other than nor-

mal. “Normal” valences for each element are defined in the Isotopes Table file in the Chem-Draw Items folder.

*NOTE: The Abnormal Valence atom property does not provide a visual indicator.*

Table 20: Abnormal valence options

Option	Search Result
Not allowed	<i>Default.</i> Finds compounds where the selected atoms only have valences that are normal for that element. If necessary, hydrogen atoms are automatically added to or removed from the atom before transferring it to the chemical database. If the Check Structure When Copying to Clipboard or Exporting preference is turned on, an error message warns of abnormal valences.
Allowed	Finds compounds with the specific valence drawn.

*NOTE: If Abnormal Valence is Allowed, any Invalid Valence messages for those atoms are ignored automatically by the Check Structure command.*

## Bond Properties

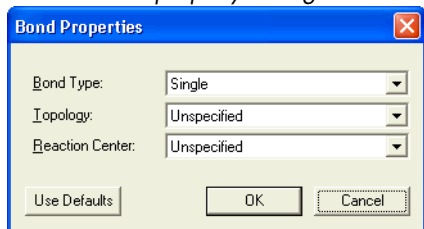
To define bond properties of selected bonds in a structure:

1. Do one of the following:
  - Select a bond using a selection tool.
  - Shift+click to select multiple bonds.
2. Then do one of the following:
  - Right-click, point to **Bond** on the context menu, point to the property you want, and choose the appropriate option.



- Click the **Properties** command on the Structure menu. On the **Bond Properties** tab, select the bond properties to associate with the selected bonds from the drop-down lists. Click **OK**.
- Point to a bond and press the Hotkey “/”. The Bond Properties dialog box appears.

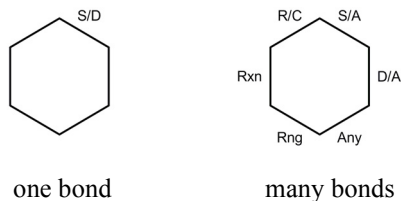
Figure 5.208: Bond property dialog box



In the Bond Properties dialog box, select the properties to associate with the selected atoms. Click **OK**.

Query indicators appear next to bonds that have associated bond properties.

Figure 5.209: Displaying bond properties



The characters that appears depends on which query properties have been assigned. If more than one property is assigned, more than one descriptor appears adjacent to the atoms. For more information, see “Query Indicators” on page 96.

The indicators are described in the following table.

Table 21: Bond property descriptors

Indicator	Bond Query Property
Any	Bond Type: Any

Table 21: Bond property descriptors

Indicator	Bond Query Property
S/D	Bond Type: Single/Double
D/A	Bond Type: Double/Aromatic
S/A	Bond Type: Single/Aromatic
Rng	Topology: Ring
Chn	Topology: Chain
R/C	Topology: Ring or Chain
Rxn	Reaction Center

## Viewing Bond Property Values

The descriptor for the Reaction Center query property indicates that the property is applied, but not the value of the property.

To find the value of a query bond property setting:

- Select the bond.
- Do one of the following:
  - Right-click, point to **Bond**, and point to the appropriate property.
  - Click the **Bond Properties** command on the Structure menu, and view the settings of the drop-down list boxes.

## Removing Bond Properties

To remove all bond properties from selected bonds:

- Select the bonds.
- Click the **Properties** command on the Structure menu.
- Click **Use Defaults**.

The bond properties are removed and the indicators are no longer adjacent to the selected bonds.

To remove specific bond properties:

1. Select the bond.
2. Do one of the following:
  - Right-click, point to the appropriate property, and click the property to remove.

- Click the **Properties** command on the Structure menu, and click the bond property to remove.

## Bond Property Options

The following are the atom properties that you can associate with an atom:

### Bond Type

This property specifies the bond type of the selected bonds. The default bond type corresponds

to the current type of the bond (single, double, etc.) as drawn.

Table 22: Bond type options

Option	Search Result
Single (all) and Dative	Finds compounds with the bond type you select for the selected bonds.
Double <i>or</i> Double Bold	Finds compounds whose selected bonds are double.
Double Either	Finds compounds whose selected bonds are double bonds and have either <i>cis/trans</i> stereochemical configuration.
Aromatic	Finds compounds whose selected bonds are aromatic.
Tautomeric	Finds compounds whose selected bonds are tautomeric.
Triple	Finds compounds whose selected bonds are triple.
Quadruple	Finds compounds whose selected bonds are quadruple.
Any	Finds compounds regardless of the bond type of the selected bonds.
S/D	Finds compounds whose selected bonds are single or double.

Table 22: Bond type options

Option	Search Result
D/A	Finds compounds whose selected bonds are double or aromatic.
S/A	Finds compounds whose selected bonds are single or aromatic.

*NOTE: Not all bond types are supported in all file formats. When an unsupported bond type is saved to a given file format, it is converted to the closest equivalent that is supported.*

## Topology

The Topology property specifies the ring environment of the selected bonds.

Table 23: Topology options

Option	Search Result
Unspecified	<i>Default.</i> Finds compounds regardless of environment.
Ring	Finds compounds where the selected bonds are part of a ring.
Chain	Finds compounds where the selected bonds are part of a chain (and are specifically not part of a ring).
Ring or Chain	Finds compounds where the selected bonds are part of either a ring or a chain.

## Reaction Center

The Reaction Center property specifies how the selected bonds are affected in a reaction. This property is only meaningful when searching a database containing chemical reactions.

Table 24: Reaction center options

Option	Search Result
Unspecified	<i>Default.</i> Finds compounds regardless of whether the selected bonds are affected by the reaction.
Center	Finds compounds where the selected bonds are affected by a reaction, but the type of change is unspecified.
Make/Break	Finds compounds where the selected bonds are either broken or created in a reaction.
Change	Finds compounds where the bond order of the selected bonds changes in a reaction.
Make& Change	Finds compounds where the selected bonds are formed, broken, or undergo a change in bond order.
Not Center	Finds compounds where the selected bonds are not part of the reaction center.
Not Modified	Finds compounds where the selected bond's orders do not change, but which may or may not be part of the reaction center.

Table 24: Reaction center options

Option	Search Result
Unmapped	Finds all compounds.

## 3D Properties

3D queries are particularly useful in pharmacophore searching where the user is looking for a particular 3D relationship among atoms and bonds, for example in a series of potential receptor ligands. To create a 3D query, you add geometries (lines, planes, etc.) and constraints (specified as ranges) to a query structure. For example, you might specify that two atoms must be between 4 and 5 Å apart, or that two planes must be separated by 80-100 degrees.

To assign 3D properties to a structure, select the structure or sub-structure and select one of the following options from the **Add 3D Property** command on the Structure menu.

*NOTE: Because some 3D properties specify an order, you should use Shift+Click to select them in the proper order rather than using the Marquee or Lasso tool to select them all at once.*

In the table below, *points* may be atoms, centroids or points. *Lines* may be lines or Normals.

Table 25: 3D property options

Option	Search Result
Angle	Defines an angle constraint between three points (in order). Indicated as a range.

Table 25: 3D property options

Option	Search Result
Dihedral	Defines a dihedral (torsional) angle constraint among four points (in order), between two lines, or two planes. Indicated as a range.
Distance	Defines a distance constraint between two points, a point and a line, or a point and a plane. Indicated as a range, in Angstroms.
Line	Defines the best-fit line for the selected points.
Plane	Defines the best-fit plane for the selected points, or for a point and a line.
Exclusion Sphere	Defines an exclusion sphere around a point. If more than one point is selected, the exclusion sphere is around the first selected point, and the subsequent points are allowed within the exclusion sphere when the query is evaluated. Indicated as a range, in Å, beginning at 0.
Normal	Defines the normal from a defined plane in the direction of a point.
Point	Defines a point positioned at a specified distance from a first point in the direction of a second point (in order), or in the direction of the normal.

Table 25: 3D property options

Option	Search Result
Centroid	Defines a point positioned at the average position of all other points selected.

All constraint values can be edited with the text tool. Only exclusion spheres show the change visually.

When you create a point, a dialog box is displayed. Specify the distance from the first selected point to the calculated point. The distance may be specified as an absolute value in Å or as a percentage of the distance between the selected points. Negative values indicate that the calculated point is further from the second point than the first point is, rather than being between them.

Geometry and constraint objects update dynamically when you change the structure; they cannot be moved independently. They may be used with CDX, MOL, SKC, and TGF files (full read-write compatibility); they are not compatible with other formats. They can, however, be saved in print-only formats such as TIFF.

## Query Tools Palette

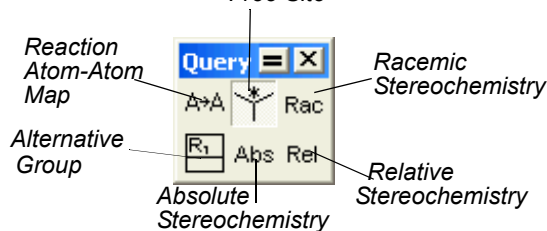
ChemDraw provides Query tools to enable you to draw query structures.

To display the Query tools, select **Show Query Tools** from the **Other Tools** command on the View menu, or click the Query Tools icon on the Main Tool Palette:

- Click .

The Query tools palette appears.

Figure 5.210: Query tools palette  
Free Site



## Query Indicators

You can display small characters to indicate query properties you assign to atoms and bonds.

### Viewing Query Indicators

To display query indicators for a structure, select a structure to which query indicators are assigned, right-click, point to **Atom** or **Bond** on the context menu, and click the **Show Query Indicator** command.

To display query indicators for individual atoms or bonds, select the atom or bond, right-click, and choose the **Show Query Indicator** command on the context menu.

### Hiding Query Indicators

To hide an individual indicator:

1. Select the indicator to hide.
2. Right-click and select **Hide Indicator**.

### Removing Query Indicators

To delete a query indicator:

1. Click the indicator.
2. Click the eraser tool and click the indicator.

### Positioning Query Indicators

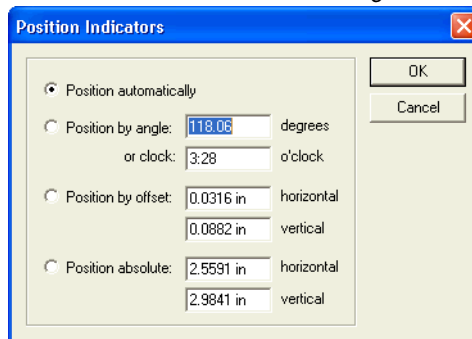
Query indicators are positioned automatically and move appropriately if a structure is modified. You can reposition them by dragging them to the desired position or with the Indicator Position dialog box.

To reposition an indicator numerically:

1. With a selection tool, click the indicator to move.
2. Right-click and choose **Position**.

The Position Indicator dialog box appears.

Figure 5.211: Position Indicators dialog box



3. Click the appropriate Position option, and type a value:

Table 26: Position options

To Position ...	Type a value for...
from the atom or bond center to indicator center	angle, degrees or clock, o'clock
from the atom or bond center to bottom left of indicator baseline	offset, horizontal and vertical
at specified coordinates	absolute, horizontal and vertical

## Drawing Stereochemical Symbols

ChemDraw provides three types of stereochemical flags that indicate that the molecule with which they are associated represents one of the following:

- **Racemic**—A racemic mixture.
- **Absolute**—A pure enantiomer of known configuration.
- **Relative**—A pure enantiomer of unknown configuration.

See “Relative Stereochemistry” on page 114 for changes in ChemDraw 10.

The font and size for stereochemical flags is determined by the default Atom Label size for the document.

To draw a stereochemical flag:

1. Click the tool for the flag you want to use on the Query tools palette.
2. Position the pointer next to the structure to which you want to assign the flag.
3. Click to deposit the symbol.

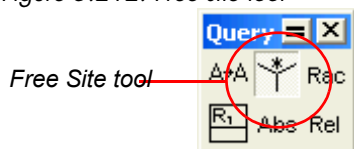
## Drawing Free Sites

Use the Free Sites tool to increment or decrement the number of free sites in a query structure.

To increment the number of Free Sites:

1. Click the Free Site tool on the Query tools palette.

Figure 5.212: Free site tool



2. Position the pointer over the atom to which you want to apply free sites.
3. Click to add the symbol.
4. Continue to click the atom to increment the free site number.

To decrement the number of free sites, hold the **Alt** or **option** key while clicking the atom.

You can also change the free sites by using the Atom Properties dialog box or the shortcut menu. For more information see “Atom Properties” on page 85.

## Generic Nicknames

Generic nicknames represent a class of elements or structural moieties. The generic nicknames recognized as chemically significant by ChemDraw are:

- **A**: used to represent any moiety
- **M**: used to represent metal
- **Q**: used to represent a non-hydrogen heteroatom
- **X**: used to represent any halide
- **R**: undefined; used in the usual way

If you are using a query system that recognizes generic nicknames, you can use these nicknames in your ChemDraw query structure.

To label an atomic position with a generic nickname, do one of the following:

- Double-click on the atom to open a text box, and type in the nickname.
- Right-click on the atom, point to **Insert Generic Label** on the context menu, and click the label you wish to insert on the sub-menu.

You can assign Generic nicknames, like other nicknames, to HotKeys. For information on assigning a Hotkey to a nickname, see “Creating HotKeys” on page 210.

You cannot define the *meaning* of a generic nickname in ChemDraw because generic nicknames represent multiple (and perhaps an infinite number of) substituents. Generic nicknames have meaning only in the context of the search system you are using.

The generic nicknames recognized as chemically meaningful to ChemDraw are listed in Generic Nicknames file in the ChemDraw Items folder.

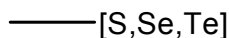
To edit the generic nickname files, open the Generic Nicknames file in a text editor and make your changes. Follow examples in the file for the correct format.

NOTE: If you perform *Check Structure* on a structure with a generic nickname, a message is displayed because the structure contains variable substituents. If you ignore this message, the generic nicknames are ignored and ChemDraw reports the chemical formula, mass, and so on as if the atom label containing the generic nickname were not selected.

## Element Lists

You can define your search query more concisely with the element list. By labeling an atom position as a list of elements you specify that one of these elements must match in the structure for which you are searching. The elements in the element list must be separated by commas. A space after each comma and brackets are optional. An example of an element list is shown below.

Figure 5.213: Element list



NOTE: An element list may contain only atomic symbols, plus D (deuterium) and T (tritium).

To create an element list:

1. Open an atom label text box.
2. Type an open bracket (“[”) followed by a list of elements separated by commas (“Cl, Br, I”), followed by a close bracket (“]”).
3. Close the text box.

Figure 5.214: Adding an element list to an atom label

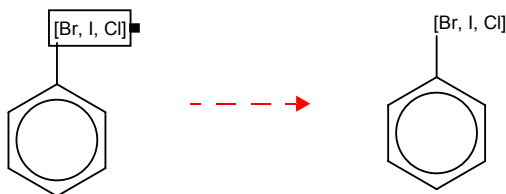
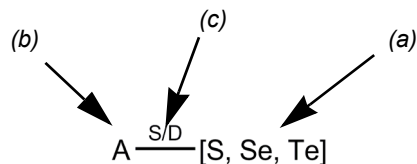


Figure 5.215 shows a query structure created to find compounds matching the following criteria:

- Non-oxygen chalcogenide bonded to another atom.
- Not necessarily carbon (a generic nickname).

- The bond type between the chalcogenide and the other atom to be a single or double bond.

Figure 5.215: Query example



The “A” label indicates that the atom may match any atom except hydrogen. The mark near the bond indicates that the bond has special properties. The bond type specified in the Bond Properties dialog box must be single or double, S/D. The “[S,Se,Te]” specifies that one of these elements must match in the target structures.

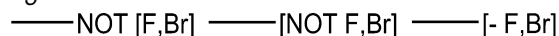
## Element Not-Lists

The element not-list specifies that the elements in the list match must not match in the structure for which you are searching. Commas must separate the elements in the element not-list. A space after each comma and brackets are optional.

The word NOT must be in all-caps and must be followed by a space. Alternatively, the word NOT may be replaced with a minus sign.

For example:

Figure 5.216: Element NOT lists



NOTE: An element not-list may contain only atomic elements, plus D (deuterium) and T (tritium).

To create an element not-list:

1. Open an atom label text box.
2. Type an open bracket, the word NOT, and a space (“[NOT”) followed by a list of elements separated by commas (“Cl, Br, I”), followed by a close bracket (“]”).



## Link Nodes

You can specify a variable-length chain or ring by indicating that one of the atoms can be repeated some number of times using link nodes.

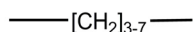
Link nodes must have exactly two connecting bonds. The atom label must conform to the following conditions:

- No more than a single element symbol or a generic nickname
- The last part of the label in the form: *number hyphen number*, with the number and hyphen subscripted
- Parentheses or braces may be used instead of brackets
- Brackets can be omitted if not needed for clarity, for example with O<sub>1-3</sub>

To create a link node:

1. Open an atom label text box.
2. Type in the following format:


Figure 5.217: Link node



## Representing Polymers and Other Repeating Units

Brackets, parentheses, and braces enclose structures or structural fragments that are to be repeated a number of times. The bracket properties in ChemDraw allow you to specify the context and orientation of the repeating units.

To enclose structures with brackets:

1. Click the Bracket tool  and select one of the double bracket tools.
2. Drag across the structure to draw the brackets.
3. Right-click or control-click and select the appropriate bracket properties from the menu that appears.

The bracket properties are described in the following sections.

*NOTE: This method will give a default value for component order, multiple group repeat count, or SRU label. To change a default value, use the Bracket Properties dialog box.*

### Setting Bracket Properties

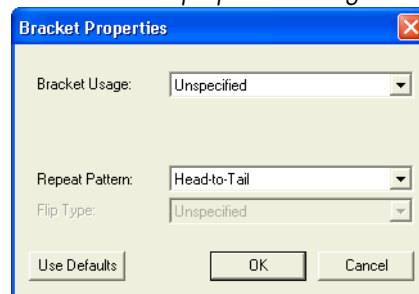
You can change the properties of brackets by the context menus or Bracket Properties dialog box.

To use the Bracket Properties dialog box:

1. Select the right bracket with a selection tool.
2. Click **Bracket Properties** on the Structure menu.

The Bracket Properties dialog box appears.

Figure 5.218: Bracket properties dialog box



The Flip Type option appears only for brackets with exactly two crossing bonds, and is disabled in other cases.

You can customize the text that appears to the bottom right of the bracket for the following bracket types.

- Component (c#)—the Component Order must be a non-negative integer, and is displayed as the letter “c” followed by that integer (or “c” alone if an order of zero is specified).
- Multiple Group (#)—the Repeat Count must be a positive integer.
- SRU (n)—the SRU label can be any text.

You can also edit the text for these Bracket Usage types directly in the document using the Text tool.

You cannot edit the text displayed for the other Bracket Usage types.

## Bracket Usage

Representations of polymers are either structure-based or source-based. The type of bracket you use depends on which type of representation you need. For references, see “Polymer Representations” on page 235.

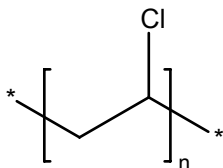
### Structure-based Polymer Representations

Structure-based polymer representations enclose only a portion of a structure within brackets. One or more bonds cross each of the enclosing brackets. The crossing bonds “match up”, making the polymer structure more explicit.

You create a structure-based polymer representation by enclosing a portion of a structure in brackets with a bracket type of SRU (n). The subscript “n” is recommended by IUPAC to notate structure-based representations of unknown size, but you can edit the text using the text tool.

A structure-based representation of poly(vinyl chloride) is shown in *Figure 5.219*.

*Figure 5.219: Structure-based polymer representation*



You can also use the Bracket Usage types “Crosslink (xl)”, “Graft (grf)”, and “Modification (mod)” to represent specific types of repeating units in a structure-based representation, but they are rarely encountered and using them is discouraged.

### Source-based Polymer Representations

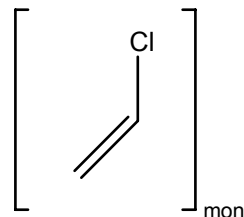
Source-based polymer representations enclose an entire discrete chemical substance in brackets. The

mode of polymerization may be obvious from context, or it might be unknown. Source-based representations are useful when describing processes where the starting materials are known, but the exact structure of the reaction product is not.

You can create a source-based representation by enclosing a structure in “Monomer (mon)” brackets.

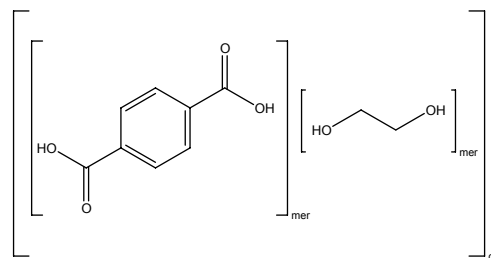
A source-based representation of poly(vinyl chloride) is shown in *Figure 5.220*.

*Figure 5.220: Source-based polymer representation*



You can use “Mer (mer)” brackets for components of a copolymer where those individual components are known not to repeat themselves or alternate with the other components. An example is shown in *Figure 5.221*.

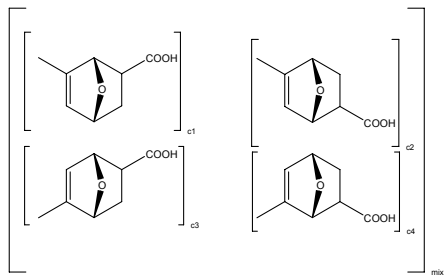
*Figure 5.221: Copolymer representation*



Copolymers represent substances with more than one repeating unit. In general, you can use bracket type “Component (co)”. You can also use “Copolymer, alternating (alt)”, “Copolymer, random (ran)”, and “Copolymer, block (blk)” to represent different specific types of copolymers in a source-based representation, but they are rarely used and their use is discouraged.

The bracket type, “Mixture, unordered (mix)” is not for polymers, but to represent a collection of substances that may all be present, but not necessarily in known amounts. Bracket type “Component (c)” indicates individual mixture elements. An example is shown in *Figure 5.222*.

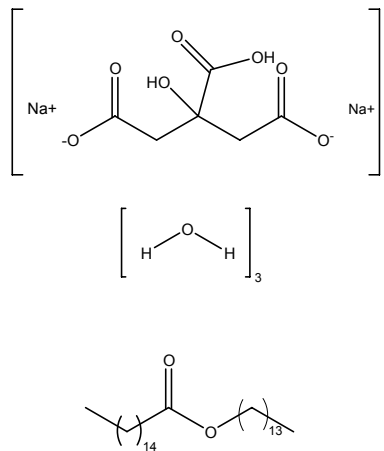
*Figure 5.222: Brackets used to indicate mixtures*



Bracket type “Mixture, ordered (f)” is primarily used to describe manufacturing processes, where the ordering of components is a critical part of the process (and where a different ordering might produce a different final product. As with Unordered Mixtures, individual elements of an ordered mixture should be surrounded by brackets with a bracket usage of “Component (c)”. Unlike with Unordered Mixtures, however, components of Ordered Mixtures must represent their ordering. You can do this by editing the “c” label with the text tool to include a number (“c1”, “c2”, and so on.)

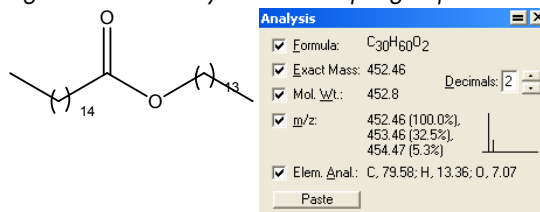
You use the bracket type, “Multiple Group (#)” to indicate that the enclosed items are repeated a specific known number of times. Multiple Group brackets may enclose entire structures, or may enclose a portion of the structures only. You can edit the numeric repeat count with the text tool. Examples are shown in *Figure 5.223*.

*Figure 5.223: Brackets used to indicate multiple groups*



Because Multiple Group brackets represent a specific repeat count (unlike the unknown repeat count of the other bracket types), it is possible to calculate accurate molecular weights (and related data) for such structures. That data is displayed in the Analysis window as with any other structure.

*Figure 5.224: Analysis with multiple groups.*

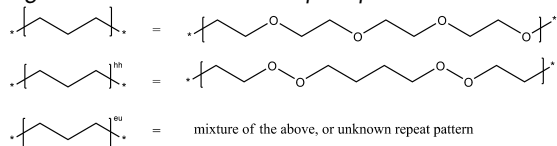


## Repeat Pattern

For simple linear polymers, the repeating units may connect head-to-tail or head-to-head (or their repeat pattern might be a mixture or unknown). You can also assign this property to brackets.

Because of its prevalence, the Head-to-Tail type is assumed to be the default Repeat Pattern, and does not receive any special annotation on the brackets, as shown in *Figure 5.225*.

Figure 5.225: Head-to-tail repeat pattern

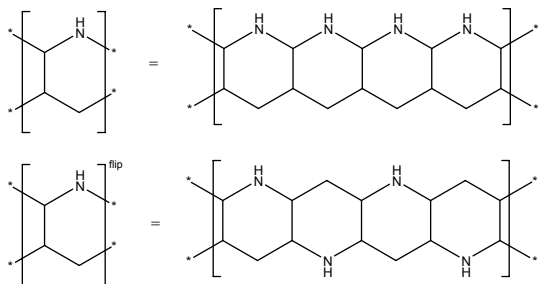


## Flip Type

For ladder-type polymers (those polymers with two connecting bonds on each side), there is a potential ambiguity in the order of the connections. You can assign the Flip Type property to resolve that ambiguity. This property is appropriate only for brackets with exactly two crossing bonds, and is disabled in other cases.

Because of its prevalence the No Flip type does not receive any special annotation.

Figure 5.226: Indicating flip type in ladder-type polymers

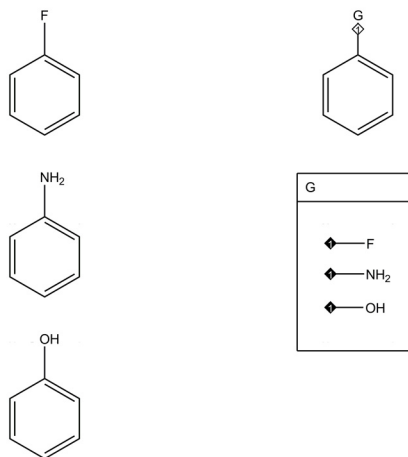


## Alternative Groups

You can create a search query that contains variable functional groups or substructures. Instead of submitting multiple queries on structures that share a common substructure, you can submit a single query with the parent structure. The parent structure can have attachment points to a list of alternative groups that you can define.

Alternative groups, sometimes called R-Groups or G-Groups (Generic Groups), are shown below.

Figure 5.227: Alternative groups



## Defining an Alternative Group

In ChemDraw Pro, you can create alternative group definitions (R, G, etc.) that represent a set of substituents, any one of which will match the query.

To define an alternative group:


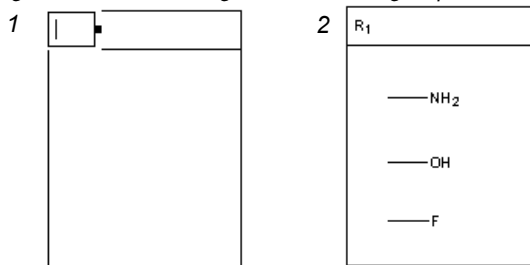

1. Click the Alternative Group query tool  and drag with the tool to create an area large enough to draw the alternative groups.
2. Type a title, such as R<sub>1</sub>, in the Alternative Group Title box, then draw the substructure fragments in the Alternative Group box.

Figure 5.228: Defining an alternative group



Specify where the fragments should bond to the parent structure on the alternative group label by defining Attachment Points

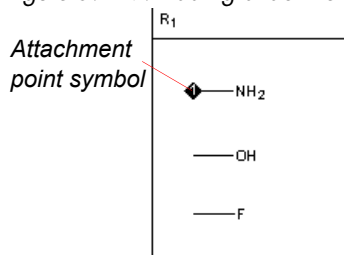
3. Do one of the following:

- Select the diamond shaped Attachment Point tool  on the Chemical Symbols palette, and click a substructure fragment where you want to place the attachment point.
- Point to a substructure fragment where you want to place the attachment point and press the Hotkey “.” (period).

An attachment point symbol appears.

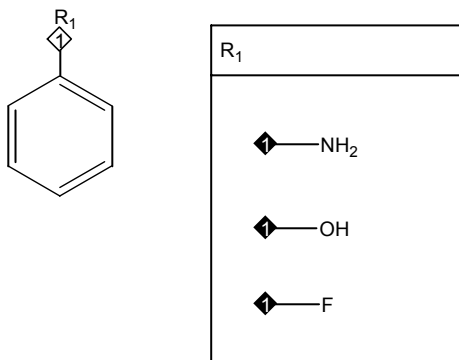
4. Repeat for all fragments.

Figure 5.229: Adding attachment points



When you create a parent compound that contains an alternative group you defined, an attachment point symbol appears next to the label. The attachment point number matches that found in the definition.

Figure 5.230: Structure with R-group table



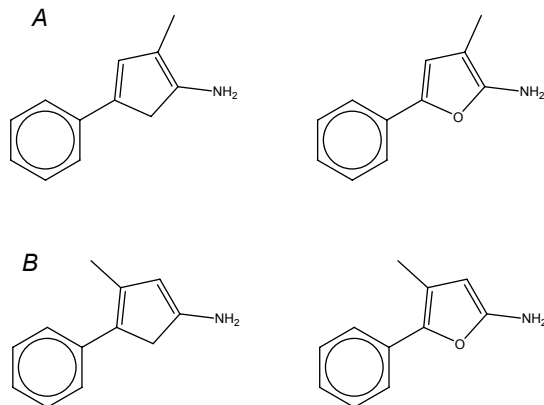
The number displayed in the attachment point symbol is the attachment rank order. See the example in “Multiple Attachment Points” on page 103.

## Multiple Attachment Points

If you have well-defined multiple attachment points on your structure fragments, you can perform searches for specific materials. This type of search is especially useful for searching for conformationally similar structures.

For example, you want to find the two compounds in *Figure 5.231A*. However, you are not interested in the two compounds in *Figure 5.231B*.

Figure 5.231: Multiple attachment points

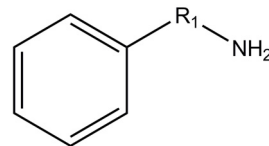


By specifying the attachment point order, you can exclude the unwanted compounds. The parent structure in *Figure 5.232* satisfies the necessary requirements.

To specify the attachment points order:

1. Draw the parent structure shown below.

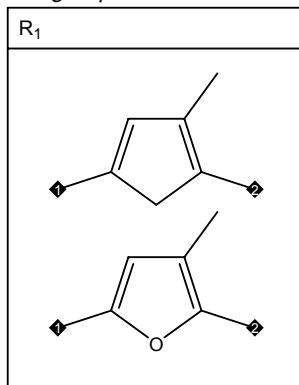
Figure 5.232: Specifying the attachment point order



2. Create an Alternative Group Box labeled “R1”.
3. Draw the structure fragments and label them with attachment points.

When the alternative group definition is complete, the attachment point symbols appear in the parent compound.

Figure 5.233: R-groups with multi-attachment points



By numbering your attachment points, you have unambiguously specified that the methyl group must be adjacent to the amine group. The conformations that are not of interest are excluded.

## Showing Attachment Rank Indicators

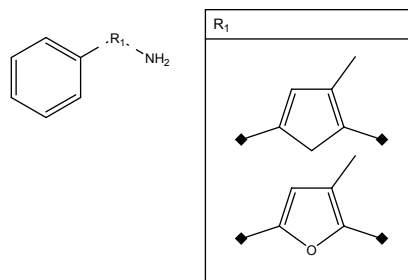
You can hide the attachment rank indicators if required. For example, sometimes—particularly in publication-quality drawings—the numbering of attachment points is implicit and the numbered attachment rank indicators are superfluous.

To hide the attachment rank indicators and remove the numbers from the attachment points:

1. Click the **Preferences** command on the File menu.
2. In the Preferences dialog box, click **Display**.
3. Deselect **Show Attachment Rank Indicators**.

Figure 5.234 shows an alternative group definition and a parent structure with the attachment rank indicators hidden.

Figure 5.234: Hidden attachment rank indicators



This change affects all documents.

## Attachment Point Numbering

Numbered attachment points allow you to specify precisely how the structure fragments are connected to your parent structure.

The numbering of the attachment points is related to the front to back order of the attachment points. To set the order of the attachment points, click the ends of the bonds in order.

The last point clicked has the highest number.

To change the ordering of the attachment points do one of the following:

- Click the attachment points with the Attachment Point tool.
- Select an attachment point with a selection tool, and click either the **Bring to Front** or the **Send To Back** command on the Object menu.

The attachment point numbers are highest in the front.

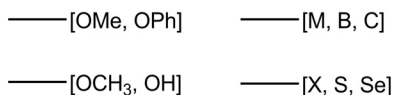
## Anonymous Alternative Groups

An anonymous alternative group is a cross between an element list and an alternative group. Element lists are restricted to single elements, but anonymous alternative groups can contain any structure that can be represented by text. Nicknames and generic nicknames are allowed in anon-

ymous alternative groups. Anonymous alternative groups are shortcut notation for regular alternative groups, eliminating the need to specify a name such as “R1”.

You can define your search query more concisely with the anonymous alternative group. By labeling an atom position as a list of substructures you specify that one of these substructures must match in the structure for which you are searching. Commas must separate the items in the anonymous alternative group. A space after each comma and the brackets are optional. Examples of anonymous alternative groups are shown in *Figure 5.235*.

*Figure 5.235: Anonymous alternative groups*




To create anonymous alternative groups:

1. Open an atom label text box.
2. Type an open bracket “[” followed by a list of elements, fragments, nicknames, or generic nicknames separated by commas, followed by a close bracket “]”.

## Atom-to-Atom Mapping

You can create correspondences between atoms in different structures for use in creating queries for searching a reaction database. The reactions mapped can be single or multi-step. You can assign atom-to-atom mapping for creating records for a reaction database and for creating queries for searching a reaction database. You can assign atom mapping in two ways:

- Automatic mapping, using the **Map Reaction Atoms** command from the Structure menu.
- Manual mapping, using the Reaction Atom-Atom Map tool  on the main tools palette.

During either type of mapping process, the mapping algorithm perceives and assigns a reaction center for the reactants and products.

When a reaction map is established, you can point to an atom in one structure with the Reaction Atom-Atom Map tool selected to highlight the mapped atom in the other structure.

## Always Display and Print Atom Mapping

To make the symbols always appear and print on the atoms when reaction mapping has been performed:

1. Click the **Preferences** command on the File menu.
2. In the Preferences dialog box, click **Display**.
3. Select **Always Display and Print Reaction Mapping**.
4. Click **OK**.

Deselect **Always Display and Print Atom Mapping** to show the symbols only when you select the Reaction Atom-Atom Map tool. When this option is deselected, atom mapping symbols do not print, even though a reaction map has been created.

## Automatic Mapping

To automatically create a reaction map:

1. Draw the reaction you want to map and select the reactants and products.

---

*TIP: Double-click the arrow with a selection tool to select the entire reaction.*

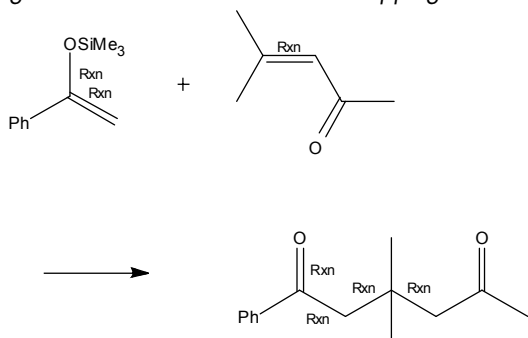
---

2. Click the **Map Reaction Atoms** command on the Structure menu.

The symbol **Rxn** appears next to the bonds in the reactant and product that are perceived by the algorithm as being modified by the reaction. These symbols are bond properties that

are automatically applied. For more information about the Reaction Center bond property, see “Bond Properties” on page 90.

Figure 5.236: Automatic reaction mapping

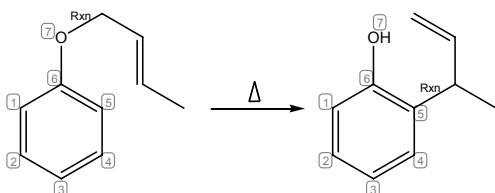


## Manual Mapping

In situations that require manual mapping of atoms, you can use the Reaction Atom-Atom Map tool. This might be necessary when the automatic mapping is applied to complicated reactions, and gives incorrect results. In these cases you can manually readjust the reaction mapping.

Figure 5.237 shows the initial mapping being amended by using the Reaction Atom-Atom Map tool.

Figure 5.237: Automatic mapping to be amended



When you perform manual mapping with the Reaction Atom-Atom Map tool, you can suppress automatic re-mapping of atoms other than your target atom.

To suppress automatic re-mapping:

1. Click the **Preferences** command on the File menu.
2. Select **Automatic Reaction Mapping** on the General tab.

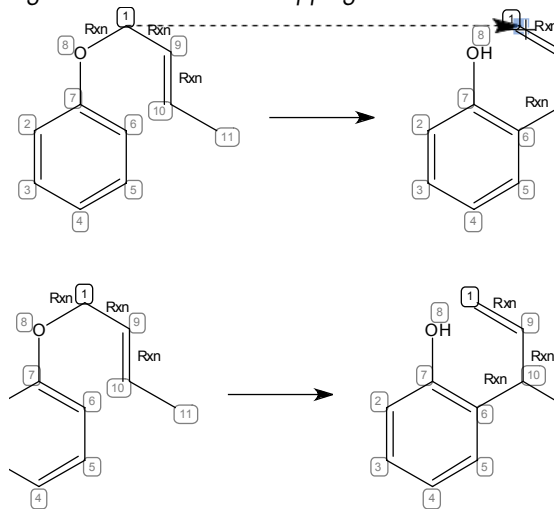
3. Click **OK**.

To use the Reaction Atom-Atom Map tool to supplement the automatic mapping:

1. Click the Reaction Atom-Atom Map tool **A→A**.
2. Point to the atom in the reactant whose mapping you want to establish. For example, in the following drawing you would point to the acyclic carbon adjacent to the ether oxygen.
3. Drag from the reactant atom to the corresponding product atom.

The remaining atoms are automatically mapped based on the manual mapping you performed.

Figure 5.238: Finalized mapping



You can continue to set or change the mapping for other atoms in the reaction if necessary until you get exactly the mapping you want. For this example additional manual mapping is not necessary.

## Clearing Reaction Mapping

To clear all reaction mapping:

1. Select the structures whose mapping you want to remove.
2. Click the **Clear Reaction Map** command on the Structure menu.



## Exporting Reaction Mapping

Reaction mapping and reaction center perception information are stored in the native ChemDraw file format (\*.cdx) for reopening in ChemDraw and the ISIS Reaction file format for transfer to other applications that read atom mapping, such as ChemFinder and ISIS/Base. You can also copy mapped reactions to these same applications using the Clipboard.

## Export Compatibility

Because query properties are only useful in a chemical database, you must transfer your structures from ChemDraw into your search system. Not all file formats support the same query properties and not all chemical databases support the same file formats. Consult the documentation for your database to see which file formats are supported.

The following table lists the query properties that ChemDraw writes to ISIS (SKC, TGF, and Clipboard) file formats. All query properties are written to the ChemDraw (CDX) file format. CDX is the preferred format to use to retain all query properties in a drawing.

Table 27: Query properties by export format

Exported Query Properties	ISIS	Mol	Rxn
Atom Properties			
Substituents			
Unspecified	<b>X</b>	<b>X</b>	<b>X</b>
Free Sites	<b>b</b>	<b>b</b>	<b>b</b>
Up to	<b>a</b>	<b>a</b>	<b>a</b>

Table 27: Query properties by export format

Exported Query Properties	ISIS	Mol	Rxn
Exactly	<b>X<sup>c</sup></b>	<b>X<sup>c</sup></b>	<b>X<sup>c</sup></b>
Implicit Hydrogens			
Not allowed	<b>X</b>	<b>X</b>	<b>X</b>
Allowed	<b>X</b>	<b>X</b>	<b>X</b>
Ring Bond Count			
Any	<b>X</b>	<b>X</b>	<b>X</b>
No ring bonds	<b>X</b>	<b>X</b>	<b>X</b>
As drawn	<b>X</b>	<b>X</b>	<b>X</b>
Simple ring	<b>X</b>	<b>X</b>	<b>X</b>
Fusion	<b>X</b>	<b>X</b>	<b>X</b>
Spiro or higher	<b>X</b>	<b>X</b>	<b>X</b>
Unsaturation			
Unspecified	<b>X</b>	<b>X</b>	<b>X</b>
Must be absent			
Must be present	<b>X</b>	<b>X</b>	<b>X</b>
Reaction Change			

Table 27: Query properties by export format

Exported Query Properties	ISIS	Mol	Rxn
May be anything	<b>X</b>		<b>X</b>
Must be as specified	<b>X</b>		<b>X</b>
Reaction Stereo			
Any	<b>X</b>		<b>X</b>
Inversion	<b>X</b>		<b>X</b>
Retention	<b>X</b>		<b>X</b>
Translation			
Equal			
Broad			
Any			
Narrow			
Abnormal Valence			
Not Allowed	<b>X</b>	<b>X</b>	<b>X</b>
Allowed	<b>X</b>	<b>X</b>	<b>X</b>
<b>Bond Properties</b>			

Table 27: Query properties by export format

Exported Query Properties	ISIS	Mol	Rxn
Bond Type			
Single	<b>X</b>	<b>X</b>	<b>X</b>
Dashed	<b>X</b>	<b>X</b>	<b>X</b>
Hashed	<b>d</b>	<b>d</b>	<b>d</b>
Wedge Hashed	<b>X</b>	<b>X</b>	<b>X</b>
Bold	<b>X</b>	<b>e</b>	<b>e</b>
Wedge	<b>X</b>	<b>X</b>	<b>X</b>
Wavy	<b>X</b>	<b>X</b>	<b>X</b>
Hollow Wedge	<b>e</b>	<b>e</b>	<b>e</b>
Dative	<b>f</b>	<b>f</b>	<b>f</b>
Double	<b>X<sup>g</sup></b>	<b>X<sup>g</sup></b>	<b>X<sup>g</sup></b>
Double Either	<b>X</b>	<b>X</b>	<b>X</b>
Double Bold	<b>h</b>	<b>h</b>	<b>h</b>
Aromatic	<b>X</b>	<b>X</b>	<b>X</b>
Tautomeric	<b>i</b>	<b>i</b>	<b>i</b>

Table 27: Query properties by export format

Exported Query Properties	ISIS	Mol	Rxn
Triple	<b>X</b>	<b>X</b>	<b>X</b>
Quadruple	<b>I</b>	<b>I</b>	<b>I</b>
Any	<b>X</b>	<b>X</b>	<b>X</b>
S/D	<b>X</b>	<b>X</b>	<b>X</b>
D/A	<b>X</b>	<b>X</b>	<b>X</b>
S/A	<b>X</b>	<b>X</b>	<b>X</b>
Topology			
Unspecified	<b>X</b>	<b>X</b>	<b>X</b>
Ring	<b>X</b>	<b>X</b>	<b>X</b>
Chain	<b>X</b>	<b>X</b>	<b>X</b>
Reaction Center			
Unspecified	<b>X</b>		<b>X</b>
Center	<b>X</b>		<b>X</b>
Make/Break	<b>X</b>		<b>X</b>
Change	<b>X</b>		<b>X</b>
Make&Change	<b>X</b>		<b>X</b>

Table 27: Query properties by export format

Exported Query Properties	ISIS	Mol	Rxn
Not Center	<b>X</b>		<b>X</b>
Other Query Attributes			
Generic Nicknames	<b>X<sup>i</sup></b>	<b>X<sup>i</sup></b>	<b>X<sup>i</sup></b>
Element Lists	<b>X<sup>ko</sup></b>	<b>X<sup>ko</sup></b>	<b>X<sup>ko</sup></b>
Element Not-Lists	<b>X<sup>k</sup></b>	<b>X<sup>k</sup></b>	<b>X<sup>k</sup></b>
Alternative Groups	<b>X</b>	<b>X<sup>m</sup></b>	
Anonymous Alternative Groups	<b>n</b>	<b>n</b>	
Link Nodes	<b>p</b>	<b>p</b>	<b>p</b>
Bracket properties	<b>X</b>	<b>X</b>	<b>X</b>
Atom-Atom mapping	<b>X</b>		<b>X</b>
Variable Attachment Positions			
3D query properties			

<sup>a</sup>Converted to the appropriate number of exact substituents

<sup>b</sup>Free Sites counts of zero translated to “Substitution as drawn”; all other Free Sites values written as substitution counts equal to the total current valence plus the free sites value.

<sup>c</sup>Substituent counts of greater than 5 are translated to “6 or more”

<sup>d</sup>Converted to Wedged Hashed

<sup>e</sup>Converted to Wedged

<sup>f</sup>Converted to a Single, with a positive charge applied to that atom at the base of the dative bond and a negative charge applied to the atom at the point of the dative bond

<sup>g</sup>Interpreted by ISIS as unspecified *cis/trans* stereochemistry

<sup>h</sup>Converted to Double

<sup>i</sup>Converted to S/D

<sup>j</sup>Only M, X, Q, A; others written as aliases

<sup>k</sup>Truncated to the first 5 elements

<sup>l</sup>Converted to single.

<sup>m</sup>An RGFile will be created automatically.

<sup>n</sup>Converted to non-anonymous alternative groups.

<sup>o</sup>Lists of greater than 5 elements converted to alternative groups.

<sup>p</sup>The low end of the repeat range is always treated as 1.

# Chapter 6: Chemistry Features

## Checking Chemistry

### Check Structure

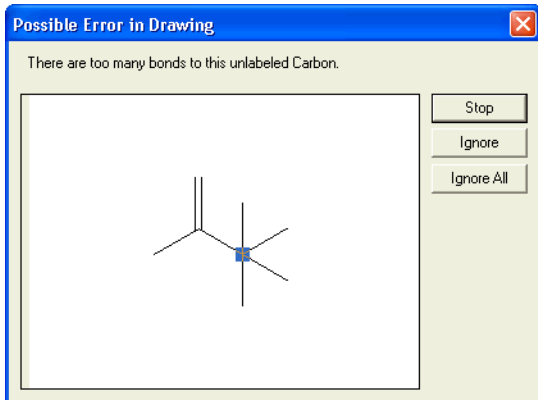
You can check the chemistry of a selected structure, part of a structure, or caption (in Formula style). The Check Structure command identifies errors in valences, labels and defined Nicknames.

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.

Figure 6.239: Check structure information window



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**.

### Check Structure when Copying to Clipboard or Exporting

To have ChemDraw perform a check structure analysis on any structure copied to the Clipboard:

1. Click the **Preferences** command on the File menu.
2. Click the **Check Structure When Copying to Clipboard or Exporting** check box.

This change affects all documents.

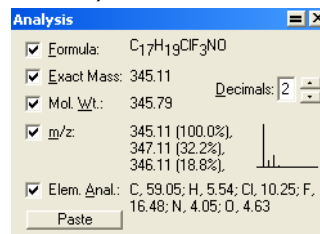
## Viewing Analysis Information

The Analysis window displays the chemical formula, exact mass, molecular weight, m/z, and elemental analysis for the entire document, a structure, part of a structure, or a caption in Formula style.

To view analysis information, click the **Show Analysis Window** command on the View menu.

The Analysis window appears.

Figure 6.240: Analysis window



Values for selected objects in the document window are shown. If no structure is selected in your document, values for the entire document are shown.

You can have this window open as you draw in the document. It shows the current values as you draw.

The Decimals setting applies to Exact Mass, Molecular Weight, and m/z only.

Table 28: Analysis properties

Property	Description
Formula	The molecular formula showing the exact number of atoms of each element in the molecule and charges, radicals, and isotopes.
Exact Mass	The exact molecular mass of the structure, where atomic masses of each atom are based on the most common isotope for the element.
Molecular Weight	The average molecular mass of the structure, where atomic masses are based on the natural abundance of all isotopes of the element.
m/z	Mass/charge, where charge = 1. The weights of the most common isotopes and a graphical representation of the isotopic abundance is shown.  The molecular weight shown takes the isotopes for each atom and their natural abundance into account. Where there is more than one abundant isotope, ChemDraw computes multiple molecular weights. Low abundance combinations (whether because the isotope is in low abundance or because it includes many moderate-abundance contributions) are not taken into account.  You cannot paste the graph in a document.

Table 28: Analysis properties

## Property Description

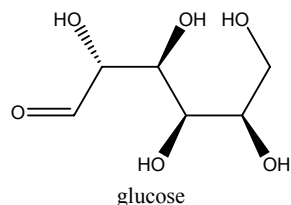
Elemental Analysis The percent by weight of each element in the structure.

To paste information about a structure as a caption:

1. Click the check boxes for the information that you want to paste.
2. Click **Paste**.

The information appears as a multiline caption below the structure. You can edit this information with the text tool.

Figure 6.241: Adding analysis information to a structure

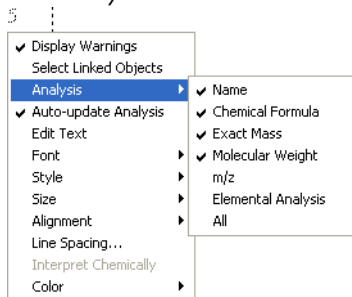


Chemical Formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>  
Exact Mass: 180.06  
Molecular Weight: 180.16  
m/z: 180.06 (100.0%), 181.07 (6.9%), 182.07 (1.4%)  
Elemental Analysis: C, 40.00; H, 6.71; O, 53.29

The information in the label updates automatically as you edit the structure. You can show or hide the information as follows:

1. Right-click in the label. It does not matter which tool you are using.
2. Point to **Analysis**, and select or deselect the item you want to show/hide.

Figure 6.242: Analysis context menu



## Showing Stereochemistry

When the Show Stereochemistry option is selected, ChemDraw calculates the absolute stereochemistry for tetrahedral atoms and double bonds according to the Cahn-Ingold-Prelog (CIP) priority rules. For more information about the CIP rules, see “Stereochemistry” on page 234.

Only tetrahedral and double-bond stereochemistry are supported, and only non-racemic stereochemistry is interpreted. Stereochemical indicators for aromatic bonds are not shown.

ChemDraw calculates and displays the following stereochemical terms:

- **(R), (S)**—Standard tetrahedral stereochemistry
- **(r), (s)**—Tetrahedral stereochemistry determined by other stereochemical centers. For example: *cis*-decalin and *myo*-inositol.
- **(E), (Z)**—Standard double-bond stereochemistry

The atom label settings determine the font style and size of the terms. A setting on the Building/Display tab of the Preferences dialog box determines whether or not the term will be displayed in parentheses. (The default is to display parentheses.)

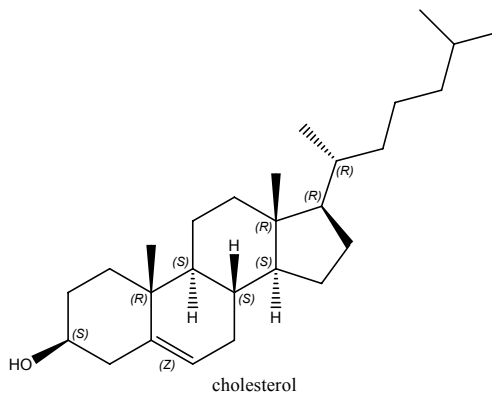
## Stereochemistry Indicators

To show the stereochemistry of a structure:

1. Select the entire structure.
2. Right-click and click **Object Settings**.
3. Check the appropriate boxes for atom and bond stereochemistry.

The stereo-centers are marked as shown in the following example.

Figure 6.243: Stereochemistry indicators



If you make changes to the drawing that affect the stereochemistry, the stereochemistry is recalculated.

## Hiding Indicators

To hide an individual indicator:

1. Select the indicator to hide.
2. Right-click and choose **Hide Indicator**.

## Removing Indicators

To delete an indicator:

1. Click the indicator.
2. Click the eraser tool and click the indicator.

## Positioning Indicators

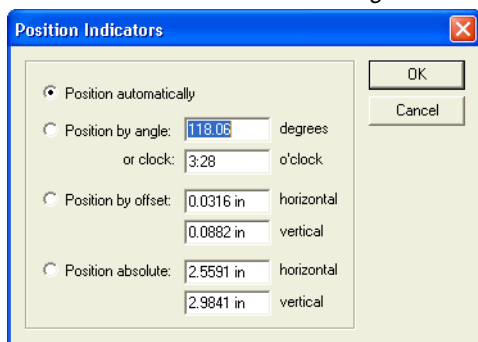
Stereochemistry indicators are positioned automatically and move appropriately if a structure is modified. You can reposition them by dragging them to the desired position or with the Indicator Position dialog box.

To reposition an indicator numerically:

1. With a selection tool, click the indicator to move.
2. Right-click and choose **Position**.

The Position Indicator dialog box appears.

Figure 6.244: Position Indicators dialog box



3. Click the appropriate Position option, and type a value:

Table 29: Indicator positioning options

To Position ...	Type a value for the position by...
-----------------	-------------------------------------

from the atom or bond center to indicator center	angle, in degrees or clock, in clock time
--	---

from the atom or bond center to bottom left of indicator baseline	offset, horizontal and vertical
---	------------------------------------

at specified coordinates	absolute, horizontal and vertical
--------------------------	--------------------------------------

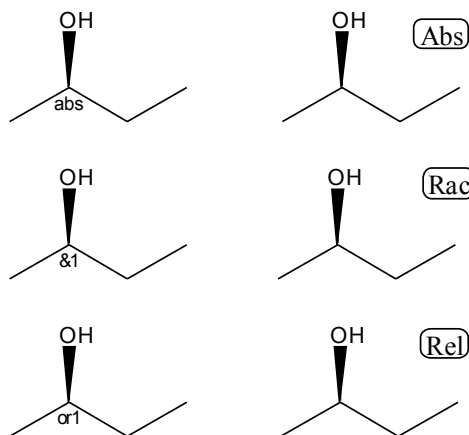
## **Pro** Relative Stereochemistry

Stereochemical representation has been enhanced to allow specification of relationships between groups of stereo-centers within a molecule. The

new notation gives you the ability to describe complex enantiomers in a compact form.

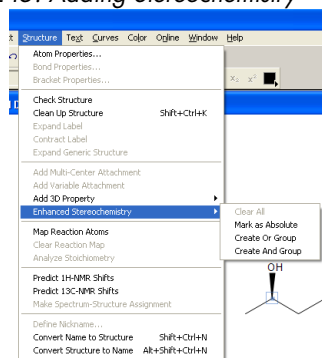
Table 30: Stereochemical Notation

New Notation	Old Notation
--------------	--------------



The new notation is added to a structure by selecting an atom and choosing **Enhanced Stereochemistry** from the Structure menu.

Figure 6.245: Adding Stereochemistry



See “Stereochemistry Indicators” on page 113 for information on showing and hiding indicators.

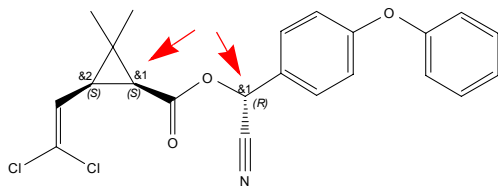
The power of this new notation becomes clear when you draw complex enantiomers. For example, beta-Cypermethrin is a mixture of four distinct stereo isomers consisting of two enantiomeric



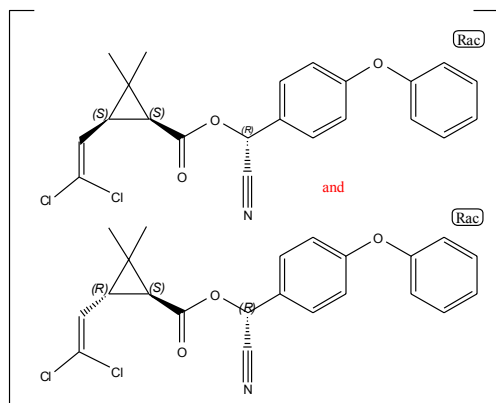
pairs. Drawing this with the old notation requires two structures.

Figure 6.246: beta-Cypermethrin

New notation



Old notation



Both stereo-centers marked with arrows in Figure 6.246 have the &1 designation because of their fixed relative configuration: when one is (R) the other must be (S). In other words, they form a group.

To indicate stereochemistry for a group:

1. Select all atoms in the group using Shift + click.
2. Select the appropriate Enhanced Stereochemistry from the Structure menu.

The third stereo center varies independently, and thus gets the &2 designation. Group numbers are incremented automatically, but can be edited manually.

ChemDraw Enhanced Stereochemistry can be saved in the following formats:

- CDX
- CDXML

- MOL V3000
- RXN V3000
- SKC
- TGF

When saving to SKC or TGF format, the indicators are converted into corresponding Data SGroups. When ChemDraw opens SKC or TGF files containing such Data SGroups, they are converted into true Enhanced Stereochemistry values.

## Converting Structures to 3D

You can convert a two-dimensional structure drawn in ChemDraw to a three-dimensional structure. To use this feature, you must have CambridgeSoft Chem3D installed on your computer.

To convert a structure to 3D:

1. Select the structure to convert.
2. Click the **Get 3D Model** command on the Edit menu.

The 3D structure appears in the document window.

*NOTE: 3D Objects inserted in this way cannot be transferred between platforms. For more information see "File Formats" on page 170.*

To edit the 3D structure:

1. Double-click the 3D structure.  
Chem3D opens.
2. Edit the structure and close Chem3D when you are finished.

The edited structure appears in the ChemDraw document window.

## Pro Viewing Chemical Properties

ChemDraw Pro and Ultra, using an add-on, ChemProp, calculate predicted values for the physical and thermodynamic properties of a selected

structure of up to 100 atoms. You can view the values in the Chemical Properties window.

The properties are calculated using the most reliable methods for calculation for the given structure. Log P and MR values based on literature values rather than a calculation are included in the report file.

## Viewing the Chemical Properties Window

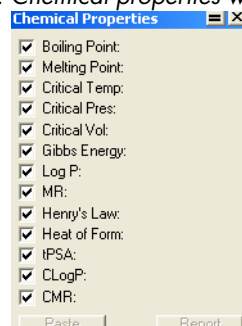
To view predicted properties for a selected structure:

1. Select the structure to analyze.

2. Click the **Show Chemical Properties Window** command on the View menu.

The Chemical Properties window appears.

Figure 6.247: Chemical properties window



The following basic values are displayed.

Table 31: ChemDraw chemical properties

Property	Description
Boiling Point	The boiling point for the structure. Reported in Kelvin at 1 atm.
Melting Point	The melting point for the structure. Reported in Kelvin at 1 atm.
Critical Temperature	The temperature above which the gas form of the structure cannot be liquefied, no matter the applied pressure ( $T_c$ ). Reported in Kelvin.
Critical Pressure	The minimum pressure that must be applied to liquefy the structure at the critical temperature ( $P_c$ ). Reported in bars.
Critical Volume	The volume occupied at the compound's critical temperature and pressure ( $V_c$ ). Reported in $\text{cm}^3/\text{mol}$ .
Gibbs Energy	The Gibbs free energy, $\Delta G$ , for the structure. Reported in $\text{kJ}/\text{mol}$ at 1 atm and 298.15K.
Henry's Law	The inverse of the logarithm of Henry's law constant [ $-\log(H)$ ] (no units).

Table 31: ChemDraw chemical properties

Property	Description
Heat of Formation	The heat of formation, $\Delta H_f$ , for the structure. Reported in $\text{kJ}/\text{mol}$ at 1 atm and 298.15K.
tPSA	Calculation of polar surface area based on fragment contributions.
CLogP <b>Ultra</b>	The calculated <i>n</i> -octanol/water partition coefficient ( $\log P_{ow}$ ).
CMR <b>Ultra</b>	The calculated Molar Refractivity

NOTE: The CLogP and CMR algorithms incorporated in ChemDraw are licensed from BioByte Corp, and have been extensively tested and peer-reviewed as providing highly accurate results. The values produced by these algorithms in ChemDraw should be exactly the same as values produced by the standalone CLogP and CMR applications from BioByte.

For further information about CLogP and CMR, please refer to the BioByte web site at:

<http://www.biobyte.com>

To paste the basic properties into your document:

- Click **Paste**.

To create a report and view results for other fragmentation methods including the Broto, Crippen, Viswanadhan, Joback, and Joback/Stein methods:

- Click **Report**.

When you create a report, a detailed list of information used for performing the calculation is shown in a text file. The list includes additional

properties and literature references used to perform the calculation.

Figure 6.248: Fragmentation tools palette



## Ultra Stoichiometry Grid

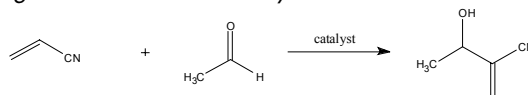
The Stoichiometry Grid is a tool that calculates stoichiometric data for a reaction. It is filled in automatically as you modify a reaction drawing.

To create a Stoichiometry Grid:

1. Draw a reaction, or open a file containing a reaction, and select the entire reaction.
2. Click the **Analyze Stoichiometry** command on the Structure menu.

The Grid appears under the reaction.

Figure 6.249: Stoichiometry Grid



Reactants			Products	
Formula	C <sub>3</sub> H <sub>3</sub> N	C <sub>2</sub> H <sub>4</sub> O	Formula	C <sub>5</sub> H <sub>7</sub> NO
MW	53.06	44.05	MW	97.12
Limiting?	Yes	No	Equivalents	
Equivalents			Expected Mass	
Sample Mass			Expected Moles	
%Weight			Measured Mass	
Molarity			Purity	
Density			Product Mass	
Volume			Product Moles	
Reactant Moles			%Yield	
Reactant Mass				

*TIP: If you have a chemical label on the arrow that does not enter in the reaction, but rather indicates a catalyst or condition, right+click on the label and deselect **Interpret Chemically** in the context menu before creating the grid.*

To enter data in the grid:

1. Select the Text tool, and click in the empty column to enter a value.

Figure 6.250: Entering data in the Grid

Reactants		
Formula	C <sub>3</sub> H <sub>3</sub> N	C <sub>2</sub> H <sub>4</sub> O
MW	53.06	44.05
Limiting?	Yes	No
Equivalents		
Sample Mass		
%Weight		
Molarity		
Density	0.00g/l	
Volume		
Reactant Moles		
Reactant Mass		

2. Set the limiting compound. If the default setting is incorrect, point to the word “No” in the correct column, right-click or control-click, and select **Set Limiting** from the context menu.

3. Enter values for all reactants, as applicable. If you are using units other than the defaults, type in the units along with the values (no space required).

Table 32: Stoichiometry Input Values

Value	Comments
Limiting reactant	Only one reactant may be specified as limiting.
Sample Mass	Weight of reactant. Default units: g
%Weight	Reactant purity. Defaults to 100%.
Volume	Default units: ml Requires either a Molarity or a Density value to also be entered.
Molarity	Default units: M
Density	Default units: g/ml

As soon as you have entered the minimum amount of information required, ChemDraw will calculate values. As you continue entering information, or edit inputs, the values are re-calculated. Entered values are in bold-face; calculated values are in normal font.

Figure 6.251: Calculated stoichiometric values

Reactants		Products		
Formula	<b>C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>S</b>	<b>C<sub>2</sub>H<sub>4</sub>O</b>	Formula	<b>C<sub>5</sub>H<sub>10</sub>O<sub>2</sub>S</b>
MW	106.14	44.05	MW	150.20
Limiting?	Yes	No	Equivalents	
Equivalents			Expected Mass	114.26g
Sample Mass	<b>Entered values</b>		Expected Moles	760.76mmol
%Weight			Measured Mass	
Molarity			Purity	
Density	<b>807.50g/l</b>	<b>788.00g/l</b>	Product Mass	
Volume	<b>100.00ml</b>		Product Moles	
Reactant Moles	760.76mmol	760.76mmol	%Yield	
Reactant Mass	80.75g	33.51g		

You can edit the grid for presentation with the context menu, showing or hiding either rows or columns. You can also change the color of the text.

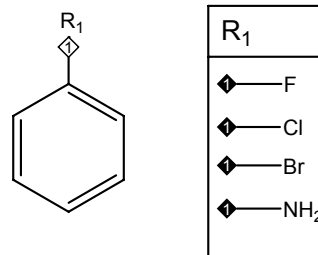
## Pro Expand Generic Structures

You can generate multiple structures from an abbreviated combinatorial structure with ChemDraw's **Expand Labels** tool. The tool is designed for "small" expansions, and is limited to a maximum of 500 generated structures. For large combinatorial expansions, use CambridgeSoft's *CombiChem for Excel*. Four kinds of abbreviated combinatorial definitions may be used:

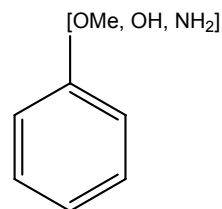
Table 33: Combinatorial definition types

### definition example

Alternative Groups and R-tables

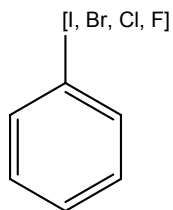


Anonymous Alternative Groups

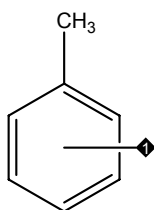


**definition example**

Element  
Lists



Variable  
Attachment

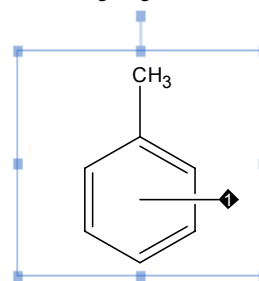


Definitions are expanded into multiple complete molecules. If more than one site is present in the selection, the expansion will include all permutations of substitutions. Expansions are generated into a new document.

To generate a combinatorial library:

1. Select at least one combinatorial substitution definition.

Figure 6.252: Selecting a generic structure

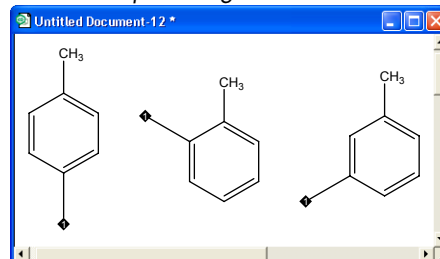


*NOTE: For alternative group/R-tables, both the alternative group label and the table must be selected. If the label is selected but not the table, the label will not be modified by the expansion, and will appear as a label in all generated structures.*

2. Choose **Expand Generic Structure** from the **Structure** menu.

The structures are generated to a new document.

Figure 6.253: Expanded generic structure



# Chapter 7: Struct<=>Name

## Overview

Struct<=>Name is CambridgeSoft's package of structure-to-name and name-to-structure algorithms included with ChemDraw Ultra. Together, they give you unprecedented power and convenience in creating and naming structures.

Struct=Name generates systematic names for chemical structures with support for the Cahn-Ingold-Prelog rules for stereochemistry. It is under continuing development to improve the range of compounds covered.

Name=Struct is a comprehensive algorithm for converting English chemical names into chemical structure diagrams. It is designed to interpret chemical names as they are actually used by chemists. In other words, it recognizes the shorthand and slang of everyday usage, in addition to recognizing most of the official IUPAC, IUBMB, and CAS rules and recommendations. In addition, it has an extensive algorithm for the identification of common "typos" (typing errors, such as "mehtyl") to increase the odds of generating structures for the names it is given.

## Improvements to Struct=Name

In ChemDraw 10, Struct=Name has added support for the following nomenclature types:

- Ring assemblies of two ring systems of any type, such as binaphthyl. (added in 9.0.1)
- Spiro fusions between two ring systems of any type. (added in 9.0.1)
- Ring fusions involving multiple rings attached to a single core, such as dibenzo[b,d]furan.

## Struct=Name

You can insert the name of a selected structure as a caption using the **Convert Structure to Name** command from the Structure menu.

The Struct=Name algorithm in use since ChemDraw 8.0 is a new proprietary naming algorithm developed by CambridgeSoft. It replaces Beilstein's AutoNom algorithm used in earlier versions of ChemDraw. In ChemDraw 10.0, an auto-update feature has been added that renames the structure as you modify it.

The conversion of a structure to a name is limited by many factors. Specifically, Struct=Name makes little or no attempt to name the following:

- Bridged ring systems with more than one bridge (for example, tricycles.)
- Radicals.
- Compounds with non-standard valence states.
- Spiro ring systems.
- Isotopically modified compounds.
- Polymers.
- Biochemicals, including specialized nomenclature for amino acids, carbohydrates, and steroids. For such compounds, only the fully systematic organic name is produced.

Nomenclature types added in ChemDraw 10.0 include:

- Most of the most-common fused ring systems, both those with trivial names (naphthalene, indole) and those with systematic names (benzo[e][1,4]diazepine, thieno[3,2-b]thiophene).
- Most salts.
- Structures with a net charge.

- Simple mixtures and multicomponent systems.
- Heterochains.
- Multiplicative nomenclature.
- Ring assemblies.
- Bicyclics.
- Basic inorganics.

Nomenclature types added in ChemDraw 10.0 include:

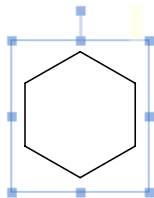
- Ring assemblies of two ring systems of any type, such as binaphthyl. (added in 9.0.1)
- Spiro fusions between two ring systems of any type. (added in 9.0.1)
- Ring fusions involving multiple rings attached to a single core, such as dibenzo[b,d]furan.

Struct=Name generates names with proper CIP stereochemistry descriptors. It has no theoretical limits to the size of the structures that can be named.

To insert the name of a structure into your drawing:

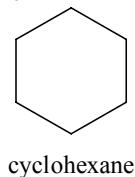
1. Select the drawing for which you want to insert a name.

Figure 7.254: Selecting the drawing



2. Click the **Convert Structure to Name** command on the Structure menu.

Figure 7.255: Adding a name



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

## Auto Update

ChemDraw 10.0 captions include a “hot-link” feature. Chemical properties, including the chemical name and analysis, can be included in a caption, and will update automatically when you modify the structure. For more information on adding data to captions, see “Adding Analysis Data to a Caption” on page 58.

To toggle the hot-link feature:

1. Point to the label.
2. Right-click and select **Auto-update**.

A check mark appears next to the command when it is selected. Successive clicks toggle the command on and off.

When auto-update is on (default) the label updates each time you modify the structure.

*NOTE: For large complex structures, it may take the new label a few seconds to appear on the screen, depending on the speed of your processor. You do not have to wait for the new label to appear before continuing to modify your structure.*

## Name=Struct

You can draw a structure automatically from a chemical name using Name=Struct.

Name=Struct recognizes most organic nomenclature. Inorganic chemistry is also usually recognized, especially when the rules closely match those for organic chemistry.

The following are not supported:

- Coordination complexes
- Polyboranes
- Polymers
- Some highly-bridged ring systems, including fullerenes and porphyrins/porphines
- Some stereochemistry designators: +, -, +/-, +/-, D, L, DL, *endo*, *exo*, *syn*, *anti*, *r*, *t*, *c*



Although some trade names are supported, Name=Struct is not intended to interpret trade or common names. A chemical database, such as chemfinder.com, is more appropriate for obtaining structures for trade or common names. See “Finding Information on ChemFinder.com” on page 272 for more information.

*NOTE: Because the syntax of German is very similar to that of English, Name=Struct can also interpret many German names. Chemical names in other languages, however, will generally not be recognized.*

## Converting Names to Structures

There are two ways to insert a name into the document window as a structure:

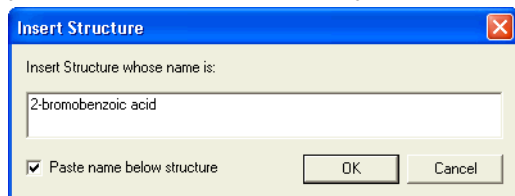
- Insert Structure dialog box
- Paste Special command

### Insert Structure

**Insert Structure** is designed for typed-in entries. For example, to insert 2-bromobenzoic acid:

1. Choose **Convert Name to Structure** from the Structure menu.  
The Insert Structure dialog box appears.
2. Type 2-bromobenzoic acid.

Figure 7.256: Insert Structure dialog box

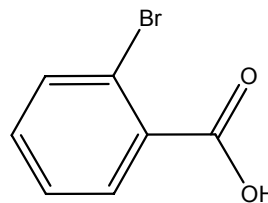


*NOTE: You can also copy a name to the clipboard and type Ctrl+V or Command+V to paste the name into the dialog box.*

3. Click **OK**.

The molecular structure and name (if “Paste name below structure” is selected) appear in the drawing area.

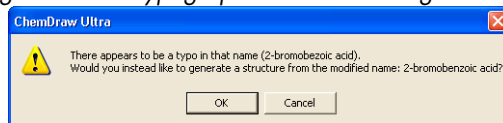
Figure 7.257: Inserting a named structure



2-bromobenzoic acid

If you should happen to type the name incorrectly, Insert Structure will try to correct the error.

Figure 7.258: Typographical error warning



Click **OK** to accept the suggested spelling, or click **Cancel** and start again to make a manual correction.

### Paste Special

The **Paste Special** command allows you to paste a name, copied to the clipboard from another application, as a structure in ChemDraw.

To paste a name from the clipboard:

1. Click in the document window.
2. Point to **Paste Special** on the Edit menu, and choose **Name as Structure**.

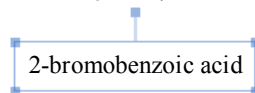
The structure appears in your document.

## Converting Captions to Structures

If a caption is already present in the drawing area you can convert it to a structure as follows:

1. Select the caption.

Figure 7.259: Selecting a caption



2. Choose **Convert Name to Structure** from the Structure menu.

The molecular structure and name appear in the drawing area.

## Types of Structures Supported by Struct=Name

Struct=Name can name compounds in the following classes of structures:

Table 34: Struct=Name supported structure types

<b>category</b>	<b>ChemDraw 8 supports...</b>	<b>ChemDraw 9 adds...</b>
<b>principal groups in both rings and chains</b>	Acid Halides	Amide derivatives of acids
	Alcohols and chalcogen analogs	Anhydrides
	Aldehydes and chalcogen analogs	Carbonic acids
	Amides	Imides
	Amines and Imines	Nitric acids
	Carboxylic Acids	Peroxy acids
	Carboxylic Esters	Salts
	Heteroatomic acid halides	Sulfides and chalcogen analogs
	Heteroatomic acids (P, B, As)	Sulfoxides and chalcogen analogs
	Heteroatomic esters	
	Hydrazides	
	Hydrazines	
	Hydroperoxides	
	Ketones and chalcogen analogs	
	Nitriles	
	Peroxides	
	S, Se and Te Amides	
	S, Se, and Te Acid Halides	
	S, Se, and Te Acids	
	S, Se, and Te Esters	
<b>Ringed structures</b>	Carbomonocyclic structures	Bridged monocyclic structures
	Heteromonocyclic structures	

Table 34: Struct=Name supported structure types

<b>category</b>	<b>ChemDraw 8 supports...</b>	<b>ChemDraw 9 adds...</b>
	Fused polycyclic trivially-named structures	
	Ring fusions of only two rings	
	Ring fusions of two multiple ring systems	
<b>Other compounds</b>		Phosphorous and Arsenic compounds
		Si, Ge, Sn, and Pb compounds
		Boron compounds
		Organometallic compounds



# Chapter 8: ChemNMR

## Ultra Spectrum-Structure Assignments

ChemDraw Ultra enables you to assign structures to spectra. You can then display the structure associated with a specific peak by placing the pointer on that peak.

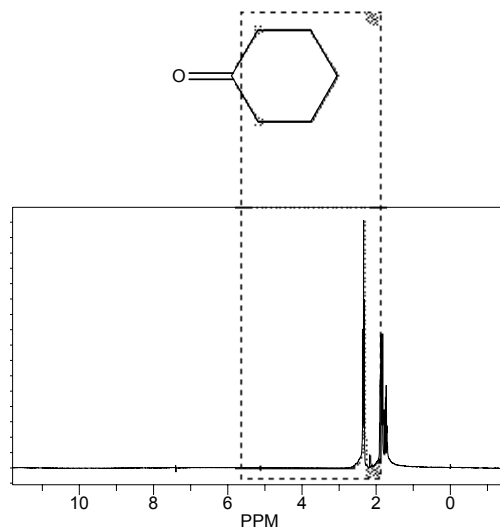
### Assigning Structures to Spectra

To assign structures to a spectrum:

1. Open a spectral file.
2. Draw the structure or structures you want to assign to the spectrum.
3. Select specific atoms and bonds in the structure.
4. Shift-click the peak or peaks to which you want the structure assigned.

The selection rectangle surrounds the selected objects.

Figure 8.260: Selecting the structure and related spectrum



5. Click the **Make Spectrum-Structure Assignment** command on the Structure menu.

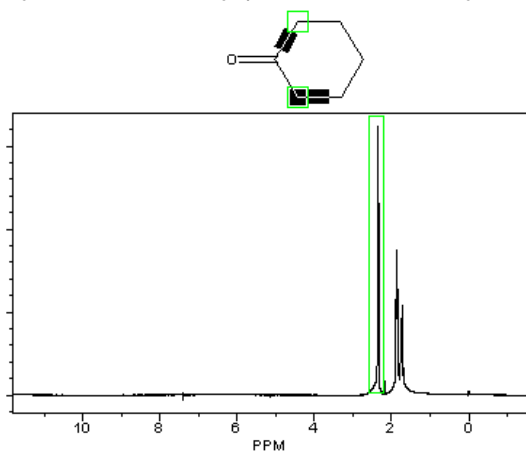
The selected atoms and bonds in the structure are associated with the selected spectral peaks.

### Viewing Spectral Assignments

To view the spectral assignments:

1. Click the Lasso or Marquee tool.
2. Place the pointer over a peak.  
The assigned atoms or bonds are highlighted.

Figure 8.261: Viewing spectrum-structure assignments



## Removing Spectral Assignments

To remove spectrum to structure assignments:

1. Click the Lasso or Marquee tool.
2. Select the objects from which to remove the assignment.
3. Click the **Clear Spectrum-Structure Assignment** command on the Structure menu.

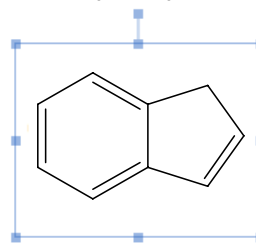
## Ultra NMR Shift Information—ChemNMR

ChemNMR is a feature of ChemDraw Ultra only. ChemNMR estimates and displays proton and carbon-13 chemical shifts in ppm for a selected molecule.

To view  $^1\text{H}$  or  $^{13}\text{C}$  NMR information:

1. Select the target chemical structure.

Figure 8.262: Selecting a target

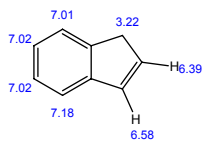


2. Click the  **$^1\text{H}$ -NMR Shifts** or  **$^{13}\text{C}$ -NMR Shifts** command on the Structure menu.

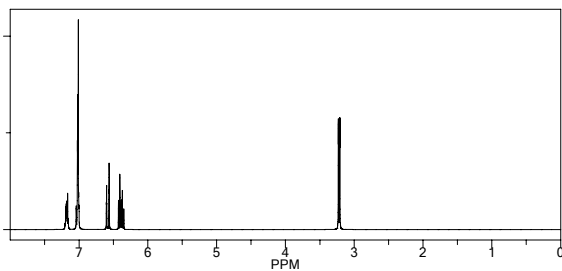
ChemNMR redraws the molecule with the estimated shifts and displays the information and line spectrum in a new window as shown below.

Figure 8.263: Displaying the NMR spectrum

ChemNMR H-1 Estimation



Estimation Quality: blue = good, magenta = medium, red = rough



Protocol of the H-1 NMR Prediction:


Node	Shift	Base + Inc.	Comment (ppm rel. to TMS)
CH	7.02	7.26	1-benzene
		-0.12	1 -C=C
		-0.12	1 -C
CH	7.02	7.26	1-benzene
		-0.05	1 -C=C
		-0.19	1 -C
CH	7.18	7.26	1-benzene
		0.04	1 -C=C
		-0.12	1 -C
CH	7.01	7.26	1-benzene
		-0.05	1 -C=C
		-0.20	1 -C
CH2	3.22	1.37	methylene
		1.22	1 alpha -1:C*C*C*C*C*1
		0.63	1 alpha -C=C
H	6.58	5.25	1-ethylene
		1.65	1 -1:C*C(R)*C*C*C*C*1 gem
		-0.32	1 -C-1:C*C*C*C*C*1 trans
H	6.39	5.25	1-ethylene
		0.09	1 -1:C*C(R)*C*C*C*C*1 trans
		1.05	1 -C-1:C*C*C*C*C*1 gem













# Chapter 9: Drawing Objects

## Overview

ChemDraw provides the following tools and tool palettes that enable you to add chemical symbols and shapes to your documents (A tool palette is indicated by a  in the lower right corner of the tool.):

- **Orbital tools palette** —to draw orbitals.
- **Chemical Symbols tools palette** —to draw charges, radicals, and other symbols.
- **Arrow tools palette** —to draw arrows.
- **Drawing Elements tools palette** —to draw boxes, circles, and lines.
- **Brackets tools palette** —to draw brackets, braces, parentheses, and daggers.
- **Arc tools palette** —to draw arcs.
- **Pen tool** —to draw freehand shapes.
- **TLC tool** . to reproduce TLC experiments.

You can use the tool palettes as extensions of the Main Tool Palette, or you can tear them off and place them anywhere on your screen.

Object behavior has improved in ChemDraw 10.0. Most objects, with the exception of daggers and some symbols, can now be rotated as well as scaled. Arrows have been completely revamped.

## Selecting Tools From a Palette

Some tools have a palette containing different types of that tool. When you choose a tool type from the palette, it becomes the default tool. To use a different tool type, select it.

To select a tool and use its default tool type, click the tool's icon to select it.

To choose a different tool type from the palette:

1. Click the tool's icon and hold down the mouse button.  
The palette appears.
2. Drag to select a tool type from the palette.
3. Release the mouse button over the tool you want to select.

The selected tool is now displayed on the Main Tools Palette.

To display a tools palette, do one of the following:

- Select the **Other Toolbars** command on the View menu, then select one of the palettes.
- Click the tool's icon and drag to the palette's title bar. Release the mouse button over the title bar.

The selected palette is displayed, and can be dragged anywhere on the screen.

## The Orbital Tools Palette

Use the Orbital tools to add orbitals to your chemical structures.

Figure 9.264: Orbital tools palette



You draw orbitals so that the node appears first. Depending on the orbital type, available fill patterns are:

- Background color
- Shaded
- Solid color

You can modify the fill colors with the Color menu.

Display the Info window to view the orbital's length and angle relative to the X-axis while you draw it. You can constrain the length and angle of an orbital by selecting Fixed Lengths and Fixed Angles on the Object menu.

*NOTE: Orbitals are not normally part of the structure they are drawn near and are not selected when you double-click a bond, atom, or atom label with a selection tool. To group the orbitals with the structure, use the Group command from the Object menu. For more information, see "Grouping Objects" on page 68.*

## s-orbitals

The s-orbital tools are shown in Figure 9.265:

Figure 9.265: s-orbital tools



To draw an s-orbital:


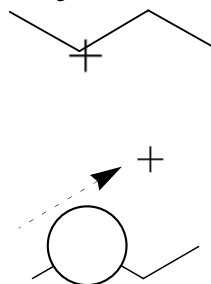
1. Hold down the mouse button over the Orbital tool  and drag to select the **s-orbital** tool from the palette.
2. Point to an atom where the orbital will be centered.
3. Drag outward.

Figure 9.266: Adding an s-orbital to an atom



## Sigma Orbitals

The  $\sigma$ -orbital tools are shown in Figure 9.267:

Figure 9.267: Sigma orbital tools



To draw a  $\sigma$ -orbital:


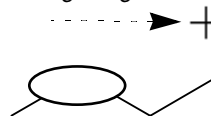
1. Hold down the mouse button over the Orbital tool  and drag to select the  $\sigma$ -orbital tool from the palette.
2. Point where the orbital will be centered.
3. Drag outward along the long axis of the orbital.

Figure 9.268: Adding a sigma orbital to an atom




## Single Lobe Orbitals

Single lobe orbitals are commonly used for indicating a lone pair. The single lobe orbital tools are shown in Figure 9.269:

Figure 9.269: Single lobe orbital tools

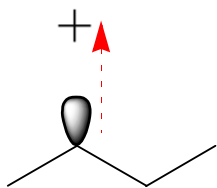


To draw a single lobe orbital:

1. Hold down the mouse button over the Orbital tool  and drag to select the single lobe orbital tool from the palette.
2. Point to an atom where the narrow end of the orbital is to be attached.

3. Drag from the narrow end of the lobe to its wide end.

Figure 9.270: Adding a single lobe orbital



## p-orbitals

The p-orbital tools are shown in Figure 9.271:

Figure 9.271: p-orbital tools



To draw a p-orbital:


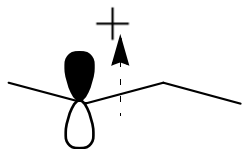
1. Hold down the mouse button over the Orbital tool  and drag to select the **p-orbital** tool from the palette.
2. Point to an atom where the node of the orbital is to be attached.
3. Drag from the orbital node to the wide end of the filled lobe.

Figure 9.272: Adding a p-orbital to an atom




## Hybrid Orbitals

The hybrid-orbital tools are shown in Figure 9.273:

Figure 9.273: Hybrid orbital tools

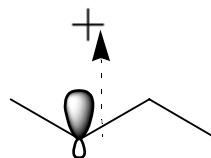


To draw a hybrid orbital:

1. Hold down the mouse button over the Orbital tool  and drag to select the **hybrid-orbital** tool from the palette.

2. Point to an atom where the node of the orbital is to be attached.
3. Drag from the orbital node to the wide end of the major lobe of the orbital.

Figure 9.274: Adding a hybrid orbital to an atom



## d-orbitals

The d-orbital tools are shown in Figure 9.275:

Figure 9.275: d-orbital tools



To draw a d-orbital:


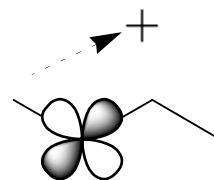
1. Hold down the mouse button over the Orbital tool  and drag to select the d-orbital tool from the palette.
2. Point to an atom where the node of the orbital is to be attached.
3. Drag from the center of the orbital to the wide end of a filled lobe.

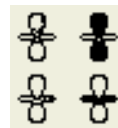
Figure 9.276: Adding a d-orbital to an atom



## $d_{z^2}$ -orbitals

The  $d_{z^2}$  orbital tools are shown in Figure 9.277:

Figure 9.277:  $d_{z^2}$ -orbital tools



To draw a  $d_{z^2}$  orbital:


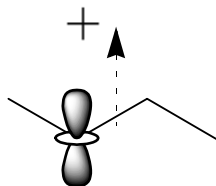
1. Hold down the mouse button over the Orbital tool  and drag to select the  $d_{z^2}$ -orbital tool from the palette.
2. Point to an atom where the node of the orbital will be attached.
3. Drag from the center of the orbital to the wide end of a lobe.

Figure 9.278: Adding a  $d_{z^2}$ -orbital



## The Chemical Symbols Tools Palette


Use the Chemical Symbols tools  to add chemical symbols to your structure. When you click the Chemical Symbols tool, the palette shown in Figure 9.279 appears:


Figure 9.279: Chemical symbols palette




When you attach a symbol (other than H-dot or H-dash) to an atom, it remains at a fixed distance from the central character of the atom label. If you drag the symbol, it will maintain that fixed distance as it moves around the atom.

You can, however, use a symbol without attaching it to an atom, place or move it anywhere, and resize it.

### H-dot and H-dash

To represent a hydrogen atom that is coming out of the plane toward you along the Z-axis, use the H-dot symbol .

To represent a hydrogen atom that is directed backwards into the plane away from you along the Z-axis, use the H-dash symbol . You can draw H-dots and H-dashes only by clicking atoms.

To draw an H-dot or an H-dash:


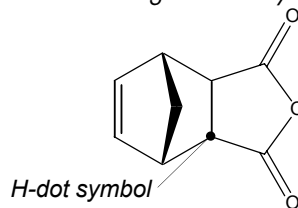
1. Hold down the mouse button over the Chemical Symbols tool  and drag to select the symbol from the palette.
2. Click an atom.


Figure 9.280: Adding an H-dot symbol to an atom



### Lone Pair

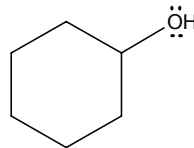
Use the lone pair symbol  to indicate a lone pair of electrons common in Lewis structure representations.

To draw a lone pair:

1. Hold down the mouse button over the Chemical Symbols tool  and drag to select the lone pair from the palette.
2. Click the atom where you want the lone pair located, or drag in the appropriate direction to position it.

The lone pair is offset from the atom at a fixed position.


Figure 9.281: Adding a lone pair to an atom





## Radical

Use the radical symbol  to indicate a single non-bonded electron.


To draw a radical symbol:

1. Hold down the mouse button over the Chemical Symbols tool  and drag to select the radical from the palette.
2. Point to the atom where you want the radical to appear.
3. Click to draw the symbol.

## Radical Cation and Radical Anion



Use the charge radical symbols   to represent radicals that are charged.

To draw a radical cation or radical anion symbol:


1. Hold down the mouse button over the Chemical Symbols tool  and drag to select the symbol from the palette.
2. Point to the atom where you want the symbol to appear.
3. Drag from the charge portion of the symbol to the radical portion of the symbol.

To add a radical cation or radical anion symbol in a horizontal orientation, click an atom.

## Charge Symbols

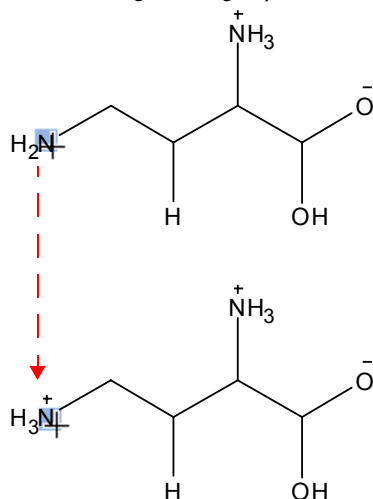
Use the charge symbols to represent charges on structures.    

To draw a charge and associate it with a structure:

1. Hold down the mouse button over the Chemical Symbols tool  and drag to select the charge symbol from the palette.
2. Click to the atom to which you want the charge to correspond.

The number of hydrogen atoms increases or decreases as appropriate for the addition of the charge.

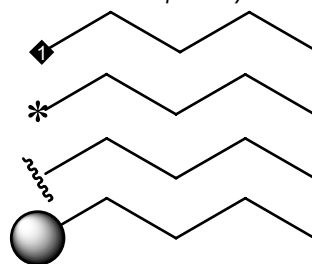
Figure 9.282: Adding a charge symbol



## Attachment Points

The ability to indicate an attachment point is useful in polymer-bound combinatorial synthesis, protein chemistry, and other situations. ChemDraw has four standard attachment point drawing tools that allow you to indicate a point of attachment while maintaining chemical meaning.

Figure 9.283: Attachment point symbols



The bead tool is specifically intended to indicate attachment to a resin, but the tools are interchangeable. Any of these tools may be used for variable attachments in queries (see “Multi-Center and Variable Attachments” on page 73), but only the diamond tool will show rank numbers. That is, if you add more than one diamond to a structure, the points will automatically number sequentially.

## Rotating a Symbol

You can rotate the radical anion, cation, and lone pair symbols by dragging the rotation handle on the selection Rectangle. All symbols are rotated around the same end from which they were originally drawn. For example, the radical cation symbol is rotated and resized from the charge. The Info window shows the angle that one of the ends of a symbol makes with the X-axis as you rotate symbols.

To rotate a chemical symbol:

1. Select the chemical symbol with a selection tool.
2. Drag the rotation handle on the chemical symbol.

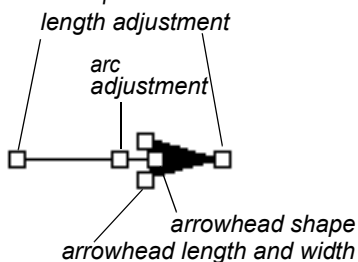
For more information about rotating and resizing, see “Rotating Objects” on page 65.


## The Arrow Tools Palette

Arrows are now customizable not only for length and angle, but for arrowhead width and shape. You can drag an arrow from the middle to create an arc, allowing you to create arcs of any length.

When you mouse-over an arrow with the Lasso, Marquee, or an Arrow tool selected, ChemDraw switches into edit mode and adjustment handles appear on the arrow.

Figure 9.284: Arrow adjustment handles



Drag the adjustment handles to change the arrow length, angle, or shape. Two different cursors appear, one for arcs and arrowhead shape , the


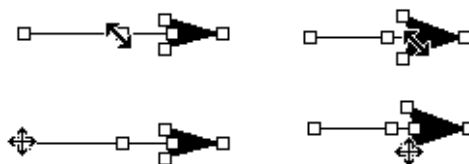
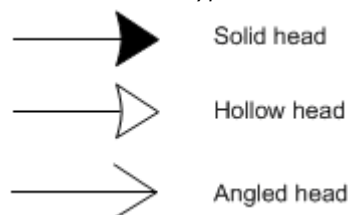
other for arrow length or arrowhead length and width.  When changing the angle of an arrow, you are restricted to multiples of 15° if the **Fixed Angles** option in the Object menu is selected. Hold down the **Alt** or **option** key to drag to any angle.

Figure 9.285: Arrow Cursors



There are three basic arrowhead shapes, solid, hollow, and angled. Change the arrowhead type from the context menu (see Figure 9.292) after creating an arrow.

Figure 9.286: Arrow head types



Angled-head, or “line segments”, was a user-requested feature. Another user-requested feature is “square” heads.

Figure 9.287: Square arrow head

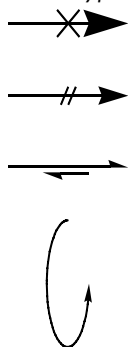


ChemDraw 10.0 introduces four new arrow types: two types of crossed (no-go) arrows, equilibrium arrows of unequal lengths, and elliptical arcs. In addition, you can create several new arc types (see Figure 9.290).

For equilibrium arrows, changing the length changes both arrows proportionately; changing the shape of the arrowhead changes both arrowheads identically. To change the length of only one arrow, hold down the **Alt** or **option** key. Two new

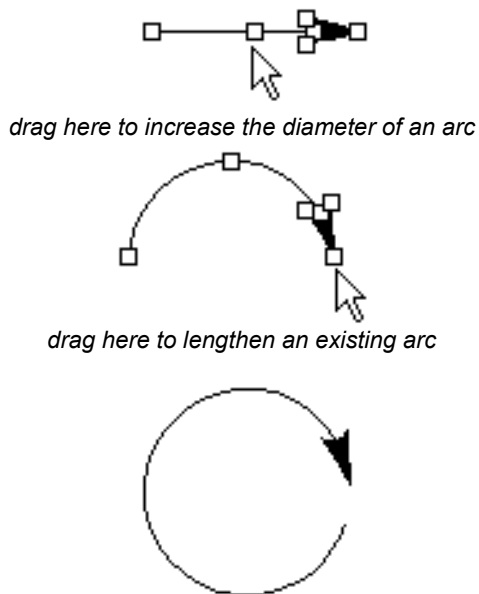
adjustment handles appear. When you have created a disequilibrium arrow, only the shorter side can be adjusted further.

Figure 9.288: New Arrow Types



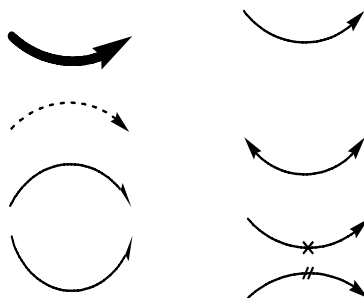
Dragging the adjustment handle on the line segment creates an arc of increasing radius. After choosing a radius, you can then adjust the arc from  $1^\circ$  to  $359^\circ$  by dragging the length. (At  $360^\circ$ , the line becomes a point, and the arc starts over again.) The assortment of pre-drawn arcs on the Arrows Palette are for your convenience, and are customizable like other arrows. Figure 9.289 shows an arrow and two arcs created from it.

Figure 9.289: Arc Variations from a Single Arrow



All arrows, except hollow or equilibrium arrows, can be made into arcs. This means that dashed, thick, double-headed, and crossed (no-go) arrows can all be arcs.

Figure 9.290: Arc Variations

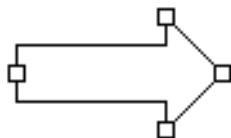


Click a modified arrow (with the same arrow tool) to undo all changes to the shape, but not length, of the arrow. Use Undo (**Ctrl+Z**) to step back through multiple changes, or to undo changed length. Click an unmodified arrow, or one that has had only its length changed, to reverse its direction.

Hollow arrows have only two types of adjustment handle—length and width. Changing the arrow-

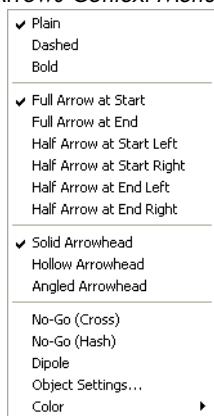
head width also changes the width of the line segment.

Figure 9.291: Hollow Arrow adjustment handles



You can modify arrows with a Context menu. Some of the context menu commands are also available on the Curves menu. Use the Context menu to create arrows for which there are no tools, such as bold-dashed or dipole.

Figure 9.292: Arrows Context Menu



Arrows “snap” together at their end or midpoints. To snap an arrow to an existing arrow, hold the Shift key down to disable the adjustment handles on the original arrow.

*NOTE: The terms “left” and “right” in the context menu are relative, and refer to the direction the arrowhead is pointing.*

Figure 9.293: Snapping arrows

1. Hold the Shift key down. This disables the adjust handle and displays the snap point.

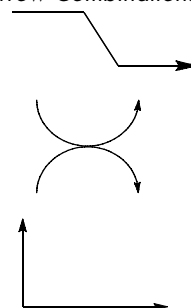


2. Continue to hold the Shift key down as you drag arrow up.



You can also drag existing arrows and snap them. This method allows you to connect two arrows at their midpoints.

Figure 9.294: Arrow Combinations



Finally, arrows can be rotated with the Structure Perspective tool as well as the Lasso or Marquee. Combining these methods allows you to draw an unlimited number of arrows that are otherwise difficult to create.

## The Drawing Elements Tools Palette

The Drawing Elements tools provides shapes you can add to your drawing.

Drawing elements are not a part of the structure they are drawn near. If you double-click on a bond, atom, or atom label with a drawing tool, they are not selected. To group drawing elements with a



structure, use the Group command in the Object menu. For more information, see “Grouping Objects” on page 68.

Some drawing element types are available with fill patterns: hollow (no fill pattern), gray, and black. You can change the type of box, circle, or oval using the Curves menu.

The Info window indicates the length and angle relative to the X-axis while you use any of the drawing element types.

Figure 9.295: Drawing elements palette



## Drawing Boxes

To draw a box:

1. Select one of the box tools.

Figure 9.296: Box tools



2. Point where you want a corner of the box to be located.
3. Drag from one corner of the box diagonally to the opposite corner.

## Drawing Circles and Ovals

To draw a circle or oval:

1. Select one of the circle or oval tools.

Figure 9.297; Circle and oval tools



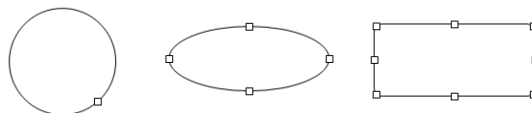
2. Point where you want the center of the circle to be located.
3. Drag outward from the center.

## Resizing or Rotating Drawing Elements

Rectangles, circles, and ovals can now be adjusted in a similar manner to the new arrows. You no longer need to delete them and redraw from scratch.

Pointing to a rectangle, circle, or oval with the same tool or a selection tool displays adjustment handles that can be dragged to reshape the object.

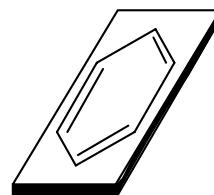
Figure 9.298: Object adjustment handles



Circles have only a radius adjustment, but ovals and rectangles can be resized for both length and width. Rectangles also have corner handles that adjust length and width proportionately.

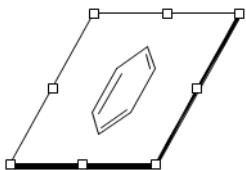
Rectangles, circles, and ellipses can now be freely rotated in three dimensions using the Structure Perspective tool.

Figure 9.299: Perspective rotation of an objects



When an object has been distorted by such rotation, dragging an adjustment point will modify the shape while preserving the perspective.

Figure 9.300: Dragging a distorted drawing object



## Drawing Lines

Lines drawn with the line tool differ in two significant ways from bonds drawn with the bond tools:

- They are not included in chemical interpretation of the drawing
- Lines that cross appear solid

To draw using a line tool:

1. Select a line tool.

Figure 9.301: Line tools



2. Point where you want the line to start.
3. Drag from one end of the line to the other end.

## The Brackets Tools Palette

Brackets includes braces { }, brackets [ ], and parentheses ( ).

### Drawing Single Brackets

A single bracket can be drawn in any orientation.

To draw a single bracket:

1. Select a single bracket tool.

Figure 9.302: Single bracket tools



2. Point where you want the bracket to start.
3. Drag from one end of the bracket to the other end.

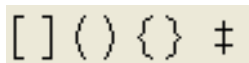
## Drawing Paired Brackets

Paired brackets can only be placed in a vertical orientation. A rectangle or box defines their position.

To draw a paired brackets:

1. Select a paired bracket tool.

Figure 9.303: Paired bracketed tools



2. Point where you want a corner of the bracket to be located.
3. Drag from one corner of the box diagonally to the opposite corner.

## Drawing Daggers

To draw a dagger:

1. Select a dagger tool.

Figure 9.304: Dagger tools



2. Point where you want the symbol to be located.
3. Click to deposit the dagger.

*NOTE: The size of the dagger symbol is proportional to the Atom Label font size specified in the Text Settings dialog box.*

## Framing Objects

You can enclose your drawings or group structures with a rectangle, brackets, parentheses, or braces.

To enclose your object:

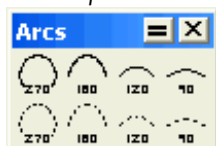
1. Select the drawing to enclose.
2. Point to the **Add Frame** command on the Object menu, and choose the type of frame to add.

The frame you selected is inserted in your drawing.

## The Arc Tools Palette

Use the Arc tools to draw solid or dashed arcs of different angles: 90°, 120°, 180°, and 270°.



Figure 9.305: Arc tools palette



### Drawing Arcs

Where you access the arc tools depends on which version of ChemDraw you are using.

To draw an arc:

1. Do one of the following:
  - In ChemDraw Std, point to the Arc tool  and drag in the palette to select the angle.
  - In ChemDraw Pro or Ultra, point to the Drawing Elements tool  and drag in the tool palette to select the angle.
2. Dragging from left to right creates a convex arc; from right to left a concave one.

The Info window shows the length between the ends, and the angle the clockwise end makes with the X-axis while you draw an arc.

### Editing Arcs

To resize or rotate an arc using the Arc tool:

1. Select the Arc tool, and position it over the arc. Three drag points appear – one on each end and one in the middle.

2. Drag either end of the arc to lengthen it.
3. Drag the center point to change the radius.

The arc is resized and rotated. The Info window indicates the distance between the ends of the arc and the angle the clockwise end makes with the X-axis.

You can resize and rotate an arc by dragging the Resize or Rotation handle on the Selection rectangle. The resize or rotation occurs around the center defined by the Selection rectangle. When you drag the Resize handle, the Info window indicates the percentage enlarged or reduced. When you drag the Rotation handle, the Info window indicates the degree rotated. For more information, see “Rotating Objects” on page 65 and “New Selection Box” on page 61.

## The Pen Tool

Use the Pen tool to draw shapes that are not provided in the Arrow, Orbital, or Drawing Elements palettes. For example, you can draw irregularly shaped arrows, curves depicting graphs or reaction coordinate diagrams, and other irregularly shaped solids.

The Pen tool has two modes:

- **Drawing**—Used to create shapes. The hand cursor appears with a “+” sign inside.
- **Edit**—Used to edit shapes. The hand cursor appears without a “+” sign inside.

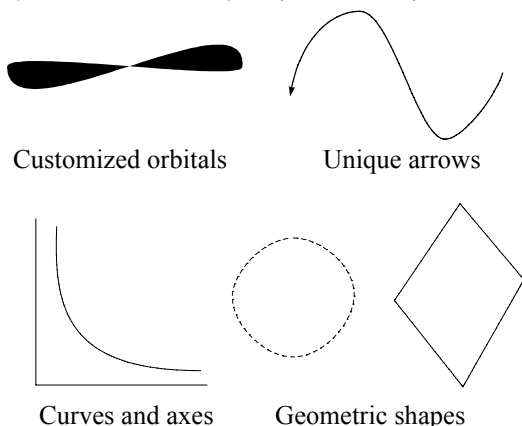
---

*NOTE: To enter edit mode directly from drawing mode, press the Esc key.*

---

Some examples of shapes that you can draw using the Pen tool are shown below.

Figure 9.306: Drawing shapes with the pen tool



To toggle between a selection tool and the Pen tool do one of the following:

- Press **Ctrl+Alt+Tab** or **command+option+tab**
- Click a selection tool.

The last drawn curve and a selection tool are selected.

## Drawing Bézier Curves by Dragging

A Bézier curve is a curve that is calculated to connect separate points into a smooth line. You can draw Bézier curves with the Pen tool by clicking and dragging repeatedly to create curved segments.

To draw a Bézier Curve:


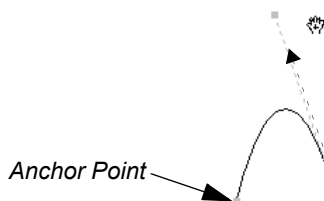
1. Select the Pen  tool.
2. Point to where you want the beginning of the curve to appear and click.  
An anchor point appears, and the cursor changes from a “+” to a hand.
3. Move the cursor to another position and click.  
A line connects the two points.
4. Position the cursor on one of the points (the “+” in the hand will disappear when you are correctly positioned) and drag to create an arc.

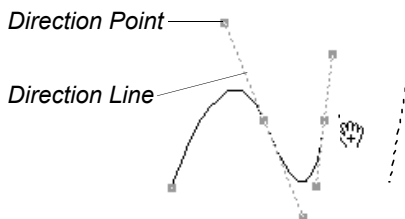
Figure 9.307: Drawing Bézier curves with the pen tool



A direction line appears tangentially to the curve. Use the direction line to control the “curviness” of the segment. The slope of the direction line determines the slope of the curve. The length of the direction line determines the height of the curve.

Direction points appear at the ends of the direction line. Use the direction points to adjust the curve by dragging a point. You can further adjust the shape by dragging an endpoint of the curve.

Figure 9.308: Adjusting a curve with the pen tool



## Drawing Segments by Clicking

You can draw shapes with corners by clicking repeatedly in an outline of the shape you want.

To draw segments:


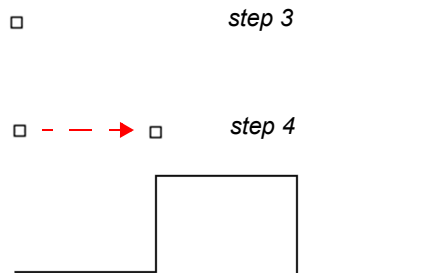
1. Select the Pen  tool.
2. Point to where you want the beginning of the curve to appear.
3. Click to deposit an anchor point.
4. Move the cursor and click again to add a second point.
5. Continue until you have the curve you want.

Figure 9.309: Drawing line segments with the pen tool




6. Press the **Esc** key or click another tool.

*NOTE: To place the fewest strategically placed control points for obtaining the smoothest curve, work in a magnified view.*

## Editing a Curve

You can edit a curve by selecting it and manipulating it with the direction lines.

To select an existing curve:

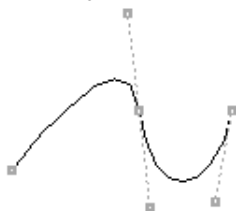
1. Select the Pen  tool.
2. Point at the curve.

The cursor will change from a “+” to an arrow when you are positioned correctly.

3. Click to select the curve.

The direction lines appear.

Figure 9.310: Editing curves with the pen tool



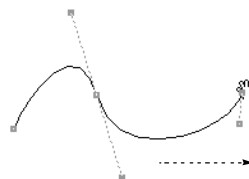
## Changing the Shape of a Curve

Use the endpoints of the direction lines to increase or decrease the breadth of the curve or change its direction.

To change the shape of a curve:

1. Select the Pen tool and click the existing curve you want to edit.
2. Drag the direction lines to create the shape you want.

Figure 9.311: Changing the shape of a curve



## Adding a Segment

To extend an existing curve by adding a segment:

1. Select the Pen tool and click the existing curve you want to edit.
2. Point to the endpoint of a curve until the cursor appears as a hand.

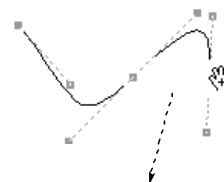
Figure 9.312: Adding a segment to a curve



3. **Alt+click** or **option+click** the endpoint.

The cursor appears as a hand with a “+” sign inside.

Figure 9.313: Adding a segment; continued



4. Drag to connect more segments to your curve.

## Deleting a Segment

To delete a curve segment, in the edit mode of the Pen tool, **Alt+Shift+click** or **option+shift+click**

the control point where you want to delete a curve segment.

The cursor appears as the Eraser tool before you click.

You can also delete entire curves using a selection tool or the Eraser tool.

## Applying a Style to a Shape

All curves are drawn with the last curve style chosen until you change the selections. Certain styles are mutually exclusive. For example, if you choose Closed, you cannot also choose Arrow at Start.

You can use the Doubled style to represent cell membranes. The lines are separated by twice the Bold Width setting for the drawing. Doubled lines cannot be dashed or include arrows.

To apply a style to a curve:

1. Select a curve using either the Pen tool or a selection tool.
2. Choose a style from the Curves menu.

## Filled and Closed Styles

Figure 9.314 shows a shape with the Plain style applied. Figure 9.315 shows the same shape with the Filled and Closed styles applied. If you do not want to fill the shape with a solid color, choose **Faded** rather than **Filled**.

Figure 9.314: Plain style curve

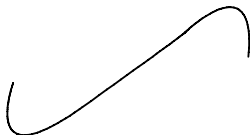
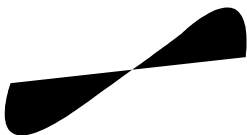


Figure 9.315: Filled and closed style curve



## Shaded Style

You can apply shading to any curve, however the shaded style works best with convex or slightly concave shapes. Shading may not appear as desired in extremely concave shapes.

Figure 9.316 below shows shapes with the Plain style applied. Figure 9.317 shows the same shapes with the Shaded style applied.

Figure 9.316: Plain closed curves

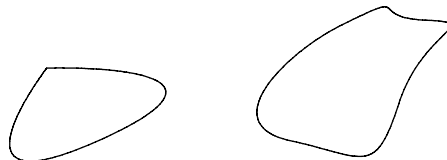
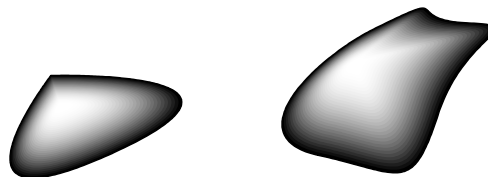


Figure 9.317: Shaded closed curves




## Plain Style

To remove all styles from a curve, with a curve selected, choose Plain from the Curves menu.

## Pro The TLC Tool

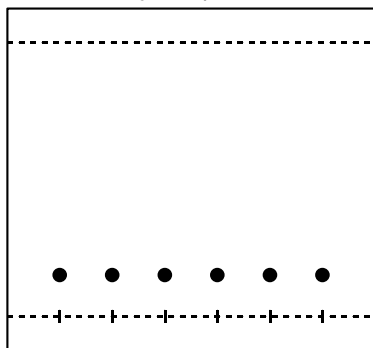
The TLC Tool is a drawing tool that allows you to easily depict Thin Layer Chromatography plates within a ChemDraw document. The tool creates a rectangular plate with origin line, solvent front, and one or more lanes. The lanes can be populated with spots of different  $R_f$  size, shape, or color.

To create a TLC plate:

1. Select the TLC tool .
2. Drag in any direction from the point of origin.

The number of lanes is a function of the width of the plate you create.

Figure 9.318: Drawing TLC plates



You can manipulate parts of the plate as follows:




Table 35: TLC plate tool options

If you want to...	then...
Change the height or width of the plate.	Drag a border or corner. The number of lanes will not change.
Move the origin or solvent front.	Drag the origin or solvent front line.
Show or hide the origin, solvent front, borders, or side ticks.	<ol style="list-style-type: none"> <li><b>Right-click</b> or <b>control-click</b> in the plate.</li> <li>Select the appropriate action.</li> </ol> <p><i>NOTE: Use the Transparent option if you want to overlay the TLC plate on a scanned plate.</i></p>
Change the order of lanes.	Drag the origin tick to the new location.

Table 35: TLC plate tool options

If you want to...	then...
Add, delete, or duplicate a lane.	<ol style="list-style-type: none"> <li>Position the cursor on the lane you want to delete or duplicate (or between lanes to add).</li> <li><b>Right-click</b> or <b>control-click</b> in the plate.</li> <li>Select the appropriate action.</li> </ol> <p><i>NOTE: You can also delete lanes with the Eraser tool.</i></p>
Move a spot.	Drag the spot. The $R_f$ displays as you drag.
Duplicate a spot.	<b>Ctrl+drag</b> or <b>option+drag</b> the spot.
Delete a spot.	Click on the spot with the Eraser tool.
Display or set the $R_f$ for a spot; add a custom spot	<ol style="list-style-type: none"> <li><b>Right-click</b> or <b>control-click</b> on a spot.</li> <li>Point to <b>TLC Spots</b>, and take the appropriate action.</li> </ol> <p><i>NOTE: To display <math>R_f</math> for all spots, <b>Right-click</b> or <b>control-click</b> in the plate and select <b>Show <math>R_f</math></b> from the TLC Spots submenu.</i></p>

Table 35: TLC plate tool options

If you want to...	then...
Change the style or color of a spot.	<ol style="list-style-type: none"> <li><b>Right-click</b> or <b>control-click</b> on a spot.</li> <li>Choose the style or color.</li> </ol> <p><i>NOTE: To change the style for all spots, <b>Right-click</b> or <b>control-click</b> in the plate and choose the style from the TLC Spots submenu.</i></p>
Enlarge or “smear” a spot.	<p><b>Shift+drag</b> the spot. When you position the cursor on a spot and press “Shift”, the cursor assumes one of three shapes, depending on how it is positioned:</p> <ol style="list-style-type: none"> <li>Cross arrows  used to enlarge a spot.</li> <li>Horizontal arrow  used to widen a spot.</li> <li>Vertical arrow  used to elongate a spot or create a crescent.</li> </ol> <p><i>NOTE: You may want to zoom in to make positioning easier.</i></p>

## R<sub>f</sub> Display

When you select Show R<sub>f</sub>, a text label appears near the spot showing the spot's retention factor value. By default, the tag will show the R<sub>f</sub> to two decimal places. You can change the tag as follows:

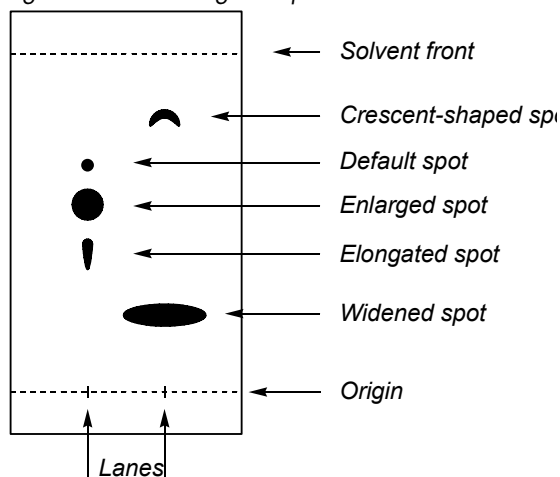
- Select the tag with the Lasso or Marquee tool and drag it to a new location, or **Right-click** or **control-click** on the tag and choose **Position...**

- Select the tag with the Text tool and edit the R<sub>f</sub> value.  
If you change the R<sub>f</sub> the spot will move to the new position indicated.  
If you edit the R<sub>f</sub> to have different precision, that precision will be preserved.

## Resizing Spots

You can resize spots by holding down the Shift key while pointing at an edge of the spot. Dragging the left or right sides of the spot will adjust the spot's width only. Dragging from the top will adjust its height only. Dragging from the bottom will adjust the tail only. Dragging from any of the other four corners will scale all three values. By using combinations of these dragging motions, you can reproduce any sized or shape spot you want.

Figure 9.319: Editing TLC spots



## Custom Spots

The TLC tool can create the most common spot shapes. Other types of spots, such as smears, can be reproduced as custom spots. The **Add Custom Spot** command allows you to insert a graphic file for a spot. Typically, these files would be produced by scanning a TLC plate and saving the spots in a library of spot shapes.







# Chapter 10: Page Layout

## Overview

The presentation quality of your ChemDraw document is determined by how well the chemical structures and other objects are placed on the page (layout). Effective layout of a drawing includes proper alignment of chemical structures and other objects, appropriate page size, and page orientation. The page layout tools include: setup of the page and the use of the ruler, and the grouping, layering, aligning, and distributing commands. You can also organize information on the page using tables.

## Controlling the Drawing Area

The size of a document window is not necessarily the same as the size of the drawing area of the page. A document window, in most cases, actually covers only a portion of the drawing area.

The following options allow you to set the drawing area displayed on your screen.

- Document Settings and Page Setup from the File menu allow you to set the size and orientation of the page, margins, headers, footers, and the document type and size.
- View menu options: Actual Size, Fit to Window, Magnify, and Reduce.
- Magnification Controls: enlarge and reduce
- Dragging to enlarge the drawing area.
- **Windows:** Point to a border or corner of a document window and drag to resize.
- **Macintosh:** Drag the Size box in the lower right corner of the document window.

The size of drawing area displayed depends on the size and resolution of your monitor. In some cases you can see the entire document.

If you magnify a document, the drawing area size and drawing objects become bigger. If you increase the magnification so that the page size becomes bigger than the screen, scroll bars become available.

## Setting up Pages

You can create two types of documents:

**Pages**—A single document containing one or more sheets, each of which is printed on a single piece of paper.

**Posters**—A single large document, composed of as many pieces of paper as necessary.

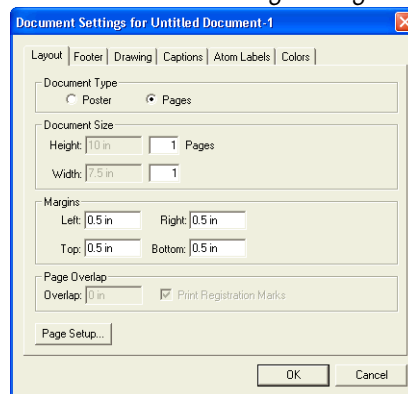
## Paged Document Setup

To create a document with one or more page:

1. Click the **Document Settings** command on the File menu.

The Document Settings dialog box appears.

Figure 10.320: Document Settings dialog box



2. On the **Layout** tab, check that **Pages** is selected.

- Specify the number of pages in the Document Size section.

The size of the pages is determined by the Page Setup settings. For more information, see “Page Setup” on page 151.

- Type the Margin settings.

The units of the margins are set in the Preferences dialog box. The paper size minus the margins determines the drawing area.

- Create Headers and Footers as described in “Creating Headers and Footers” on page 150.
- Click **OK**.

A document is created using your settings.

## Poster Documents Setup

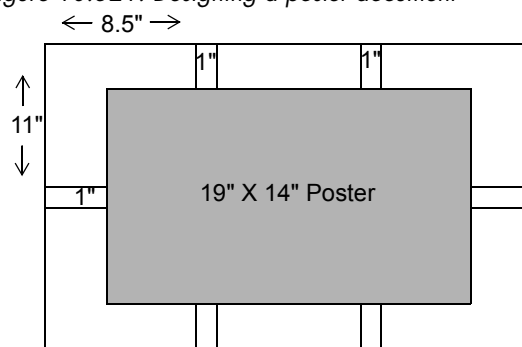
You can create a poster by creating a single large drawing area, which will be printed on as many separate pages as necessary. When you set the document size and how much each page overlaps, ChemDraw calculates the number of pages needed and the margin sizes. You can set registration marks, which mark the overlap setting on each page, to use as a guide when assembling the poster from the separate pages.

To create a poster document:

- Click the **Document Settings** command on the File menu.
- On the Layout tab, click **Poster**.
- Type the **Height**, **Width**, and **Page Overlap**.  
The number of pages and the margin dimensions are calculated.
- Select whether to **Print Registration Marks**.
- Create Headers and Footers as described in “Creating Headers and Footers” on page 150.
- Click **OK**.

An example of a 19-inch by 14-inch poster, consisting of six 8.5-inch by 11-inch pieces of paper with a 1-inch overlap is shown below.

Figure 10.321: Designing a poster document



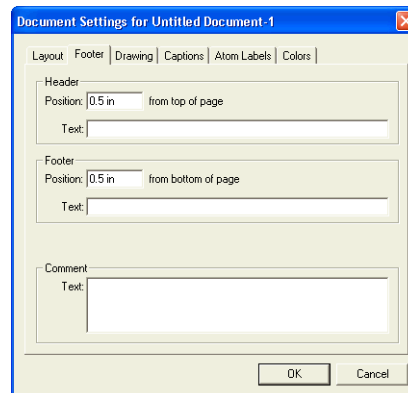
## Creating Headers and Footers

You create headers and footers in the Document Settings dialog box. In poster documents, only one header and footer appear for the entire document.

To create headers and footers:

- Click the **Document Settings** command on the File menu.
- Click the **Footer** tab.

Figure 10.322: The Footer tab of Document Settings



- Type the value of the position from the edge of the page that you want the header or footer to appear.
- Type the text to appear in the header or footer.

- Type additional information in the Text box from the following table:

Table 36: Footer additional text codes

To include the...	Type ...
file name	&f
page number	&p
date printed	&d
time printed	&t

- Position the text horizontally by typing the characters in the table below. Any text following these characters is appropriately aligned.

Table 37: Footer formatting codes

To align the text ...	Type ...
centered	&c
right	&r
left (default)	&l

## Page Setup

The Page Setup parameters that affect the size of the drawing area are:

- Page size
- Orientation

These parameters are specified in the Page Setup dialog box. The Page Setup dialog box and the options available vary depending on the printer you have chosen. For the Macintosh, the version

of the printer driver for that printer is installed in your System Folder.

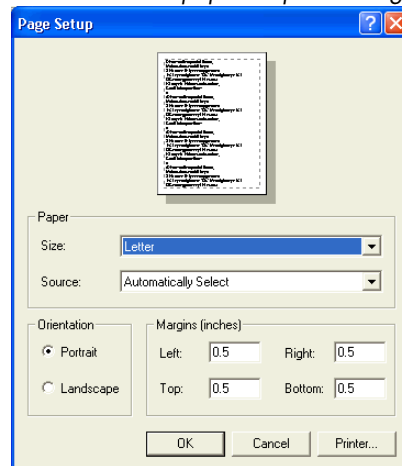
To set the paper size, orientation, and margins:

- Click the **Page Setup** command on the File menu.

The Page Setup dialog box appears. The dialog box appears slightly different depending on the printer and platform you have.

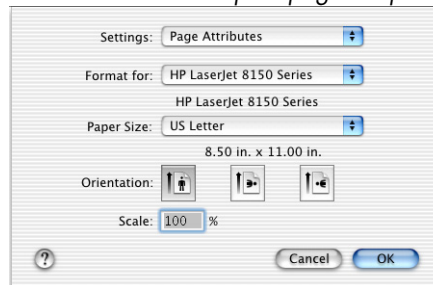
A Windows dialog box for a typical postscript printer is shown below.

Figure 10.323: Postscript printer print dialog



The Macintosh Page Setup dialog box with common settings for a LaserWriter is shown below.

Figure 10.324: Macintosh print page setup



- Select a paper size from the drop-down list.

The available page sizes vary depending on the type of printer. Listed below are common sizes available. The page orientation you choose determines which of the measurements is height and which is width:

Table 38: Standard paper sizes

Paper Type	Dimensions
US Letter	8.5 x 11 inches
US Legal	8.5 x 14 inches
A4 Letter	21 x 29.7 cm
B5 Letter	17.6 x 25 cm
Tabloid	11 x 17 inches
International	8.5 x 12 inches
Computer	14 x 11 inches

## Page Orientation

To choose the orientation of the page, click the vertical (portrait) or horizontal (landscape) orientation button.

The orientation of a document window changes to the orientation you have chosen. This is evident when the rulers are visible.

## Reduce or Enlarge

Some printers include an option to reduce or enlarge your drawings by a variable percentage (25-400%). This option scales all objects and text in the document window by the percentage specified. This is not a change in magnification. The size of

objects is changed relative to the paper size, margins, and orientation you have specified.

The enlarge or reduce option is useful for changing the size of the available drawing area, while keeping the images on the screen at the normal size when you are drawing. If your document is set so that the drawing fills the page on one printer and you use another printer that requires larger margins, the drawing may disappear off the edge of the document window. You can reduce the size of the drawing with the reduce option so that it fits in the document window.

## Saving Page Setup Settings

You can save Page Setup settings in a Style Sheet or Stationery Pad. Whenever you open a Style Sheet or Stationery Pad, these settings are automatically used. The Page Setup settings are saved in addition to the Text settings, Drawing Settings, and the Color Palette.

## 35mm Slide Boundary Guides

If you make 35mm slides from a hard copy of a ChemDraw document or from a screen shot, you can display boundary lines that appear on your screen positioned at 7 inches and 10.5 inches to match the 2:3 ratio for the 35 mm slide format. These guides help you keep your drawing within this region to maintain the proper ratio, but are not printed. The drawing area of the page must be at least 7 x 10.5 inches for these boundary lines to be visible.

To display the 35mm slide boundary lines:

1. Click the **Preferences** command on the File menu.
2. Select the **Show 35mm Slide Boundary Guides** check box.
3. Click the **OK** button.

Two 35mm Slide Boundary Guides appear in the same orientation you have chosen in the Page Setup dialog box. These guides appear in every document.

This preference affects all documents.

## Changing Perspectives

You can use a close-up view of objects in your reaction scheme to make sure they are properly positioned. At times, you may want to reduce your view so that you can move groups of objects around the page. You can change the magnification to perform these functions by using the Magnify and Reduce commands in the View menu, the Zoom tool, or the magnification controls.

## Magnifying with the View Menu

When you use the View menu to magnify or reduce, the magnification is set to the next higher or lower value. You can magnify up to 400% or reduce to 25%.

### Magnify

To magnify using the View menu:

1. Select the object around which you want to magnify your view.

---

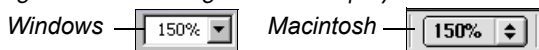
*NOTE: If you do not select an object, the last object drawn is the center point of the magnification.*

---

2. Click the **Magnify** command on the View menu.

The magnification occurs around the center of the selected object. The magnification percentage appears in the Magnification drop-down list.

Figure 10.325: Magnification display



You can continue to magnify your view to a maximum of 400%.

## Actual Size

To return to the actual size from any other magnification, click the **Actual Size** command on the View menu.

The view is returned to the original size.

## Reduce

To reduce the magnification:

1. Select an object around which you want to reduce the magnification.

---

*NOTE: If you do not select an object, the last object drawn is the center point of the magnification.*

---

2. Click **Reduce** on the View menu.

The reduction in magnification appears in the Magnification drop-down list.

Figure 10.326: Viewing reduced magnification



You can reduce the magnification until the entire page fits on the screen. In the reduced view, you can continue to use all of the drawing tools. In particular, you can use a selection tool to rearrange the drawing in order to take better advantage of the space available.

## Fit to Window

Fit to Window reduces the magnification until the entire page is visible in the document window.

To view the entire drawing area in a document window at once, click the **Fit to Window** command on the View menu.

The Magnification control shows the reduction in magnification that was required to have the entire page appear on the screen.

## Using the Magnification Control

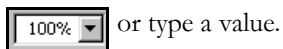
When you use the Magnification control, you can display magnifications from 10% to 999% of the

normal size of your page. The magnification control allows you to select a specific value.

To use the Magnification controls:

Windows:

- Select a value from the drop-down list

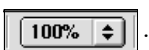


or type a value.

Macintosh:

Do one of the following:

- Select a value from the drop-down list



- Select **Other** from the drop-down list. In the dialog box that appears, type a value and click **OK**.

## Arranging Objects

This section describes methods for positioning, aligning, and layering objects in a document window.

### Using Rulers

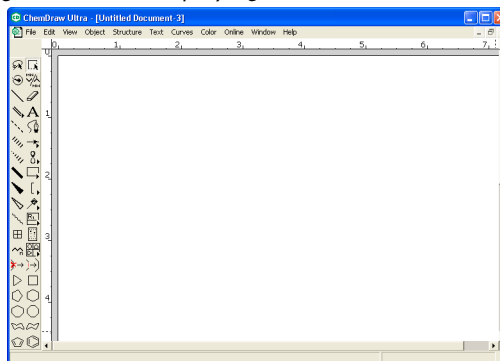
You can use the rulers to position objects a measured distance away from some reference point or create objects of an approximate size. The units used for the ruler are set in the Preferences dialog box, where you have the choice of inches, centimeters or points.

### Showing Rulers

To display the rulers, click the **Show Rulers** command on the View menu.

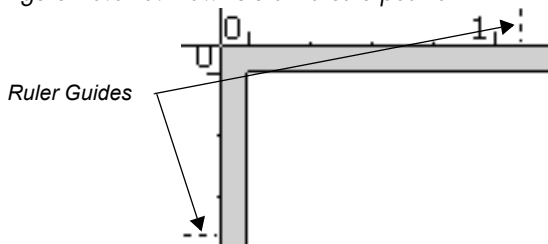
A check mark appears next to the Show Rulers command, and the rulers appear along the top and left edges of a document window.

Figure 10.327: Displaying rulers



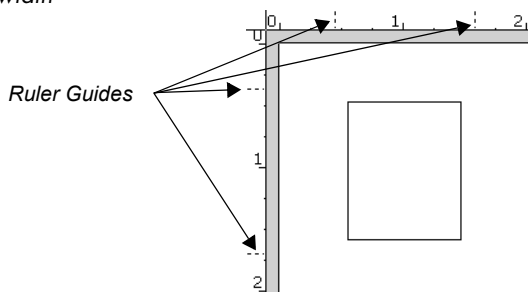
As you move the pointer, Ruler Guides appear on each ruler, indicating the position of the pointer.

Figure 10.328: How rulers indicate position



Ruler guides also appear when you drag selected objects. In this case, however, there are two Ruler guides that bracket the object. With this bracketing you can quickly establish the height and width of the selected objects.

Figure 10.329: Using ruler guides to show height and width





## Hiding Rulers

To Hide the rulers, deselect **Show Rulers** on the View menu.

The check mark disappears.

## Using the Crosshair

Use the Crosshair to align objects relative to each other, and to space objects a consistent distance apart. The axes of the Crosshair can be moved within a document window.

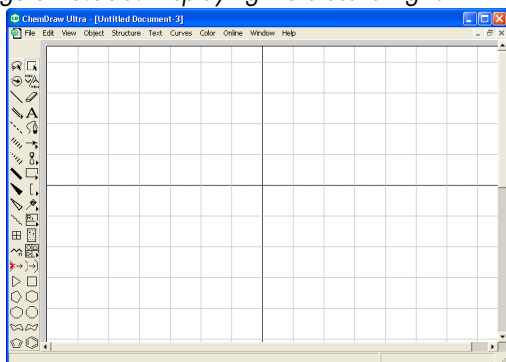
## Displaying the Crosshair

To show the Crosshair, click the **Show Crosshair** command on the View menu.

A check mark appears next to the Show Crosshair command and the Crosshair appear within a document window.

To assist you in aligning objects, the Crosshair includes grid lines that extend from the major division marks on each axis.

Figure 10.330: Displaying the crosshair grid



You can also show the Rulers while the Crosshairs are displayed so that you can see the unit measurement associated with each of the divisions on the Crosshair axes.

## Moving the Crosshair

To move the Crosshair:

1. Position the pointer where the Crosshair axes intersect.

When the pointer is near to the center of the Crosshair, it changes to an arrow.

2. Drag the Crosshair.

To constrain the movement of the Crosshair to the X- or Y-direction, shift+drag the crosshair.

## Aligning Objects using the Crosshair

To use the Crosshair to align objects do one of the following:

- Move the Crosshair axes and align it with the object.
- Select an object and drag it until it is aligned with either axis of the Crosshair, or a grid line.

In either case, if a bond or side of the object is parallel to one of the axis, it disappears when it is exactly positioned over a Crosshair axis.

To align another object on the Crosshair:

1. Select a second object.
2. Drag the second object to the Crosshair axis or grid line and align it to the first.

You can also move selected objects in small increments to align them with the Crosshair using the Arrow keys available on some keyboards:

To move 1 point in the direction of an Arrow key, select the objects and press an Arrow key.

*NOTE: 1 point equals 1/72 inch or 0.035 cm.*

To move 10 points using the Arrow key, for example, to the right, press **Alt+Right Arrow** or **option+right arrow**.

## Hiding the Crosshair

To hide the Crosshair, click the **Show Crosshair** command on the View menu.

The check mark next to the Show Crosshair command disappears.

## Centering on a Page

To center an object (or group of objects) at the center of the page:

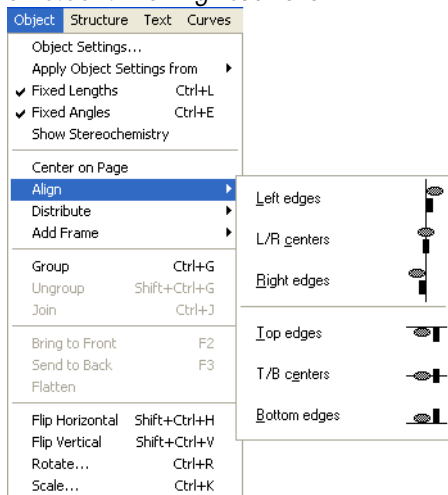
1. Select the object you want to center using a selection tool.
2. Click the **Center on Page** command on the Object menu.

The selected objects move so that the center of the Selection rectangle is positioned at the center of the page.

## Aligning Objects

Use the Align commands to align objects relative to each other. Examples of the types of alignments are shown on the menu.

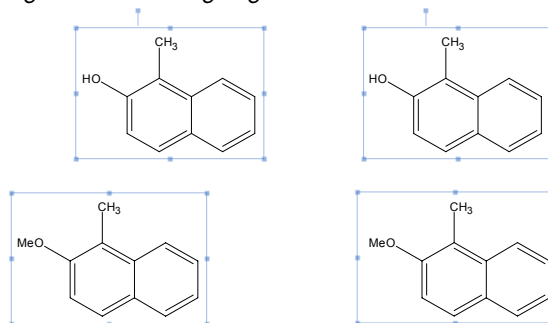
Figure 10.331: The Align submenu



To align two or more objects:

1. Select the objects with a selection tool.
2. Choose one of the **Align** commands from the Align submenu of the Object menu.

Figure 10.332: Aligning structures



NOTE: If you look closely, you can see that the structures in Figure 10.332 were aligned on left edges, not centers.

If you select only part of a structure or group with a selection tool, only that part is used for the alignment operation, but the entire structure or group is moved.

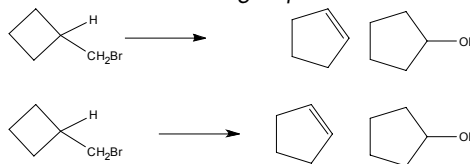
## Distributing Objects

Use the distribute commands to distribute objects horizontally or vertically and at an equal distance apart. For reactants and products with different shapes, select the parts of the objects to distribute.

To distribute 3 or more objects:

1. Select the 3 or more objects to distribute.
2. Point to the **Distribute** command on the Object menu, and choose **Vertically** or **Horizontally**.

Figure 10.333: Distributing objects



The space between the objects is equalized. The upper, lower, right, and left positions of objects in your selection remain unchanged.

## Front to Back Ordering

The front to back ordering is a useful method for changing the orientation of one object relative to another object within the same picture layer. For

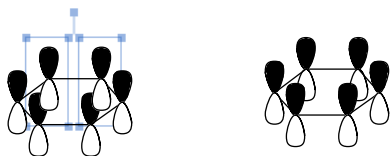
additional information specific to the layering of bonds, see “Changing Bond Crossings” on page 55.

## Send to Back

To place one object behind another within a layer:

1. Select the object that you want to send to the back, in this example, the two upper orbitals.
2. Click the **Send to Back** command on the Object menu.

Figure 10.334: Moving objects to the back



The selected object appears behind all other objects in the same layer.

## Bring to Front

To place one object in front of another within a layer:

1. Select the object that you want to move forward.
2. Click the **Bring to Front** command on the Object menu.

The selected object now appears in front of all other objects.

*NOTE: When bonds have 3D coordinates, those coordinates always determine the visible bond crossings. Bring To Front and Send To Back have no visible effect in this case.*

## Creating Tables

You can create tables of ChemDraw objects with the Table tool or tables of text with the Text tool.

### Creating Tables with the Table Tool

Tables created with the Table tool are containers for drawings and data. To place a structure in a

table, you can draw it directly in the table, or copy or drag it into the table.

The Table tool enables you to do the following:

- Create and modify tables
- Customize the borders
- Add or delete rows and columns
- Resize the table and its cells manually
- Fit a cell around its contents automatically
- Align cell contents

To create a table with the Table tool:


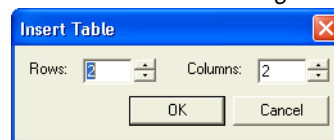
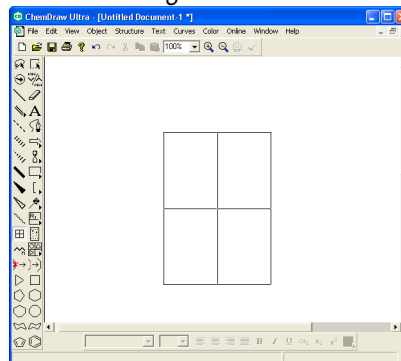
1. Select the Table tool on the Main Tools palette. 
2. Do one of the following:
  - Click and drag in the document window to create the table.  
The default table has two rows and two columns.
  - Click in the document window. Type the numbers of rows and columns in the Insert Table dialog box, and click **OK**.

Figure 10.335: The Table tool dialog box



The table appears in the document window.

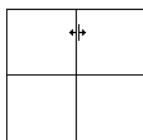
Figure 10.336: Adding a table to a document



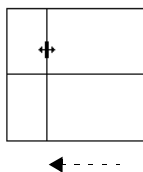
To resize the rows or columns:

1. Place your pointer on the border to resize.

The pointer changes to a double-headed arrow.



2. Drag the border to the desired size.



Changed Table tool behavior

Table 39: Table tool behavior in ChemDraw 10

when you...	ChemDraw 9	ChemDraw 10
change the width of a column:	Table width stays the same; columns to the right move. The result is that the right-most column also changes width.	Table width stays the same; only the column you are adjusting changes.
change the height of a row:	Table height stays the same; rows below move. The result is that the bottom-most column also changes height.	Table height changes with the change in the row. All other rows stay the same.

Table 39: Table tool behavior in ChemDraw 10

when you...	ChemDraw 9	ChemDraw 10
change the width of a column with the shift key:	Table width stays the same; only the column you are adjusting changes.	Table width resizes; other columns stay the same.
change the height of a row with the shift key:	Table height stays the same; only the row you are adjusting changes.	Table height stays the same; only the row you are adjusting changes.
change the table height (drag the top or bottom border)	Table resizes proportionately.	Top: table resizes proportionately. Bottom: bottom row resizes.
change the table width (drag the left or right border)	Table resizes proportionately.	Left: table resizes proportionately. Right: right column resizes.

Table 39: Table tool behavior in ChemDraw 10

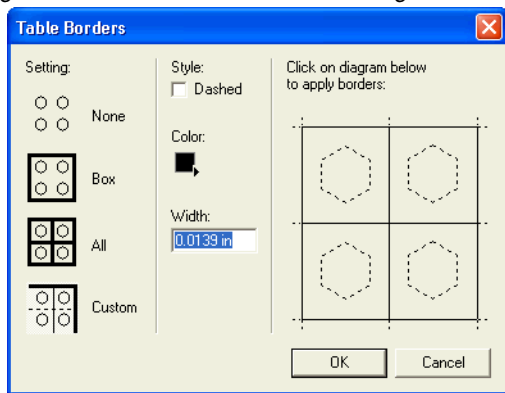
when you...	ChemDraw 9	ChemDraw 10
change the table height with the shift key	Top: table resizes proportionately. Bottom: bottom row resizes.	Top: table resizes proportionately. Bottom: bottom row resizes.
change the table width with the shift key	Left: table resizes proportionately. Right: right column resizes.	Left: table resizes proportionately. Right: right column resizes.

To customize the borders of the table:

1. With the Table tool selected, point to a border and right-click (Mac: option-click).
2. Click **Borders** on the context menu.

The Table Borders dialog box appears.

Figure 10.337: The Table Borders dialog box

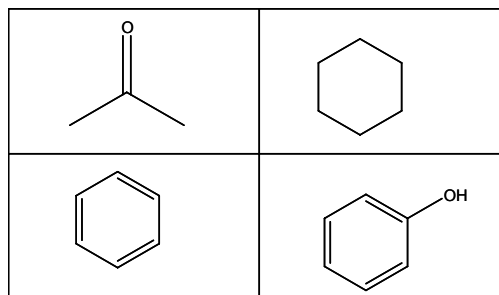


3. In the Setting section, click the borders to which you want to apply the settings.
4. In the Style section, select the style, color and width of the border to apply.
5. In the table diagram, click the borders to customize.
6. Click **OK**.

The table tool includes commands for alignment of cell contents, fit, adding or deleting cells, and clearing cells. In general, to change the whole table, work with the right or bottom borders. To change only a single row or column, work with the left or top borders.

To make a cell fit around its contents, such as in the table shown below:

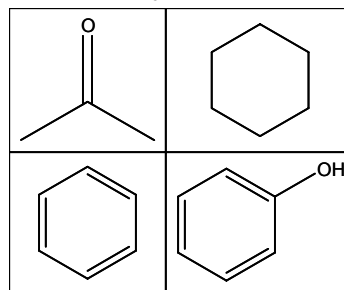
Figure 10.338: Fitting a table cell around the contents



1. Point to a border and right-click.
2. Choose **Size To Fit Contents**.

The cells resize to fit around the contents.

Figure 10.339: Resizing a table cell

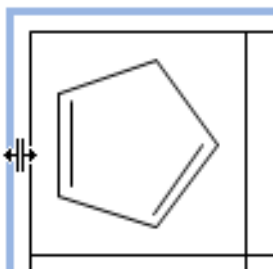


To add rows or columns to the table:

1. Point to the top or left border where you want to add the row or column.

The cursor changes as shown below.

Figure 10.340: Table cursor when dragging



2. Right-click or Option-click, and from the menu that appears, choose the appropriate option:

Table 40: Adding rows and columns to tables

<b>If you want to ...</b>	<b>Then choose ...</b>
add an empty row above the indicated row	<b>Add Row Before.</b>
add an empty row below the indicated row	<b>Add Row After.</b>
add an empty column to the left of the indicated column	<b>Add Column Before.</b>
add an empty column to the right of the indicated column	<b>Add Column After.</b>
delete the indicated row and its contents	<b>Delete Row.</b>

Table 40: Adding rows and columns to tables

### **If you want to ... Then choose ...**

delete the indicated column and its contents	<b>Delete Column.</b>
--	-----------------------

To align all of the objects in a column or row, point to a top or left border, right-click, point to the **Align** command on the context menu, and choose the alignment you want.

The cell contents shift and stay in a fixed position relative to the cell. The default alignment is unaligned.

To align all of the objects in a table, point to a bottom or right border, right-click, point to **Align**, and choose the alignment you want.

## **Creating Tables with the Text Tool**

ChemDraw allows you to create tables of text using the Tab key with the Text tool.

### **Creating the First Row (column headings)**

To create the first row and establish the columns of a table:

1. Click the Text tool.
2. Click in a document window where you want the table to start.
3. Type a caption.
4. Press Tab.  
A second caption box appears.
5. Type a second caption.

The second column is placed 20 points (20/72 inch, 0.71 cm) to the right of the first.

6. Press Tab again to create a third column, and so on.

*NOTE: The style, font, and size that you set in each column are maintained in all the rows that follow.*

Figure 10.341 shows the creation of new columns using the Tab key.

Figure 10.341: Using the Tab key in text tables

Compound    MW    LogP    LD50

To change the spacing between columns one point at a time while editing a caption:

1. Select the caption.
2. Move the caption with the arrow keys.

For more information on moving objects, see “Moving Objects” on page 64.

To create another column with this same spacing as the previous, press Tab.

A third caption text box appears.

## Creating a New Row

To start a new row that is exactly aligned with the first, press Tab twice at the end of a row.

A caption text box appears exactly aligned under the first caption positioned exactly 20 points below the first caption in the first row.

The Figure 10.342 illustrates the creation of a new row.

Figure 10.342: Creating a new row in a text table

Compound    M.W.    LogP    LD50

→ 1

To change the spacing between rows as you create the table:

1. Select the captions in a row.
2. Move the captions using the arrow keys.

For more information on moving objects, see “Moving Objects” on page 64.

To continue and fill in the row with captions, press Tab to create another caption in the row, and then press Tab twice to begin a new row.

The spacing between the newest row and the row directly before it have the same spacing that you specified between the previous two rows.

## Adjusting Row or Column Spacing

To use a selection tool to adjust the spacing in a table:

1. Select all of the captions with a selection tool.
2. Shift+drag the caption.

The movement is constrained to the X-axis or Y-axis so that you can maintain the row or column alignment.

## Moving Around In Tables

To move within an existing table, click the Text tool and select a caption.

Press **Ctrl+arrow** or **command+arrow** to move to the next caption in the direction of the arrow.

Alternatively, you can use the key combinations shown in Table 41.:

Table 41: Moving around in a text table

Use ...	To move ...
Tab	right
Shift+Tab	left
<b>Ctrl+Enter</b> or <b>command+return</b>	down
<b>Ctrl+Shift+Enter</b> or <b>command+shift+return</b>	up

## Inserting a New Row

To insert a row:

1. Select a selection tool and select a row of captions.
2. **Shift+drag** the selected row.  
Shift constrains the movement to the Y-axis to maintain the column alignment.
3. Select the first caption in the row above or below the space you created.
4. **Ctrl+Shift+drag** or **command+shift+drag** to create a copy of the caption and position it in the empty space you created.

The placement of this copied caption sets the position of the inserted row.

To fill in the inserted row with caption text:

1. Click the Text tool and select the first caption in the inserted row.
2. Type new text.

Press Tab to move to the second caption in the inserted row, and so on.

## Printing

ChemDraw uses the standard system commands to print ChemDraw documents. The options that you have available to you depend on the printer that you are using. Refer to your printer's documentation for more information.

In general, to print a ChemDraw document:

1. Click **Page Setup** on the File menu.
2. Make all appropriate selections for the printer you are using and click **OK**.
3. Click the **Print** command on the File menu.
4. Make your selections in the Print dialog box and click **OK**.

To print a document from Windows Explorer or from the Finder:

1. Select the document you want to print.
2. Click **Print** on the File menu.

The ChemDraw application is opened and the Print dialog box appears.

3. Make your selections in the Print dialog box and click **OK**.



# Chapter 11: Sharing Information

## Overview

ChemDraw includes many of the standard system commands for transferring information within and between ChemDraw documents, and between ChemDraw and documents created using other applications.

You can transfer information using:

- the Clipboard
- drag and drop
- file formats

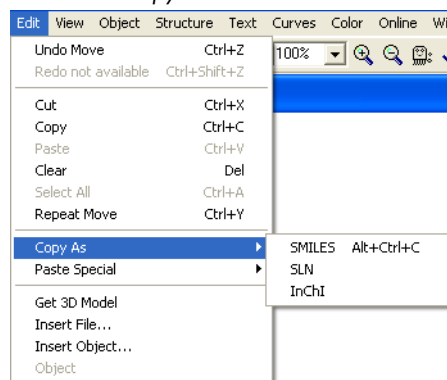
When you drag-and-drop ChemDraw information, or use the clipboard, the object you are copying can be edited.

## Using the Clipboard

You can use the clipboard to transfer part or all of the information within an active document window between applications on the same computer or a networked computer. Use the standard “Copy-and-Paste” or “Cut-and-Paste” tools to transfer information to any application that supports these tools. The information is transferred as a ChemDraw drawing object. Double-clicking on it will open ChemDraw and allow you to edit the object. See “Embedding Objects (Windows)” on page 167 and “Edit Graphic Object (Macintosh)” on page 167 for more information on editing ChemDraw objects embedded in other documents.

You may also use the Copy As tool to translate a selected structure to a SMILES, SLN, or InChI™ string.

Figure 11.343: Copy As submenu



If the Clipboard contains ChemDraw structures and you are pasting into another ChemDraw document, the pasted information is scaled to the settings in the current document. For more information, see “Autoscaling” on page 165.

If you are pasting the ChemDraw drawing into a document from which you are planning to print to a PostScript printer, see “Transferring PostScript (Macintosh)” on page 167.

## SMILES and SMIRKS Strings

A SMILES string is a way to describe a chemical structure in a line of text. Several software packages use SMILES strings as a way to enter and store chemical structure information.

A SMIRKS string is a way to describe chemical reactions in text. If you select a reaction and use the Copy As SMILES command, a SMIRKS string is copied to the clipboard. If you use the Paste Special SMILES command when a SMIRKS string is on the clipboard, a reaction is pasted into your document.

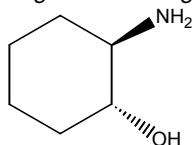
## Creating SMILES Strings

To create the SMILES string for the following structure:

1. Select the structure using a selection tool.
2. Point to the **Copy As**, command on the Edit menu, and choose **SMILES**.

The SMILES string is transferred to the Clipboard.

Figure 11 - 1: Using SMILES strings



N[C@@H]1[C@H](O)CCCC1

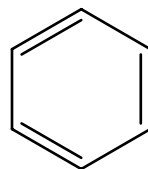
To display the SMILES string, paste the string in a document window.

When the SMILES string is on the Clipboard, you can transfer it to another application that can interpret and manipulate SMILES strings.

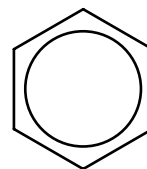
If you select more than one structure in ChemDraw, and choose Copy SMILES from the Edit menu, the SMILES string for each structure is copied to the Clipboard and separated from the previous SMILES string by a period.

SMILES supports an alternate notation for aromatic structures using lowercase letters. ChemDraw generates this type of SMILES string for any structure drawn with explicit aromatic bonds, either by using the Aromatic bond type in the Atom Properties dialog box, or by placing a circle within any ring structure.

Figure 11.2: Aromatic SMILES notation



C1=CC=CC=C1



c1ccccc1

### Pro Pasting SMILES from Clipboard

If you have a SMILES string, then you can automatically convert that text string into a ChemDraw structure.

To paste a SMILES string as a ChemDraw structure:

1. Select the SMILES string using the Text tool.
2. Click the **Copy** command on the Edit menu.
3. Point to **Paste Special** on the Edit menu, and choose **SMILES**.

The SMILES string is drawn as a structure.

*NOTE: Pasting SMILES uses the same routines as the Structure CleanUp command. For more information, see "Multi-Center and Variable Attachments" on page 73.*

### Pro Creating SLN Strings

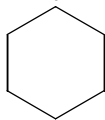
You can copy a ChemDraw structure to the Clipboard as an SLN string for export to a Tripos application.

To copy a ChemDraw structure as an SLN string:

1. Select a structure.
2. Point to **Copy As** on the Edit menu, and choose **SLN**.

The Structure is copied to the clipboard as an SLN String.

Figure 11.3: SLN strings



C[1]CCCC@1

## Pro Creating InChI™ Strings

ChemDraw 10 supports the IUPAC International Chemical Identifier (InChI™) protocol. A new addition to the Copy As submenu allows structures to be copied to other documents as InChI™ strings. It is used the same way as the SLN command.

*NOTE: InChI™ is not supported in either BioDraw Pro or Ultra.*

You may only copy legitimate InChI™ structures. If you attempt to copy a structure not supported by the InChI™ protocol, a warning appears informing you that the structure is not supported.

For more information on InChI™, and on using InChI™ strings in publications, see the InChI™ project page, <http://www.iupac.org/inchi/>, or the informal FAQ at: <http://wwwmm.ch.cam.ac.uk/inchifaq/>.

## Using Drag-and-Drop

You can use the drag-and-drop feature to copy objects to place in other documents. To use this feature in other applications, they must support drag-and-drop. As when using the clipboard, the information is transferred as a ChemDraw object and can be edited.

You can also use the drag-and-drop feature to create clipping files (Macintosh) or scrap files (Windows).

1. InChI™ is a trademark of the International Union of Pure and Applied Chemistry. InChI™ Material in ChemDraw is © IUPAC 2005.

To create a clipping file or a scrap file:

1. Select an object in a ChemDraw document.
2. Drag the selection out of the ChemDraw document window onto the desktop.

A clipping file or a scrap file is created on your desktop.

To view the information within a clipping file or a scrap file, double-click the file's icon.

A window appears showing the ChemDraw drawing. Click the close box to close the clipping file's window.

To use the contents of a clipping or scrap file in a document, drag the clipping or scrap file into an open window of an application that supports the drag-and-drop feature.

The contents of the clipping or scrap file are copied to the open window. The clipping or scrap file is unchanged.

## Transferring Between ChemDraw Documents

Whether you use the clipboard or drag-and-drop, when you move objects into another ChemDraw document they will behave in a well-defined way. In particular, you should be aware of the behavior of:

- Autoscaling
- Bonds
- Atom Labels
- Captions
- Non-bond Objects and Color
- Pasting to an Empty Document Window

### Autoscaling

When you transfer ChemDraw objects using the Clipboard or drag and drop from one ChemDraw document (the source document) to another ChemDraw document (the destination document), the objects are automatically scaled to

match the document settings of the destination document. Automatic scaling assures that the objects being transferred match the settings of the current document.

## Bonds

All bonds drawn in the source document using the values specified on the [Drawing Settings](#) tab of the Document settings dialog box can be changed to use the Drawing Settings in the destination document.

Any resized bond in the source document is scaled in the destination document. The scale factor is based on the ratio of the bond's length after resizing (source) to the Fixed Length on the Drawing Settings tab (source). This scaling process maintains the source document proportions in the destination document. All values on the Drawing Settings tab are scaled using this method.

For example, the Fixed Length is set to 1.0 cm in a source document. A benzene ring is resized in to 200%. The bond length is then 2.0 cm: a ratio of 2.0 cm:1.0 cm or a scale factor of 2. In the destination document, the Fixed Length set to 1.7 cm. When the benzene ring is pasted into the destination document, the bonds are scaled by a factor of 2 to a final bond length of 3.4 cm.

## Atom Labels

Atom labels are scaled the same way as bonds.

For example, in the source document, the atom label font size is set to 16 points. One or two atom labels in the source document are resized to 8 points, a ratio of 8:16 or a scale factor of 0.5. The destination document has an atom label font size set to 14 points. When the atom label is pasted into the destination document, the font size is scaled by a factor of 0.5 to give a final atom label font size of 7 points.

## Captions

ChemDraw autoscales captions are autoscaled using the ratio of the fixed length in the destination document to the fixed length in the source document times the caption font size. The font size of the caption can be any size and is not related to the setting in the Settings dialog box. This assures that captions are always in proportion to the bonds with which they are pasted.

For example, If the source document has a fixed length of 1.0 cm and the destination document has a fixed length of 2.0 cm, and the caption you are pasting is 12 points, then the resulting caption size after autoscaling is  $(2.0 \text{ cm} / 1.0 \text{ cm}) \times 12 \text{ points} = 24 \text{ points}$ .

## Non-bond Objects and Color

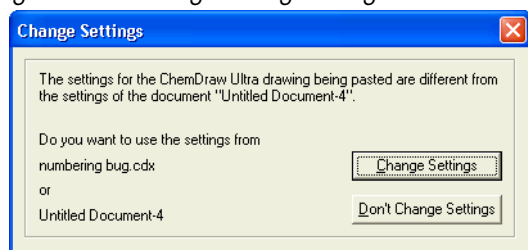
All objects that are not affected by settings in the Document Settings dialog boxes, such as arrows and boxes, are scaled to maintain the same proportions to bonds that were present in the source document.

With the exception of the foreground and background color, the other colors present in the selection to be pasted are added to the destination document's Color Palette if they are not already present (up to a maximum of 20 total colors). The background color in the destination document is unchanged, and all objects colored using the foreground color are changed to match the foreground color in the destination document.

## Pasting to an Empty Document Window

If you paste a ChemDraw drawing into an empty ChemDraw document and the settings between the documents are different, the Change Settings dialog box appears:

Figure 11.4: Change Settings dialog box



To change the settings in the destination document to match the settings in the source document, click **Change Settings**.

All of the settings in the destination document are changed to match those of the source document. All of the colors in the Color Palette of the destination document are changed to those specified in the source document.

To scale the objects from the source document to the settings in the destination document, click **Don't Change Settings**.

The settings from the source document are scaled to those in the destination document using the ratios given above.

*NOTE: If the source document was created in a ChemDraw version earlier than 3.0, the name of the document appears as "Unknown" in the dialog box.*

## Embedding Objects (Windows)

ChemDraw supports the Object Linking and Embedding (OLE) protocol on Windows. This allows you to edit ChemDraw structures that are pasted in other types of documents. ChemDraw is an OLE server, which means it can create OLE objects that can be copied and pasted into other OLE client applications.

When a drawing is transferred from ChemDraw into another document type that supports OLE, you can open the drawing and edit it from within the client application.

For example, to edit a ChemDraw drawing inserted into Microsoft Word for Windows version 6.0 or later, do one of the following:

- Select a ChemDraw drawing in a Word document and from the Edit menu, point to **CS ChemDraw Drawing Object**, and choose **Edit**.
- Double-click a ChemDraw drawing in a Word document.

The ChemDraw tools and menus replace those of Word. Use the ChemDraw tools to edit the drawing.

When you have finished making changes, click in another area of the document.

The Word tools and menus are restored.

## Edit Graphic Object (Macintosh)

ChemDraw supports the Edit Graphic Object (EGO) protocol for editing ChemDraw structures pasted into other types of documents. When you drag an object from ChemDraw into another type of document that supports the EGO protocol, or copy it with the clipboard, you can double-click on the object and it appears in a ChemDraw document window. When you close the ChemDraw document window, any changes you made are reflected in the other document.

*NOTE: As of this writing, versions of Microsoft Word after 5.0 do not support EGO.*

## Transferring PostScript (Macintosh)

To obtain the highest quality drawings possible on a PostScript printer, ChemDraw creates both a screen representation and a PostScript representation of your drawing. PostScript is a page-definition language used to describe drawings. Many

printers, including most Apple LaserWriter printers, use PostScript to create high quality output.

For best print quality under all circumstances, we recommend that you leave the Include PostScript and Include ChemDraw Laser Prep preferences selected (default) when you copy and paste from ChemDraw to other applications. The ChemDraw Laser Prep option adds approximately 11K to 12K to each drawing, but these options give you the greatest flexibility if you give your document to someone else or later want to print it on a PostScript printer.

If you never plan to print to a PostScript printer or never plan to give your document to someone who uses a PostScript printer, you can turn the preferences off.

To deselect the PostScript preferences:

1. Click the **Preferences** on the File menu.
2. Deselect **Include PostScript** and **Include ChemDraw LaserPrep**.

To transfer only a few drawings to another document, select **Include PostScript** and **Include ChemDraw Laser Prep** in the Preferences dialog box.

The PostScript commands and the ChemDraw Laser Prep are transferred with each drawing. The transferred drawings can be printed independently of ChemDraw.

If you do not check the Include PostScript check box when printing to a PostScript printer ChemDraw sends QuickDraw commands to the printer. For more information, see “Printing Background Color” on page 214.

*NOTE: You can also transfer drawings to a document in a remote location whose printer cannot be initialized by ChemDraw.*

To print to a non-PostScript printer, deselect both **Include PostScript** and **Include ChemDraw Laser Prep** on the General tab of the Preferences dialog box.

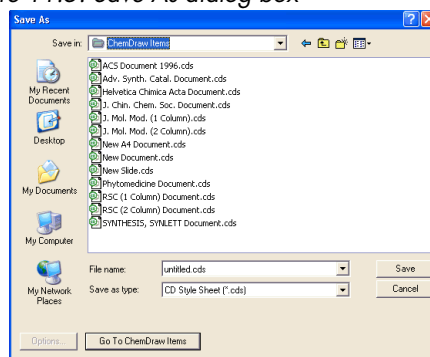
## Importing and Exporting

Many applications can use the information contained within a ChemDraw document and saved to another file format. Similarly, ChemDraw can import and work with information in a number of file formats. Not all formats are supported for both import and export. See the individual format descriptions for details. File formats are available in a pop-up menu at the bottom of the “Open” and “Save As” dialog boxes.

To export a file:

1. Click the **Save As** command on the File menu.

Figure 11.5: Save As dialog box



2. In the Save As dialog box, do the following:
  - a. Type a name for the file and choose a location in which to save it. Use the “Go To ChemDraw Items” button to quickly locate the ChemDraw Items folder.
  - b. Select a file format from the bottom of the dialog box.
  - c. Click **OK** or **Save**.

A copy of the current document is saved in the format you specified. The current document remains unchanged.

Some file formats do not support atom labels that contain nicknames or structural fragments. When you save in these formats, ChemDraw automatically expands all atom labels and saves the file using the expanded form. For more information,

see “Expanding and Contracting Labels” on page 70.

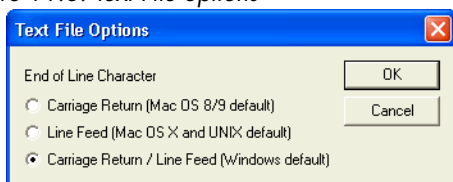
The following formats do not support nicknames or structural fragments:

- Connection Table
- MSI MolFile
- SMD

Some formats can be saved with different options. If a format has no save options, the “Options” button is grayed out. The following text-based formats can use the Text Options:

- ChemDraw XML
- CML
- Connection Table
- ISIS/TGF
- ISIS/Reactions
- MDL MolFile
- Molecular Simulations MolFile
- SMD

Figure 11.6: Text File options



Other format options are noted in format descriptions.

## Improved ISIS compatibility

ChemDraw 10 has improved support for the ISIS/Sketch (SKC), ISIS/TGF (TGF) and ISIS/Reaction (RXN) formats. Support for both import and export of the V3000 format has been added.

ChemDraw auto-detects V3000 files on import. For export, there are two new entries in the **Save**

**As** drop down menu: **ISIS Reaction V3000 (RXN)** and **MDL Molfile V3000 (MOL)**. If you have used features that require the V3000 format, you must select it manually; there is no auto-detect on save.

## Attached Data

ChemDraw 10 supports associating text fields with objects such as atoms and bonds by defining a “field name”. The feature is compatible with the “Data SGroup” in MDL formats, and will be converted to Data SGroups when saved in MDL formats if:

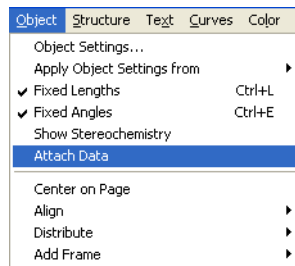
- a field name is specified *and* it is attached to:
  - a collection of atoms and bonds, *or*
  - a single set of brackets

If it is attached to both a collection of atoms and bonds and a set of brackets, it will be converted to two different Data SGroups.

To attach data to objects:

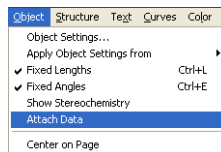
1. Select an object.
2. Click the **Attach Data** command on the Object menu.

Figure 11.7: Attach Data command



The Attach Data dialog box appears.

Figure 11.8: Attach Data dialog box



3. Enter the field name and click OK.

---

*NOTE: Field names cannot be edited in ChemDraw after they are created. While ChemDraw will allow any field name length, MDL formats have restrictions that users should be aware of before creating names.*

*Likewise, ChemDraw will allow data to be attached to any object. When saving to MDL formats, this data will be lost unless the object meets the rules noted above.*

---

4. Enter the data in the text box under the object.

## Modifying Attached Data

ChemDraw treats attached data as normal text for most purposes. However, two additional commands appear on the context menu when attached data is selected.

Figure 11.9: Attached data context menu



- **Select Linked Objects** changes the selection to include all of the objects associated with the data.
- **Position** opens up the same dialog that is used to position ObjectTags, allowing you to position the data relative to the associated structure.

---

*NOTE: Positioning information is lost when saving to MDL formats.*

---

## Graphics export border preference

An explicit preference option allows the user to specify the size of the border when exporting pictures. This preference affects the output of all graphical formats, including but not necessarily

limited to: WMF, PICT, EPS, TIFF, GIF, BMP, and PNG. It applies to both the clipboard and saved files.

The default value is 2 points (0.278 in; 0.071 cm). The value can be zero, meaning that the exported image is exactly snug against the objects in the graphic. However, this is not recommended because a bug in Windows causes clipping at the edges of metafiles when they are reduced in size. The default value should prevent clipping with reductions to about 20% of original size.

## File Formats

ChemDraw supports both import and export (except as noted below) of the following file formats. To export a ChemDraw file to one of these formats, use the **Save As...** option when saving. Not all formats are supported in all versions of ChemDraw, as noted in the table below. For additional information on importing files, see “Inserting Objects from Other Applications” on page 177.

Table 42: Import and export of different file formats

Format	Import	Export
ChemDraw (CDX)	YES	YES
ChemDraw XML (CDXML)	YES	YES
ChemDraw 3.5 (CHM)	YES	YES
ChemDraw 2.0 and ChemDraw 2.1 (CHM)	YES	NO
<b>Pro</b> ChemDraw Template (CTP)	YES	YES
<b>Pro</b> ChemDraw Template Style Sheet (CTS)	YES	YES



Table 42: Import and export of different file formats

Format	Import	Export
ChemDraw Stationery/Style Sheet (CDS)	YES	YES
<b>Pro</b> Connection Table (CT)	YES	YES
<b>Pro</b> Chemical Markup Language (CML)	YES	YES
Bitmap (BMP)	YES	YES
Encapsulated PostScript (Macintosh)	NO	YES
PostScript (EPS) (Windows)		
Graphic Image Format (GIF)	YES	YES
<b>Pro</b> ISIS (SKC, TGF, RXN)	YES	YES <sup>a</sup>
<b>Pro</b> JCAMP (JDX, DX)	YES	NO
JPEG (JPG, JPEG)	YES	NO
<b>Pro</b> MDL MolFile (MOL)	YES	YES
MDL RGFile (RGF)	YES	YES
(Macintosh) <b>Pro</b> Molecular Simulations MolFile (MSM)	YES	YES

Table 42: Import and export of different file formats

Format	Import	Export
PICT (Macintosh)	YES	YES
Portable Network Graphics (PNG)	YES	YES
<b>Pro</b> Standard Molecular Data (SMD)	YES	YES
<b>Pro</b> Galactic Industries (SPC)	YES	NO
Windows Metafile (EMF, WMF)	YES	YES
TIFF file (TIF)	YES	YES

<sup>a</sup>. May have limitations. See the appropriate section in the text.

## Bitmap BMP)

Bitmap (BMP) files store raster graphics in an array of individual bits. Bitmap images are the most common format for continuous-tone images. Because they represent a fixed number of pixels, bitmaps are resolution dependent and may appear jagged and lose detail if they are scaled on-screen or printed on a higher resolution printer than they were created for.

## ChemDraw Template (CTP, CTR)

Use the ChemDraw Template file format to save template documents that appear in the template pop-up menu.

## ChemDraw (CDX)

The ChemDraw file format is the native format for ChemDraw version 4.0 and later. This is a public

tagged file format that stores information about a ChemDraw structure in a series of data blocks. This format is designed to be easily generated and interpreted by other programs. This format accurately stores anything that can be drawn in ChemDraw.

*NOTE: Imported drawings saved within a ChemDraw file created using ChemDraw for Macintosh are lost when the file is opened using ChemDraw for Windows. The same applies for objects saved in ChemDraw for Windows and opened on a Macintosh. However, all ChemDraw specific information is preserved.*

*Imported drawings include any graphics pasted into a ChemDraw document from another Macintosh application. They also include Chem3D drawings imported using the Insert Object dialog box or the "Get 3D Model" Edit menu command in ChemDraw for Windows.*

## ChemDraw XML (XML)

The CDXML file format is an interpreted version of cdx that conforms to the XML specification unlike binary cdx format. CDXML is text-based but contains some data. For information about XML in general, see <http://www.xml.org>.

## ChemDraw 3.5 (CHM)

ChemDraw 3.5 file formats are used for saving or opening ChemDraw documents using the version 3.5.x of ChemDraw. These documents can also be opened in versions 3.0, 3.0.1, 3.0.2, and 3.1 of ChemDraw as long as atom properties are not used in the files.

*NOTE: When you save a ChemDraw file in one of these formats, all features specific to later versions are lost. For example, multi-attached atom labels, variable attachment points, and multicenter bonds are not be saved.*

## ChemDraw 2.0 and ChemDraw 2.1 (CHM) Import Only

ChemDraw 2.0 and ChemDraw 2.1 file formats are used for opening ChemDraw documents using the

version 2.x file format of ChemDraw for Macintosh. You cannot save files in these formats.

## ChemDraw Stationery/Style Sheet (CDS)

Use ChemDraw Stationery file format to save document settings and other objects.

### **Pro** Connection Table (CT)

The Connection Table file format is a simple format that saves a list of atom connectivities in terms of an element, serial number, X and Y coordinates, bond order, and bond type. For more information, see "Chemistry File Formats" on page 225

### **Pro** Chemical Markup Language (CML)

CML is an extensible, chemically-aware markup language based on XML. ChemDraw supports both import and export of the format. More information can be found at <http://www.xml-cml.org/> and <http://cml.sourceforge.net>.

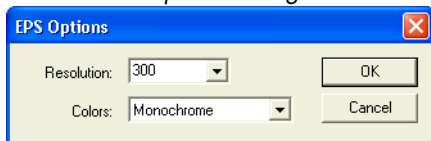
## Encapsulated PostScript (Macintosh) PostScript, EPS (Windows)

Encapsulated PostScript (EPS) files are ASCII text files containing the scalable PostScript representation of a ChemDraw drawing that can be opened using other applications and platforms. There are two types: one containing text only, and one containing a graphic representation of the drawing. The latter are known as Postscript with Preview or Postscript Mac. For text only files, programs that do not support the display of raw PostScript can only print, not view an image on screen.

Use EPS files to share ChemDraw drawings with desktop publishing applications such as Adobe PageMaker and QuarkXPress.

The Options dialog box allows you to select the resolution (in dpi) and color depth of the saved file. The defaults are 300 dpi and Monochrome. For Windows EPS with Preview, there is also a Preview option (default: WMF).

Figure 11.10: EPS Options dialog box.



If you select a color option, all colors are saved in the EPS file except for the Background color. To save an EPS file with a colored background, create a large colored rectangular box using the Drawing Elements tool and choose Send to Back before saving the file. For more information, see “Drawing Boxes” on page 139 and “Multi-Center and Variable Attachments” on page 73. These options only affect embedded images. Objects created in ChemDraw always output at maximum resolution and in full color.

To include correct PostScript font names in Windows EPS files, you must have Adobe Type Manager (ATM) installed. Only ATM fonts are saved in the EPS file.

### Resolution

Available resolutions range from 72 (computer monitor) to 1440 dpi (high resolution output). When choosing a resolution, keep in mind that the size of the file increases as the square of the resolution.

### Color

You can select from the following color options:

- **Monochrome**—Forces all objects to black and white.
- **Grayscale**—Translates colors to shades of gray.
- **24-bit RGB**—Stores colors using computer monitor style of color encoding.

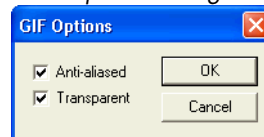
- **32-bit CMYK**—Uses printing press style of color encoding. Groups each color type sequentially. This provides better compression.

## GIF Image (GIF)

Graphics interface format (GIF) is useful for working with the hypertext markup language (HTML) used in displaying information on the World Wide Web. A GIF image can be displayed directly on a Web page rather than having to download the drawing for viewing in a Helper application.

The default GIF format conforms to the GIF 89a specifications with transparent backgrounds. You can change this from the options menu.

Figure 11.11: GIF Options dialog box



## **Pro** ISIS/SKC and ISIS/TGF

You can save a ChemDraw document in an ISIS file format for export to an ISIS application, or import a file created by an ISIS application into ChemDraw.

ChemDraw Pro provides two ISIS file formats:

- **ISIS/Sketch (SKC)**—For saving files as a binary sketch file for transfer to another ISIS application running on the same operating system (this format is used on the Clipboard).
- **ISIS/TGF (\*.tgf)**—For saving as an ASCII text file (a Transportable Graphics File) for transfer to ISIS applications on different platforms.

*NOTE: When transferring between ChemDraw and ISIS/Draw, if information in a file or on the Clipboard contains only non-bond, unsupported objects, the information is*

imported as a WMF (metafile) or PICT graphic. However, if a supported object, such as a bond, is also in the file or on the Clipboard, then only the supported object appears.

*NOTE: Object types in ISIS not supported in ChemDraw, such as polymers, are not transferred. Object types in ChemDraw not supported in ISIS are not transferred. However, in some cases, such as different arrow types, the arrow is converted to the most similar form.*

## **Pro** ISIS/Reactions (RXN)

The ISIS/Reactions format is an MDL-developed format for storing chemical reaction information used by the ISIS family of products and others.

For single step single or multi-line reactions, ChemDraw uses the point of the reaction arrow as the dividing line to determine which molecules in a reaction are reactants and which are products.

*NOTE: You cannot save a reaction with an intermediate step accurately in the RXN file format.*

Molecules whose centers are behind or above the tip of the arrow are considered reactants, and all remaining molecules are products. The reaction arrow can be at any orientation; it does not have to be parallel to the x-axis. If a reaction contains multiple arrows, then the largest arrow is used as the reaction arrow.

Reaction mapping and reaction center information is stored in the RXN output file.

## **Pro** JDX (JDX, DX) Import Only

The Joint Commission on Atomic and Molecular Properties (JCAMP) developed the JDX file format for spectral data. JDX is a public, but not well defined format that has numerous variations. ChemDraw supports many of the more common spectral variations with uniform x-axis spacing.

ChemDraw also supports Bruker NMR JCAMP data, which is saved with a DX file extension

When you import JDX files, they appear in the window with a spectrum of a standard size that can be re-sized by dragging.

You can export spectral data as part of a CDX file only.

## JPEG (JPG, JPEG) Import Only

ChemDraw supports import of digital images compressed with the widely used JPEG (Joint Photographic Experts Group) algorithm. JPEG images are imported as objects, and can be scaled after importing.

## **Pro** MDL MolFile (MOL)

MDL Information Systems, Inc. MolFile (MDL MolFile) file format is used by several other Windows, Macintosh, and UNIX chemical databases and drawing applications such as ISIS/Draw™, ISIS/Base™, MACCST™, and REACCST™.

ChemDraw Pro provides two MDL MolFile formats:

- MDL MolFile (Text)
- MDL MolFile (Mac) for Macintosh only. This file type is saved with an mMol file type and can be saved and opened with ISIS.

MDL MolFile files are ASCII text files that can be created or edited in common word processing applications or text editors. Atom and bond property information is stored in the MolFile.

MDL RGFile (RGF) file format is used by several other chemical databases and drawing applications. The MDL File RGFile supports alternate groups whereas an MDL Molfile cannot. When you save a ChemDraw file that contains alternate groups as an MDL MolFile, it is automatically saved as an MDL RGFile.

## **Pro** Molecular Simulations MolFile (MSM)

Molecular Simulations MolFile format is an ASCII text file used by applications such as ChemNote™. You can save a ChemDraw Pro document in Molecular Simulations MolFile format for export to one of these applications.

*NOTE: ChemDraw uses the file extension “MSM” for Molecular Simulations MolFiles rather than the standard “MOL”, used by Molecular Simulation, Inc. ChemDraw recognizes files with the “MOL” file extension as MDL MolFiles. In addition, the extension “MSI” used in earlier versions of ChemDraw is no longer recognized in ChemDraw. To open Molecular Simulations MolFiles that have a “MOL” or “MSI” extension you must first change the extension to “MSM”.*

## PICT (Macintosh)

PICT files contain a QuickDraw representation of a ChemDraw drawing that can be used by various drawing applications. You can save a ChemDraw document in the PICT format so it can be opened by one of these other applications. The PICT file format contains ChemDraw structural information. PICT files created by earlier versions of ChemDraw can be reopened and edited by ChemDraw version 8.0. However, the pictures contained in PICT files created by versions of CS ChemDraw earlier than version 3.5, or by other applications, are treated as a single, non-editable, imported picture.

All colors are saved in the PICT file except for the Background color.

## PICT scaled 4X (Macintosh)

PICT scaled 4X files are the same as PICT files, except that the drawing is four times larger. When these larger files are placed into certain other applications and shrunk back down to 1/4 size, they

may provide higher quality output than regular PICT files.

## PNG file (PNG)

PNG (Portable Network Graphics) format is an alternative to the GIF format for adding graphics to web pages. You can save, but not open, files in PNG format. The PNG format is fairly new and was designed to address many of the shortcomings of the GIF format. In particular, the PNG file format offers true color images, is less prone to transmission errors and offers a full alpha channel for specifying background or transparency options.

For additional information about PNG visit:

<http://www.boutell.com/boutell/png>

## **Pro** SMD (SMD)

Standard Molecular Data (SMD) file format, version 4.3, is an ASCII text file commonly used by programs that search Chemical Abstracts Databases such as STN Express™. You can save your ChemDraw document in SMD format and use the file for searching in a Chemical Abstracts database.

## **Pro** SPC (SPC) Import Only

The SPC file format was developed by Galactic Industries as part of the GRAMS software, which reads spectral data from every type of spectrometer and converts them to SPC format. SPC is a well-defined, proprietary, but open standard format for spectral data.

ChemDraw imports most one-dimensional spectral SPC formats. When you import an SPC file, it appears in the window with a spectrum of a standard size that can be re-sized by dragging.

You can export spectral data as part of a CDX file only.

## Pro Template Style Sheet (CTS)

The Template Style Sheet file format is used for saving document settings and row and column characteristics for creating ChemDraw Template documents.

## Windows Metafile (WMF)

The Windows Metafile file format saves the Graphic Device Interface (GDI) representation of a ChemDraw drawing. Using the WMF file format you can transfer ChemDraw drawings to other applications, such as Microsoft® Word, that support that WMF file format on the same or different computers rather than using the Clipboard. The WMF file format contains ChemDraw structural information.

## TIFF file (TIF)

TIFF format (Tagged Image File Format) is a high resolution format commonly used for saving graphics for importing into desktop publishing applications on the same or on different computer platforms. TIFF images can be saved using a variety of resolution, color, and compression options. As TIFF images can get rather large, choosing appropriate options is important. The TIFF format is for export only.

### Resolution

Available resolutions range from 72 (computer monitor) to 1440 dpi (high resolution output). When choosing a resolution, keep in mind that the size of the file increases as the square of the resolution.

### Color

You can select from the following color options:

- **Monochrome**—Forces all objects to black and white.

- **RGB Indexed**—Stores colors using computer monitor style of color encoding.
- **CMYK Planar**—Uses printing press style of color encoding. Groups each color type sequentially. This provides better compression. For example: CCCCCC-MMMMMMYYYYYYKKKKK rather than CMYKCMYKCMYKCMYK. This option produces far better compression than using the PackBits compression method. However, many desktop publishing packages do not support CMYK Planar files.
- **CMYK Contiguous**—Uses printing press style of color encoding. Stores colors non-sequentially. For example: CMYKCMYK. The PackBits compression type provides no compression for this type of file.

*NOTE: If objects in your document are black and white they are saved black and white regardless of which Color options you set. If you import drawings from other applications and want them to print Black and White you must set the Color option to Monochrome.*

### Compression

You can select from the following compression options:

- **PackBits**—Used to reduce files size by encoding repeating bytes of information as output when using the CMYK Planar color option. Below is a highly simplified representation of this compression scheme. For a line of color information such as: CCCCCC-MMMMMMYYYYYYKKKKK, the compression yields a smaller file by representing the information as C46M5Y5K.
- **CCITT Group 3**—Used for fax transmissions of images.
- **CCITT Group 4**—Used for fax transmissions of images.

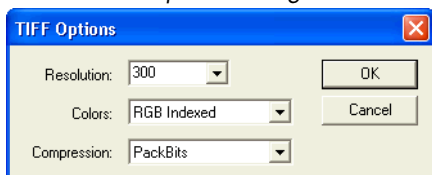
- **Deflate**—Similar to LZW compression. Works well with all Color and Resolution options.

## Setting TIFF options

To set these options:

1. click the **Options** button in the Save dialog box to display the TIFF options dialog box.

Figure 11.12: TIFF Options dialog box



2. Select the options you want and click **OK**.

*NOTE: In the Macintosh version you may want to increase the memory allocated to ChemDraw if you are saving large TIFF files.*

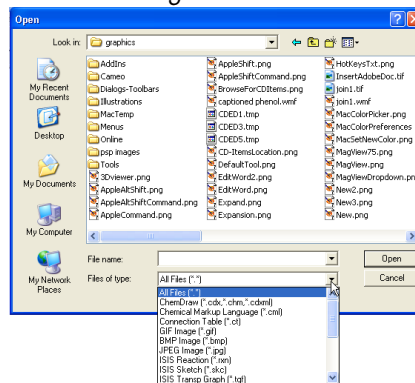
## Inserting Objects from Other Applications

You can insert graphics or documents created in other applications into ChemDraw. You can edit inserted objects using the ChemDraw Edit menu. Inserted objects can be resized or rotated using the resize and rotate handles of a selected object. You cannot flip inserted objects.

To insert a graphic from another application into ChemDraw:

1. Click **Insert File** the Edit menu.
2. In the Open dialog box, select the file type from the drop down menu.

Figure 11.13: Inserting a file into ChemDraw



3. Select the graphic and click **Open**.

The file is embedded into the ChemDraw file.

*NOTE: If you select file type "All files" and choose a file type that ChemDraw does not support (such as TXT) you will get an error message, and the file will not be embedded.*

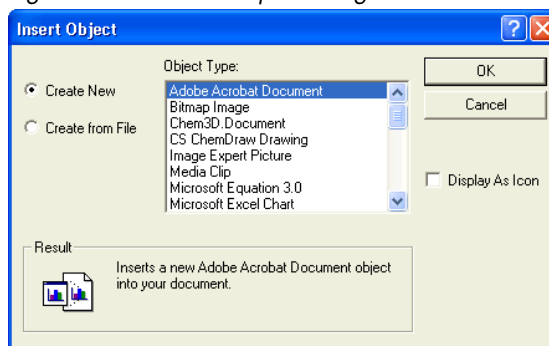
### (Windows only)

To insert an object from another application into ChemDraw:

1. Click the **Insert Object** command on the Edit menu.

The Insert Object dialog box appears.

Figure 11.14: Insert Object dialog box



2. Take the appropriate action:

Table 43: Insert object options

### If you want to ... Then ...

---

create a new object	Click <b>Create New</b> .  Select the <b>Object Type</b> .  Click <b>OK</b> .
insert an existing graphic	Click <b>Create from File</b> .  Type the path or browse to the object to insert.  Click <b>OK</b> .

## Transferring ChemDraw Documents Across Platforms

Use the following procedures to transfer ChemDraw documents across platforms. From the following table, determine the versions of the ChemDraw software between which you want to transfer documents and follow the appropriate instructions.

When you transfer ChemDraw files across platforms, fonts are not transferred. If a font in the transferred document is not available, ChemDraw substitutes fonts for those that are available on the new platform.

### Transferring from Macintosh to Windows

To be able to open a ChemDraw file created on the Macintosh in Windows, follow the instructions

for the appropriate versions shown in the table below.

Table 44: Transferring from Mac to Windows

From Mac Version	To Windows Version	Instructions
≥ 4.0	≥ 4.0	Save as ChemDraw and add .cdx to the file name.
≥ 4.0	3.x	Save as ChemDraw 3.x and add .chm to the file name.
≤ 3.5.x	= 3.x	Save as ChemDraw and add .chm to the file name.

### Transferring from Windows to Macintosh

To be able to open a ChemDraw file created in Windows on the Macintosh, follow the instructions for the appropriate versions shown in the table below.

Table 45: Transferring from Window to Mac

From Windows Version	To Mac Version	Instructions
≥ 4.0	≥ 4.0	Save as the default ChemDraw (.cdx).
≤ 3.5.x	≥ 4.0	Save as ChemDraw 3.x (.chm).



Table 45: Transferring from Window to Mac

≤ 3.5x	≤ 3.x	Save as ChemDraw 3.x (.chm) and follow the instructions in “Transferring files to ChemDraw/Plus 3.1 for the Macintosh” below.
--------	-------	---

### Transferring Files to ChemDraw/Plus 3.1 for the Macintosh

Use the following procedure to transfer a ChemDraw for Windows file to ChemDraw/Plus 3.1 for the Macintosh. A file translator such as PC Exchange or Apple File Exchange must be running on your Macintosh.

To transfer from Windows to ChemDraw/Plus 3.1 for the Macintosh:

1. In ChemDraw for Windows, save the file in the ChemDraw (CHM) format.
2. Insert the disk with the ChemDraw for Windows files into the Mac floppy drive.
3. If you are using PC Exchange, double click the floppy disk icon to display the files.
4. Select **PC Exchange** from the Control Panels.
5. Select **Add**.
6. Change the DOS suffix to **CHM**.
7. In the application selection, find **CSC ChemDraw** on your Mac and click once to highlight the selection.
8. Change the document type to **CHMS**.

If you are using a translator other than PC Exchange, you need to use an editor such as ResEdit or Desktop to change the type and creator of the files being transferred. The type should be “CHMS” and the creator should be “CHMD.”



# Chapter 12: ChemDraw/Excel

The ChemDraw/Excel add-in is an extension of Microsoft<sup>®</sup> Excel<sup>®</sup> for Windows.

ChemDraw/Excel enables you to:

- Add chemical structures and other data from ChemDraw or a ChemFinder database to an Excel spreadsheet.
- Search using the same search features as ChemFinder.
- Perform calculations on chemical structures.

See the ChemOffice manual for information on other CambridgeSoft add-ins for Excel.

*NOTE: Any commands you use operate on the cells, not the pictures in the cells.*

## Setting Up ChemDraw/Excel

When you install *ChemFinder*, ChemDraw/Excel is automatically installed. Before you use ChemDraw/Excel for the first time, do the following:

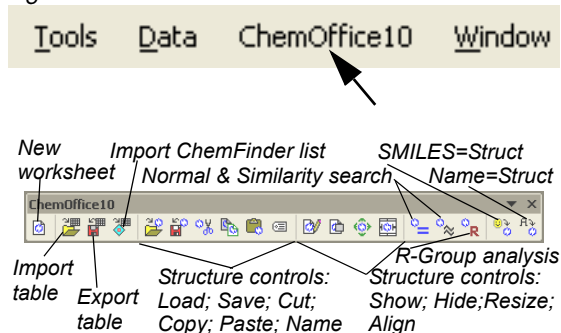
1. Select **Add-Ins** on the Tools menu.

The **Add-Ins** dialog box appears.

2. In the **Add-Ins** dialog box check the **ChemDraw for Excel** checkbox and click **OK**.

A ChemOffice menu is added to the Excel menu bar and a ChemOffice tool bar appears.

Figure 12.15: ChemOffice menu item and toolbar



3. Point to **Macro** on the Tools menu, and select **Security**.


The **Macro Security** dialog box appears.

4. In the **Macro Security** dialog box click the **Security Level** tab and set the security level to **Medium**.

*NOTE: ChemDraw/Excel no longer requires this step. You must set security to Medium only if you will be using ChemDraw/Excel worksheets from version 8 or earlier without conversion.*

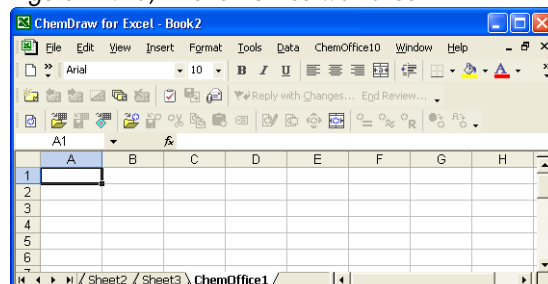
5. Click **OK** to save and exit.

To create a ChemOffice worksheet:

- Select **New ChemOffice Worksheet** on the ChemOffice menu, or click .

A ChemOffice worksheet appears. When a ChemOffice worksheet is active, ChemDraw/Excel appears in the title bar and the ChemDraw tool bar is active.

Figure 12.16: A ChemOffice worksheet



## Importing Tables

ChemDraw/Excel allows you to import from the following sources:


- **MDL SDFfiles**—Imports all records in the file. Each structure is given the name stored in the SDFfile.

- **ChemDraw databases** —Imports all fields stored in the main form. Molecular weight and formula fields are not imported because ChemDraw/Excel calculates them. Each structure is named Structure <*n*>, where *n* is a unique number.

*NOTE: In order to import CFW files into Excel, make sure you save them with the “allow CAL/OLE Automation access” security setting checked. See “Setting Security Options” in Chapter 3 of the ChemFinder manual for details.*

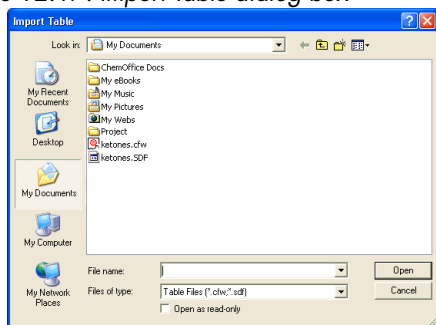
When you import a table, structure data are transformed into structure drawings in the first column, and all other fields are imported in separate columns.

To import a table:

1. Select the cell where you want the import to start. The upper left corner of the import is at this cell. Data is filled down and to the right.
2. Select **Import Table** on the ChemOffice menu, or click .

The Import Table dialog box appears.

Figure 12.17: Import Table dialog box



3. Type or select the file name to import and click **Open**.

All records are added to your spreadsheet.

## Converting and Upgrading

Instead of copying and pasting information from a non-ChemDraw/Excel worksheet, you can convert the existing worksheet into a ChemDraw/Excel worksheet.

To convert a worksheet:

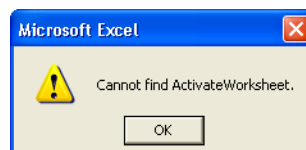
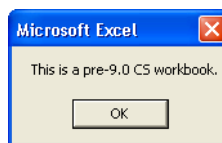
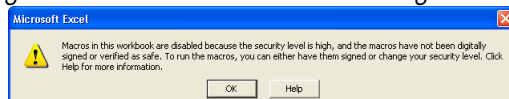
Select **Convert Worksheet** from the ChemOffice menu.

The work sheet is converted to a ChemDraw/Excel worksheet.

## Upgrading Workbooks

ChemDraw/Excel 9.0 improvements made workbooks created with older versions incompatible. You can open and maintain old workbook formats, but you may get error messages (depending on your Excel security settings) and will be asked if you want to upgrade each time you open them.

Figure 12.18: Version and macro warnings



To upgrade a workbook:

1. Point to **Macro** on the Tools menu, and select **Security**.
2. Click the **Trusted Sources** tab and make sure that CambridgeSoft Corporation is listed as a trusted source. Make sure the **Trust access to Visual Basic Project** checkbox is selected.
3. Select **Upgrade Workbook** from the ChemOffice menu.
4. To maintain tight security, go back to the **Macro Security** dialog box and deselect the **Trust access to Visual Basic Project** checkbox.


## Importing Hit Lists

You can perform a search in ChemFinder and then import the hit list structures with data into Excel using the Import ChemFinder List command.

To use the Import ChemFinder List command, ChemFinder must be open with a hit list present.

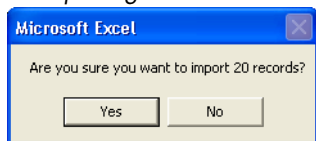
### Importing a Hit list

To import a hit list:

1. Select **Import ChemFinder List** on the ChemOffice menu, or click the  icon.

A message box similar to the one in *Figure 12.19* appears:

Figure 12.19: Importing a ChemFinder hit list



2. Click **Yes** to import the hit list.

The records are imported into Excel, starting with the currently selected cell and moving down and to the right.

### Error Messages

If all conditions required to use the Import ChemFinder List command are not met, one of the following error messages may appear.

#### **ChemFinder is not running, would you like to start it up?**


ChemFinder is not running. Do the following:

1. Click **Yes**.

The message “After loading your desired database and performing your search, return to Excel and redo the operation.” appears.

2. Click **OK**.

ChemFinder opens.


3. Open a database and perform a search.
4. Return to Excel and from the ChemOffice menu, select **Import ChemFinder List**, or click .

#### **No database loaded in ChemFinder. Load a database and perform your search. Then return to Excel and redo the operation.**

ChemFinder is running, but no database is loaded. Do the following:

1. Click **OK**.


ChemFinder moves to the front.

2. Open a database and perform a search.
3. Return to Excel and from the ChemOffice menu, select **Import ChemFinder List**, or click .

#### **Form has no database or hit list has no records. Load a database and perform your search. Then return to Excel and redo the operation.**

4. Click **OK**.

ChemFinder moves to the front.

5. Open a database and perform a search.
6. Return to Excel and from the ChemOffice menu, select **Import ChemFinder List**, or click .

## Exporting Tables

ChemDraw/Excel allows you to export tables to MDL SDFfiles.

Selected cells are exported to a specified file. If no cells are selected, the entire spreadsheet is exported. The first column of the area to export must have the word “**Structure**” in its top cell. Structures outside the first column will be discarded.

Figure 12.20: Selecting cells for export


	A	B	C	D	E
1	STRUCTURE	MOL_ID	FORMULA	MOLWEIGHT	MOLNAME
2	Structure1	1	C10H16O	152.2358	Camphor
3	Structure2	2	C6H10O	98.1444	Cyclohexano
4	Structure3	3	C13H10O	182.2214	Benzophenon

To export data:

1. Select the information to export:

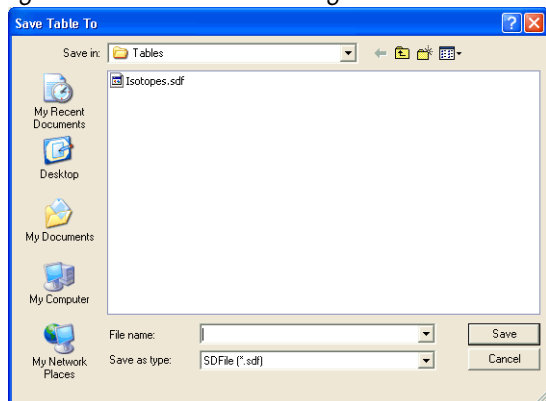
Table 12 - 1: Selecting the area to export

If you want to export	Then
a specified area of your spreadsheet	Select the area to export.
the entire spreadsheet	Do not make any selection.

2. Select **Export Table** on the ChemOffice menu, or click .

The **Save Table To** dialog box appears.

Figure 12.21: Save Table dialog box



3. Type the file name and click **Save**.

The table is saved to the specified file.

## Adding Structures

You can add chemical structures from any file format supported by ChemDraw to a spreadsheet. The names of added structures are retained. If the structure does not have a name, ChemDraw assigns the name: Structure <*n*>, where *n* is a number unique to the worksheet.

### Adding Structures with ChemDraw

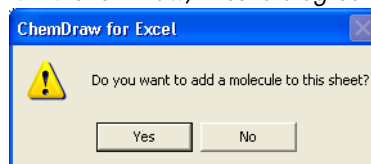
The most direct way to insert a new structure into a cell is by using ChemDraw.

To add a structure with ChemDraw:

1. Double-click in a cell.

The ChemDraw/Excel dialog box appears:

Figure 12.22: ChemDraw/Excel dialog box



2. Click **Yes**.


ChemDraw opens.

3. Draw the structure in ChemDraw.
4. Click **Close and Return to New Molecule** on the ChemDraw File menu.

The new structure appears in the cell.

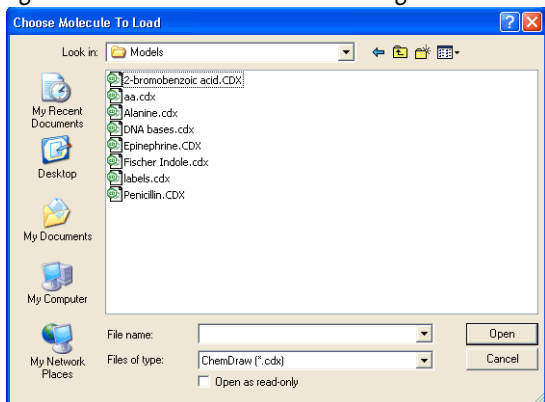
### Adding a Structure From a File

To add a structure from a file:

1. Select the cell into which you want to add the structure.
2. Select **Load Molecule** on the ChemOffice menu, or click .

The **Choose Molecule to Load** dialog box appears.

Figure 12.23: Choose Molecule dialog box



*NOTE: You can use the sample molecule file, "SAMPLE.cdx" contained in the ChemDraw system directory, or any CDX file to load.*

3. Type the file name of the structure to add and click **Open**.

The information is stored in the selected cell.


## Adding a Structure with a SMILES String


You can insert SMILES strings into cells and convert them to structures.

To insert SMILES strings:

1. Type or paste SMILES strings into cells.
2. Select the range of cells or single cell to convert.

*NOTE: If you want to keep the original text, copy it and paste it elsewhere.*

3. Select **Convert SMILES To Molecule** on the ChemOffice menu, or click .

If the cell contains a valid SMILES string, it is replaced by a structure. The cell will display a text string starting with "Structure" and followed by a number. To display the structure, click the **Show Picture**  icon.


If the cell did not contain a valid SMILES string, the string remains.

## Adding Structures by Name

You can type or paste the names of chemicals into cells and convert them into structures as follows:

1. Enter the names into cells.
2. Select the range of cells to convert.


*NOTE: If you want to keep the original text, copy it and paste it elsewhere. Note that this command can also convert names generated from Excel formulas.*

3. Select **Convert Name To Molecule** on the ChemOffice menu, or click .

If the cell contains a name supported by ChemDraw *Name=Struct*, the structure corresponding to that name is added to the cell, with the given name as the name of the cell. To show the structure, select the cell and choose **Show Picture** from the ChemOffice menu. For more information about *Name=Struct*, see the ChemDraw User's Guide.

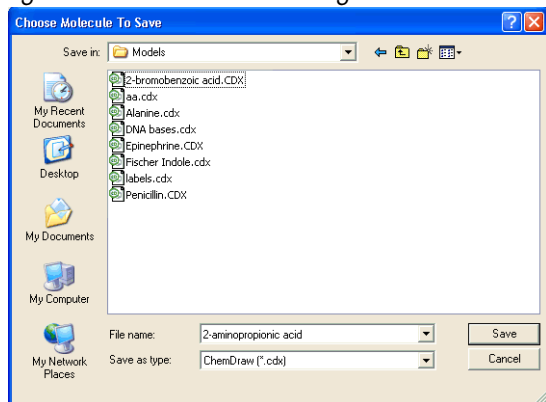
## Saving Structures

You can save a chemical structure to a separate file.

1. In the spreadsheet, select the cell containing the structure.
2. Select **Save Molecule** on the ChemOffice menu, or click .

The **Save to File** dialog box appears.

Figure 12.24: Save to File dialog box



3. Select an existing file or enter a new file name, and click **Save**.

The structure is saved with the name and in the location you selected.

## Searching


You can perform the same types of searches in ChemDraw/Excel as you can in *ChemFinder*:

- Exact structure searching
- Substructure searching
- Similarity searching

## Filter Tables

Filter tables allows you to search for exact structures and substructures.

To perform a structure search:

1. Select a cell in the data table.
2. Select **Filter Table** on the ChemOffice menu, or click .

The **Search Query** dialog box appears.

3. Select the search options:

Table 13: Search options

### If you want Then to

search for a structure	<ol style="list-style-type: none"> <li>1. To load a structure, right-click and select <b>Read Structure</b>.</li> <li>2. To edit the structure, double-click it.</li> <li>3. Select the <b>Search Type</b>.</li> <li>4. Select the <b>Filter Type</b>.</li> </ol>
search for a formula	<ol style="list-style-type: none"> <li>1. Type the molecular formula or formula query in the And/Or Formula Query box.</li> <li>2. select <b>Clear</b>.</li> </ol>
search for a structure and a formula	<ol style="list-style-type: none"> <li>1. To edit the structure, double-click it.</li> <li>2. Select the <b>Search Type</b>.</li> <li>3. Select the <b>Filter Type</b>.</li> <li>4. Type the molecular formula in the And/Or Formula Query box.</li> </ol>
see the R-Group Analysis	click the <b>Show R-Group Analysis</b> box.
see the previous query	click <b>Restore Previous Query</b> .
	<ol style="list-style-type: none"> <li>5. Click <b>Search</b>.</li> </ol>




The hit list is displayed in a column named Match. Items matching the search criteria are labeled as TRUE.

## Similarity Searches

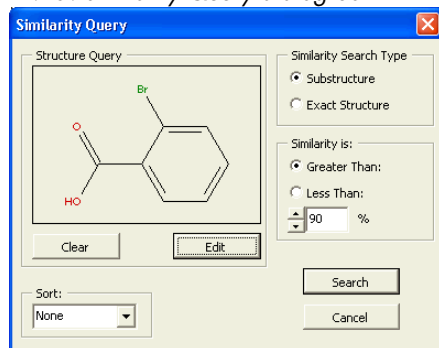
You can perform similarity searches to find structures with features corresponding to your search structure. For more information about similarity searching, see the *ChemFinder* User's Guide.

To search for similarity:

1. Select a cell containing the label **Structure**.
2. Select **Similarity Table** on the ChemOffice menu, or click .

The **Similarity Query** dialog box appears.

Figure 12.25: Similarity Query dialog box



3. Select the **Search Type**.
4. Select the **Similarity Is** value.
5. Select the **Sort** order.
6. Click **Search**.

The hit list is displayed in a column named Match. Items matching the search criteria are labeled as TRUE.


## Working with Structures

ChemDraw/Excel allows you to rename structures and use the clipboard to cut, copy, and paste structures.

## Naming Structures

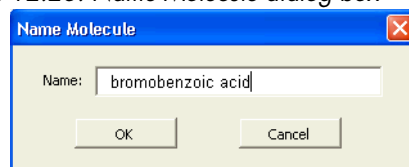
Excel recognizes certain characters as formulas. To prevent the system from interpreting a chemical structure name as an Excel formula, you can rename a structure.

To name a structure:

1. Select the structure.
2. Select **Name Molecule** on the ChemOffice menu, or click .

The **Name Molecule** dialog box appears.

Figure 12.26: Name Molecule dialog box




3. Type the name and click **OK**.

## Using the Clipboard


You can cut, copy, and paste structures using the clipboard. After you cut or copy a structure, it is placed on the clipboard. You can then paste it into another cell or another application.

To cut a structure from a cell:

1. Select the structure.
2. Select **Cut Molecule** on the ChemOffice menu, or click .

The structure is removed from the cell and is placed on the clipboard.

To copy a structure from a cell:

1. Select the structure.
2. Select **Copy Molecule** on the ChemOffice menu, or click .

The structure remains in the cell and a copy is placed on the clipboard.

To paste a structure:

1. Select the area into which you want to paste the structure.

2. Select **Paste Molecule** on the ChemOffice menu, or click .


The structure is pasted from the clipboard.

## Viewing Structures

ChemDraw/Excel allows you to select whether or not to display structures in a cell. You can also adjust the height and width of cells to display their entire contents.


## Showing and Hiding Structures

To show structures:

1. Select the cells in which you want to display pictures.
2. Select **Show Picture** on the ChemOffice menu, or click .

The structures are displayed in the selected cells.

To hide structures:


1. Select the cells in which you do not want to display pictures.
2. Select **Hide Picture** on the ChemOffice menu, or click .

The structures are hidden and the cells resize.

## Aligning Structures

A structure may fall outside the boundaries of its cell because it is too big or because it is improperly positioned within the cell. Use the **Align All Pictures** command to enlarge the cell or reposition the structure. If the entire structure is within the cell, regardless of its position, it is not affected by the **Align All Pictures**.

To align structures:

Select **Align Pictures** on the ChemOffice menu, or click .

The cells adjust to display their entire contents.

## Resizing Structures


To resize pictures use the **Resize Picture** command.

*NOTE: When pictures are resized larger than their cells, use **Align Pictures** to enlarge the cells. **Align Pictures** does not make cells smaller.*

To resize pictures:

1. Select the chemistry cells whose pictures you want to resize.

It is not necessary to only select chemistry cells. Non-chemical cells or chemical cells without pictures will be ignored.

2. Select **Resize Picture** on the ChemOffice menu, or click .

Resize handles appear on the selected structures.

3. Click-drag the resize handles to resize a picture. Any changes you make to a picture is proportionately reflected in the other pictures.
4. To end resizing, click a cell and the pictures are deselected.

## Resizing Structures With a Macro

To resize a large number of structures simultaneously, create the following macro:

```
CFXL.xls!CFxlDoSelectPicture
```

and assign it to an Excel button or menu item.

Then do the following:

1. Select the cells to be resized.
2. Run the macro.
3. Resize one structure.

All of the selected structures resize by the same amount.

4. Select the Structure column and align (see “Aligning Structures” on page 188).

For more information on creating and storing macros, see Excel Help.

## Using ChemDraw/Excel Functions

ChemDraw/Excel supplies nine functions that return information about chemistry objects in a specified cell. Seven of these functions take only one argument—the cell to which the function refers. The remaining two functions may also take a string as an optional second argument.

The function ISSTRUCTURE is an example of a function that takes only one argument. To determine whether the content of cell A1 in an Excel spreadsheet is a ChemDraw/Excel chemistry object, you type =ISSTRUCTURE(A1) into a second cell. The second cell then displays TRUE or FALSE depending on whether A1 contains a chemistry object.

The function CHEM.COMPOSITION is one of the functions that may take an optional second argument. It works in one of two ways:

### With First Argument Only—

Without the second argument, it displays elemental composition by weight percent of the entire chemical structure in cell A1 when you type =CHEM.COMPOSITION(A1) into a second cell. For benzene, it displays C, 92.26; H, 7.74.

**With Both Arguments—**The second argument lets you find the percent composition of a single element in the structure. Typing =CHEM.COMPOSITION(A1, "C") returns the weight percent of carbon in the structure. For benzene it would display 0.922582. Notice that the display format for a single element is different from that of the whole structure.

Table 14 outlines the ChemDraw/Excel functions. Only CHEM.COMPOSITION and CHEM.NUM.ATOMS take an optional second

argument. The others only take the reference cell argument.

Table 14: ChemDraw/Excel functions

Function	Action
ISSTRUCTURE	Returns TRUE if cell referred to is any ChemDraw/Excel chemistry object including reactions; otherwise it returns FALSE.
ISREACCTION	Returns TRUE if cell reference is any ChemDraw/Excel chemistry object <u>and</u> reaction; otherwise it returns FALSE.
CHEM.FORMULA	Returns formula for structure in cell reference; it returns #N/A error if cell doesn't contain a ChemDraw structure.
CHEM.MOLWEIGHT	Returns molecular weight for structure in cell reference. Returns #N/A error if cell doesn't contain ChemDraw structure.

Table 14: ChemDraw/Excel functions

Function	Action
CHEM.NUM. HBACCEPTORS	Returns number of hydrogen bond acceptors based on topology. Returns <b>#N/A</b> error if cell doesn't contain ChemDraw structure.
CHEM.NUM. HBDONORS	Returns number of hydrogen bond donors based on topology. Returns <b>#N/A</b> error if cell doesn't contain a structure.
CHEM.SMILES	Returns SMILES string for structure. Returns <b>#N/A</b> error if cell doesn't contain ChemDraw structure.

Table 14: ChemDraw/Excel functions

Function	Action
CHEM.COMPOSITION	Returns elemental percent by weight for all elements in structure unless optional second argument specifies a single element symbol as a string. In this case the elemental percent is expressed as a decimal number between 0 and 1. (75.1% would be 0.751) Returns <b>#N/A</b> error if the cell referenced in first argument doesn't contain a ChemDraw structure, or if second argument is not a valid element symbol.
CHEM.NUM.ATOMS	Returns total number of atoms in the structure unless optional second argument specifies a single element symbol as a string. In this case, it returns the number of atoms of that element only. Returns <b>#N/A</b> error if the cell referenced in first argument doesn't contain a ChemDraw structure or if second argument is not a valid element symbol.

## Using ChemProp Functions

If you are using ChemDraw Pro or Ultra with the ChemProp add-on installed, you can calculate physical and thermodynamic properties in ChemDraw/Excel. For detailed information on the properties calculated and how ChemProp calculates them, see “Viewing Chemical Properties” on page 115 and Appendix E “How ChemProp Works.”

### ChemProp Properties

In ChemDraw/Excel, you can use the ChemProp functions to calculate the following properties:

Table 15: ChemProp functions

Property	Function
LogP (Ultra only)	CHEMPROP.LOGP
Molar Refractivity (Ultra only)	CHEMPROP.MR
Henry's Law Constant	CHEMPROP.HENRY.LAW.CONSTANT
Boiling Point	CHEMPROP.BOILING
Freezing Temperature	CHEMPROP.FREEZING
Critical Temperature	CHEMPROP.CRITICAL.TEMP
Critical Pressure	CHEMPROP.CRITICAL.PRESSURE
Critical Volume	CHEMPROP.CRITICAL.VOLUME

Table 15: ChemProp functions

Property	Function
Heat of Formation	CHEMPROP.HOF
Gibbs Free Energy	CHEMPROP.GIBBS
Ideal Gas Thermal Capacity	CHEMPROP.IDEAL.GAS
tPSA	CHEMPROP.TPSA

*NOTE: Using ChemProp requires that you have a version of ChemDraw that includes ChemProp installed.*

### Inserting Functions

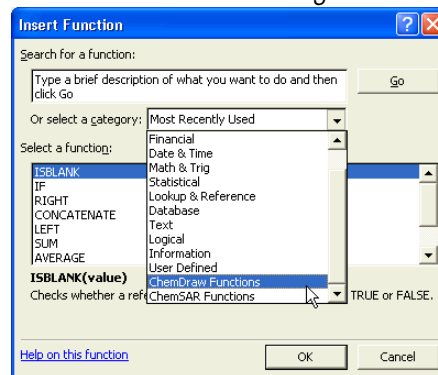
To insert a ChemDraw/Excel function into your worksheet:

1. Select an empty cell.
2. Select **Function** on the Insert menu.

The **Paste Functions** dialog box appears.

3. Select **ChemDraw Functions**.

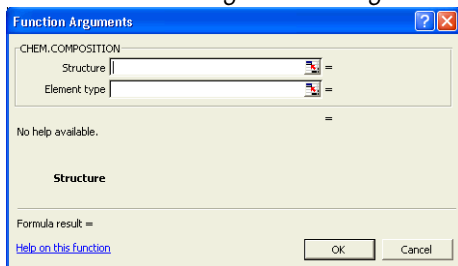
Figure 12.27: Paste Functions dialog box



4. Select the function to insert from the list and click **OK**.

A dialog box appears.

Figure 12.28: Function arguments dialog box



5. Enter the structure cell reference for which you want to calculate properties in the **Structure** box.

6. If the function takes a second argument, enter it in the **Element type** box. Element type arguments are optional.

7. Click **OK**.

Each property is calculated using the “best available” method. For more information about calculation methods, see the ChemDraw manual. If the cell reference argument does not point to a valid structure cell, #N/A appears in the cell.

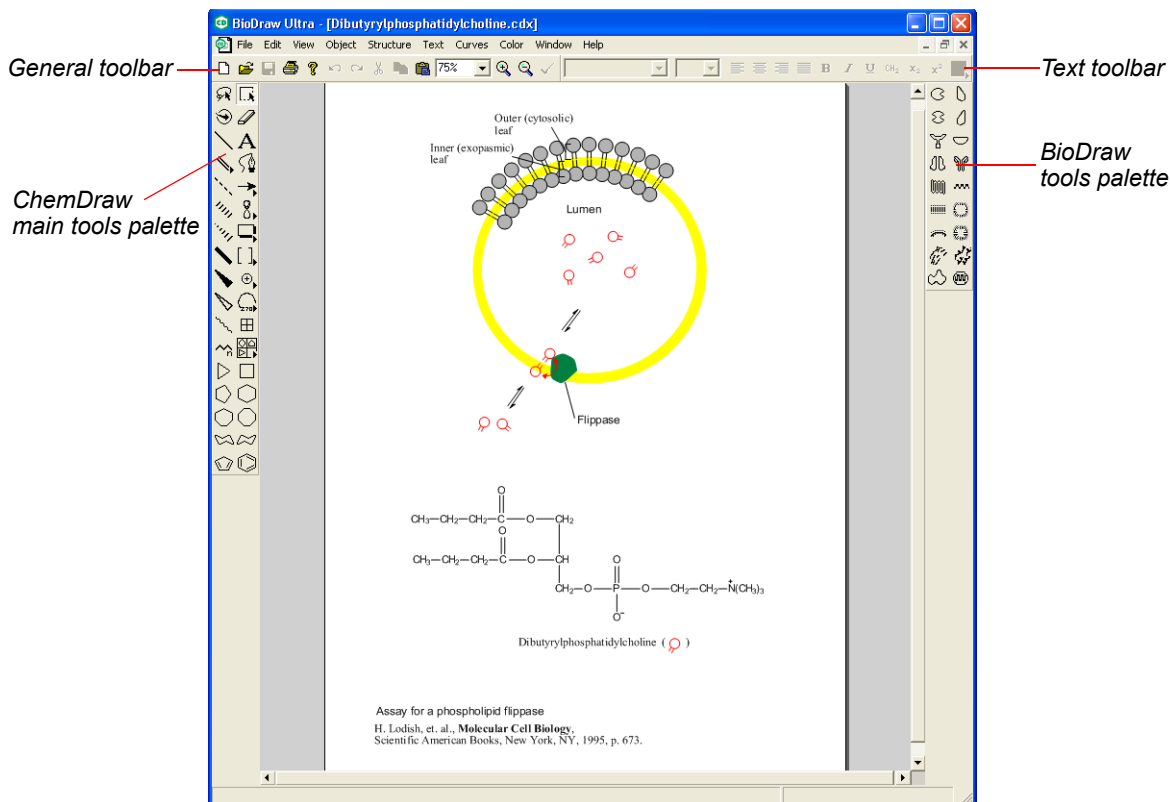
# Chapter 13: BioDraw

## Overview

BioDraw tools are drawing objects. Before reading this section, users should familiarize themselves with the general behavior of ChemDraw drawing tools by reading Chapter 9, “Drawing Objects” on

page 131. Pay particular attention to “The Arrow Tools Palette” on page 136, and “The Drawing Elements Tools Palette” on page 138, as you will want to use those tools in your BioDraw pathways.

Figure 13.29: The BioDraw Ultra GUI



## The BioDraw Tools Palette

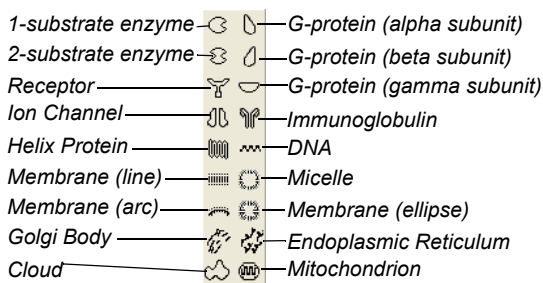
The BioDraw tools palette contains tools to draw metabolic pathways, such as enzymes and receptors. Standard shapes, such as circles, ellipses, and arrows, can be added from the Drawing Elements tool palette or the Arrows tool palette. You can also use the Pen tool to create custom shapes.

As with ChemDraw Drawing Elements, you can change the color of an object with the **Color** menu, and the line and fill properties with the **Curves** menu. You can also rotate, or change the size, after selecting it. In general, anything you can do with a ChemDraw drawing object you can do with a BioDraw object as well. We would, however caution care in the use of shading (“Shaded Style” on page

144). The effect of shading applied to irregularly shaped objects such as receptors is unpredictable, and generally quite unaesthetic.

You create a BioDraw object by either clicking or dragging on the page where you want it to appear. Clicking gives you the default size and shape, dragging allows you not only to enlarge the object, but to distort it as well by dragging differently on the x and y axes. Linear objects elongate in the direction they are dragged. The membrane and protein tools (DNA and Helix) add more subunits as they are dragged and display the subunit count.

Figure 13.30: BioDraw Toolbar



## Customizable Objects

Some of the BioDraw objects can be customized after being created. Table 16 describes the customization options. When customizing a BioDraw object, you must use the same tool used to create it, or a selection tool.

Table 16: Customizable BioDraw Objects



Tool	Customization Options
1-Substrate Enzyme 	size of the enzyme “mouth”
Receptor 	width

Table 16: Customizable BioDraw Objects








Tool	Customization Options
G-protein, gamma subunit 	shape
Helix Protein 	height, width of the strands, width of the cylinders, spacing
DNA 	height, width of the strands, offset of the second strand, spacing
Membrane (line) 	size of subunit (The overall length remains constant, and the number of subunits changes in inverse proportion to the size.)
Membrane (arc) 	length, arc, size of subunit
Membrane (ellipse) 	size of subunit
Micelle (ellipse) 	size of subunit

Table 17: Tools that are not customizable









2-Substrate Enzyme 	G-protein, alpha subunit 
Ion channel 	G-protein, beta subunit 
Immunoglobulin 	Golgi body 



Table 17: Tools that are not customizable

Endoplasmic reticulum 

Mitochondrion 

Cloud 

## Drawing a Membrane Line

To create a membrane line:

1. Select the membrane line tool.
2. Drag in the work space.

---

*TIP: You may also click to draw the default size.*

---

When orienting the membrane, note that if the **Fixed Angles** option on the Object menu is selected, you are constrained to 15 degree increments. You can override the default by holding down the **Alt** or **option** key as you drag.

The membrane line has a single adjustment handle. When you place the cursor over the handle, it turns into a double-sided arrow. Dragging the handle to the right increases the size of each subunit of the membrane; dragging to the left decreases the size of each subunit. When you change the subunit size, the length of the membrane stays constant.

Figure 13.31: Adjustment cursor

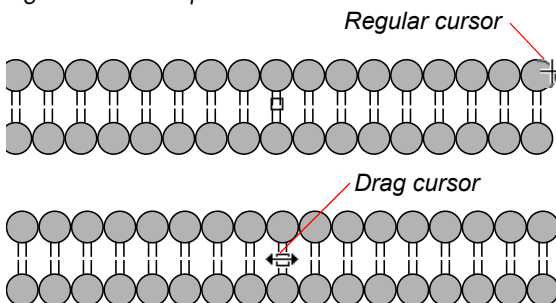
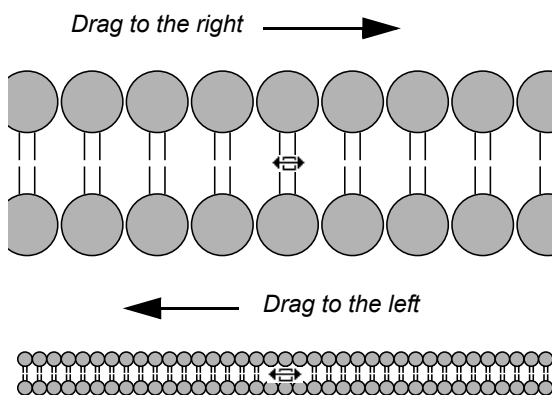


Figure 13.32: Changing the membrane size

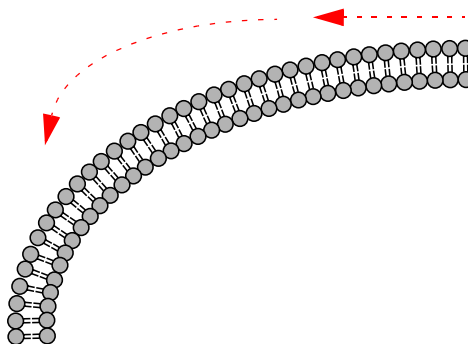


*TIP: To change the length of the membrane, select it and drag the left or right handle of the selection box. You may then deselect it and readjust the subunit size.*

## Drawing a Membrane Arc

Creating a membrane arc is similar to creating a membrane line. Begin by dragging in a straight line, then drag in a curve.

Figure 13.33: Creating a membrane arc



The membrane arc tool has three adjustment handles:

- the handle at the starting point controls the length
- the center handle controls the subunit size
- the handle at the leading edge controls the arc

## Drawing a Helix Protein

To create a helix protein:

1. Select the Helix Protein tool.
2. Drag in the work space.

---

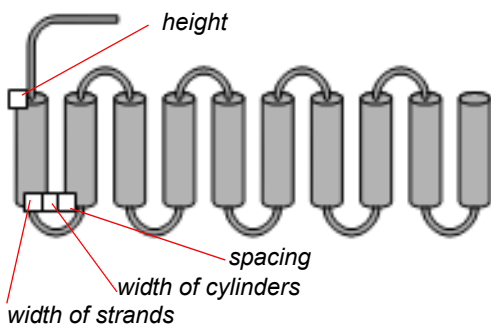
*TIP: You may also click to draw the default size.*

---

When orienting the protein, note that if the **Fixed Angles** option on the Object menu is selected, you are constrained to 15 degree increments. You can override the default by holding down the **Alt** or **option** key as you drag.

The helix protein has four adjustment handles: height, width of the strands, width of the cylinders, and spacing.

Figure 13.34: Helix protein adjustment handles



## Drawing a DNA Molecule

To create a DNA molecule:

1. Select the DNA tool.
2. Drag in the work space.

---

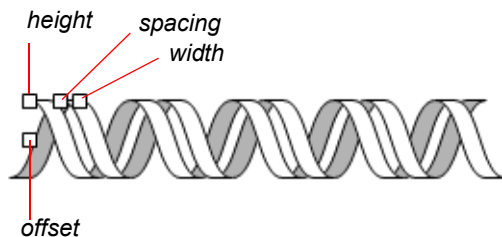
*TIP: You may also click to draw the default size.*

---

When orienting the DNA, note that if the **Fixed Angles** option on the Object menu is selected, you are constrained to 15 degree increments. You can override the default by holding down the **Alt** or **option** key as you drag.

DNA has four adjustment handles: height, width of the strands, offset of the second strand, and spacing.

Figure 13.35: DNA adjustment handles



# Appendix A: Customizing ChemDraw

## Overview

You can customize ChemDraw by configuring Preferences and Document Settings.

Preferences allow you to change the default behavior of certain options that apply to every open document. Document Settings allow you to change the default behavior of options that will affect only the active document.

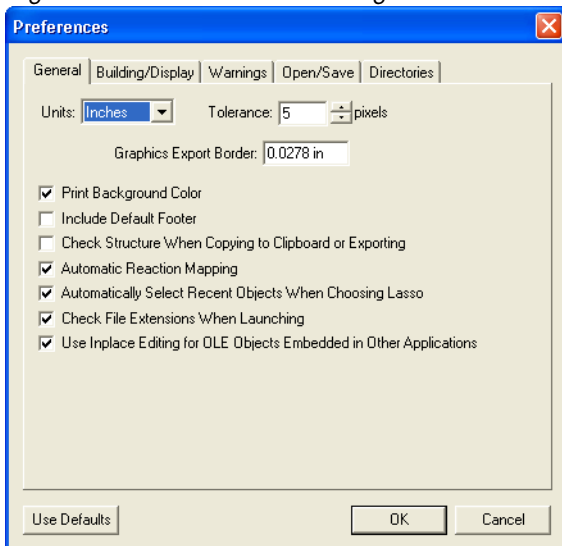
## Setting Preferences

Preferences affect the way the ChemDraw application works, regardless of the document with which you are working.

To open the Preferences dialog box click **Preferences** on the File menu.

The Preferences dialog box appears:

Figure A.36: The Preferences dialog box



To restore the CambridgeSoft default settings, click the **Use Defaults** button.

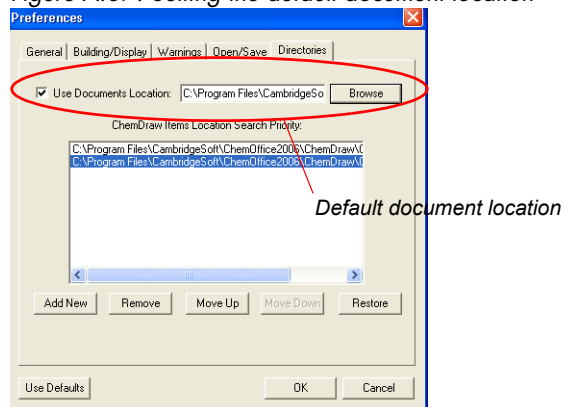
## Setting the Default Document Location

You can set what file location is shown in the Open dialog box by using the Preferences dialog box.

To set the default location:

1. Click **Preferences** on the File menu.  
The Preferences dialog box appears.
2. Click the **Directories** tab.
3. Click the checkbox next to **Use Documents Location** and type in or browse to the location to use.

Figure A.37: Setting the default document location



If **Use Documents Location** is not selected, the first time you use the Open dialog box your **My Documents** folder is shown. Subsequent uses show the last directory used.

## Setting the Default Open File Format

You can set what file format is selected by default in the Open dialog box.

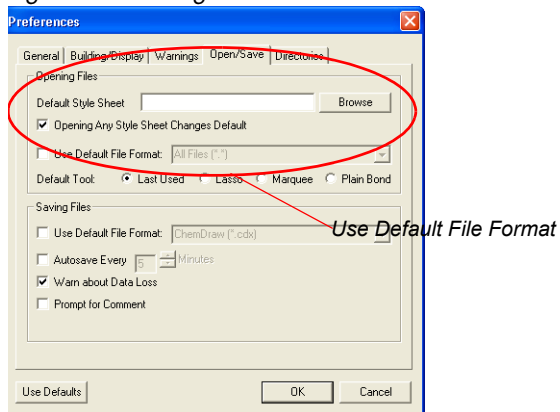
To set the default file format:

1. Click **Preferences** on the File menu.

The Preferences dialog box appears.

2. Click **Open/Save**.
3. Click **Use Default File Format** in the **Opening Files** section, and choose the format you want from the list

Figure A.38: Using default file format.



If **Use Default File Format** is not selected, the first time you use the Open dialog box the ChemDraw format is shown. Subsequent uses show the last format used.

## Setting the Default Tool

Use the Preferences dialog box to set which tool is automatically selected when you open documents.

To set the default tool:

1. Click **Preferences** on the File menu.  
The Preferences dialog box appears.
2. Click the **Open/Save** tab.
3. In the section labeled **Opening Files**, click the **Default Tool** to be automatically selected when you open a document.

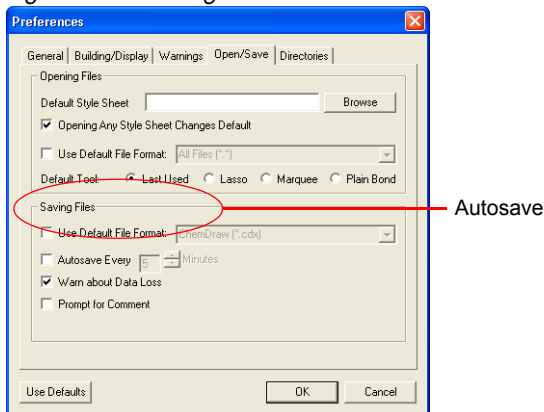
## Saving Changes Automatically

You can configure ChemDraw to save changes to a document automatically at the time interval you set.

To set the frequency at which ChemDraw automatically saves your changes:

1. Click **Preferences** on the File menu.  
The Preferences dialog box appears.
2. Click **Open/Save**.
3. Click the checkbox next to **Autosave Every** and type or select the minutes to use.

Figure A.39: Setting Autosave



The time starts counting down after the first change is made.

## Undoing Actions

To undo the last action performed, click the **Undo** command on the Edit menu,

The last action performed is reversed. The Redo command changes to reflect the undone action. The Undo command changes to reflect the next action you can undo.

For example, if you draw cyclohexane, create an atom label text box, type a label, and select and rotate the structure, you will be able to remove the actions as follows:

1. Remove the rotation.
2. Remove atom label.
3. Remove the ring.

At each step, the text of the Undo command indicates the action being removed.

## Redoing Actions

When you undo an action, the Redo command becomes active so you can reverse the effect of the Undo command.

To redo the last action undone, click the **Redo** command on the Edit menu.

The last action undone is reinstated. The Undo command changes to reflect that action. The Redo command changes to reflect the next action that can be redone.

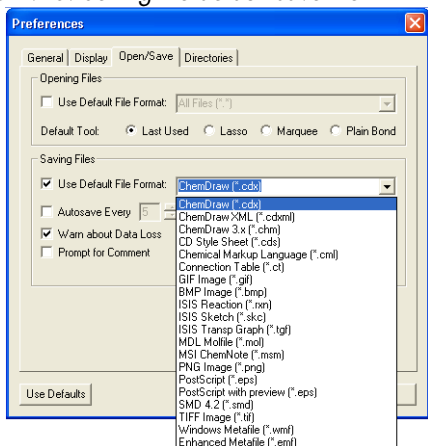
## Setting the Default Save File Format

You can set what file format is selected by default in the Save As dialog box.

To set the default file format:

1. Click **Preferences** on the File menu.  
The Preferences dialog box appears.
2. Click **Open/Save**.
3. Click the checkbox next to **Use Default File Format** in the **Saving Files** section, and choose the format you want from the list.

Figure A.40: Setting the default save file



If **Use Default File Format** is not selected, the first time you use the Save dialog box, the ChemDraw format is shown.

## Creating a New Line and Closing Text Boxes

The default way to create a new line in a caption text box is with the **Enter** or **return** key. The default way to create a new line in an atom label is with **Alt+Enter** or **option+return**. To close the text box, click outside the text box or select another tool.

To change the default do the following:

1. Click **Preferences** on the File menu.

---

*TIP: In Mac OS X, the Preferences dialog box is found on the ChemDraw menu.*

---

2. Choose the appropriate option on the **General** tab:

Table 18: Setting new line options

### To change the default for ...

---

Atom Label text	Require <b>Alt+Enter</b> or <b>Option+Return</b> to Create New Line in Atom Labels.
-----------------	---

Caption text	Require <b>Alt+Enter</b> or <b>Option+Return</b> to Create New Line in Captions.
--------------	--

3. Click **OK**.

## Using Bitmap Fonts When Available (Macintosh)

When text appears in a document on the screen, it can appear using either a bitmap or a TrueType font.

To use bitmap fonts if they are available:

1. Click **Preferences** on the File menu.
2. Select **Use Bitmap Fonts When Available**.

Text drawn using Bitmap fonts looks better and appears more quickly than text drawn using True-Type fonts. However, the size and position of text drawn using Bitmap fonts change somewhat when printed.

For accurate correspondence between what you see on the screen and what is printed, deselect **Use Bitmap Fonts When Available**.

This change affects all documents.

## Setting the Highlight Box Tolerance

You determine the size of the highlight box and how close you must get to activate an object by setting the Tolerance. The standard setting for the Tolerance is 5 pixels. At this setting, the highlight box appears on bonds if the pointer is located 5 pixels or less from any point on the bond.

To set the Tolerance:

1. Click **Preferences** on the File menu.
2. Select or type the tolerance.

This change affects all documents.

## The ChemDraw Items Folder

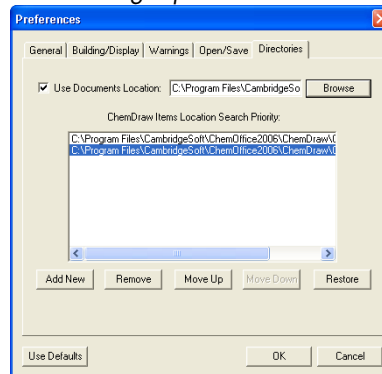
The ChemDraw Items Folder is located by default in the same folder as your ChemDraw application. It contains the ChemDraw preferences, hotkeys, nicknames, and isotopes files; scripts, and the generic nicknames file. It also contains template documents and template Stationery Pads. You can have multiple ChemDraw Items folders. This is useful in corporate installations for maintaining personal files such as nicknames as well as standard templates.

To add a path to a ChemDraw Items folder:

1. Click **Preferences** on the File menu.  
The Preferences dialog box appears.
2. Click the **Directories** tab.
3. Click the **Add New** button, browse to a location, and click **OK**.

A new path is added to the list.

Figure A.41: Adding a path to ChemDraw Items



4. To rearrange the search order, use the **Move Up** and **Move Down** buttons.
5. To delete a path, click the **Remove** button. To delete all added paths, click the **Default Paths** button.

## Accessing Documents Quickly

You can access ChemDraw documents quickly by placing them in the ChemDraw Items folder and then selecting them from the **Open Special** menu.

You can access open documents quickly by using the **Window** menu.

## The Open Special Submenu

To select documents from the ChemDraw Items folder, point to **Open Special** on the File menu and select the file to open.

The **Open Special** submenu, listing documents stored in the ChemDraw Items folder, appears.

## Document and Object Settings

Document and object settings are user-definable settings that are applied to the current document. Settings include:

- Drawing settings—set drawing options such as the fixed length used to draw bonds
- Caption and label text settings—set text options such as the font used for atom labels and captions
- Color settings—set available colors for objects and the document background
- Print/Page Setup—set options such as the page size used and text displayed in footers

You can apply document settings in the following ways:

- Customize settings for the entire document using the Document Settings dialog box
- Apply settings to the entire current document from an existing document
- Apply settings to selected objects in the current document from an existing document

## Default Style Sheet or Stationery Pad

When you open ChemDraw, the last Style Sheet or Stationery Pad used opens as the default. If you choose another Style Sheet or Stationery Pad, that file becomes the default.

You can set a default that is not changed:

1. Click Preferences on the File (Mac: Chem-Draw) menu.
2. Browse to the default Style Sheet (Stationery Pad).
3. On the Open/Save tab, deselect the **Opening Any Style Sheet (Stationery Pad) Changes Default** checkbox.

To view the default Style Sheet or Stationery Pad, click the File menu.

The **New** menu item displays the name of the Style Sheet or Stationery Pad.

## Saving Customized Settings as Style Sheets or Stationery Pads

Every new document created with ChemDraw uses a Style Sheet or Stationery Pad to obtain its document settings. Style Sheets or Stationery Pads can also contain predefined objects. When you create a new document, you actually create an untitled copy of the Style Sheet or Stationery Pad. Any changes you make to the copy of the Style Sheet or Stationery Pad do not affect the Style Sheet or Stationery Pad itself.

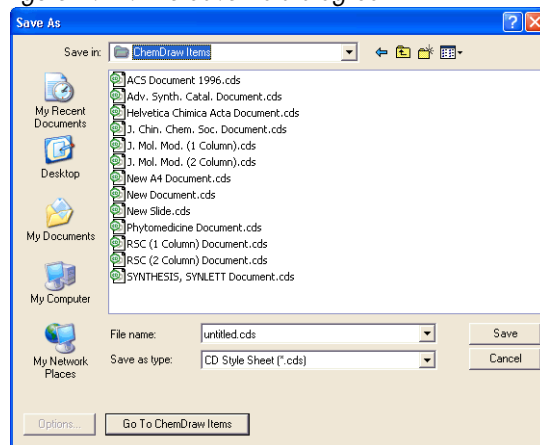
You can create a Style Sheet or Stationery Pad with your own customized setting by saving it as a CDS file. If you store the CDS file in the ChemDraw Items folder, it appears in the Open Special menu so you can access it from the File menu.

To save a document's setting as a Style Sheet or Stationery Pad:

1. Click the **Save As** command from the File menu.

The Save As dialog box appears.

Figure A.42: The Save As dialog box



2. Name the file and change the type (in OS X: format) to CD Style Sheet (cds) or ChemDraw Stationery.
3. To save the file in the ChemDraw items folder, click the **Go To ChemDraw Items** button.

4. Click **Save**.

## Applying Document Settings From Other Documents

To apply document settings to the active window that are contained in a different document, point to **Apply Document Settings from...** on the File menu, and choose the document from which to apply the settings.

The settings in the active document window change to those found in the Style Sheet or Stationery Pad that you choose.

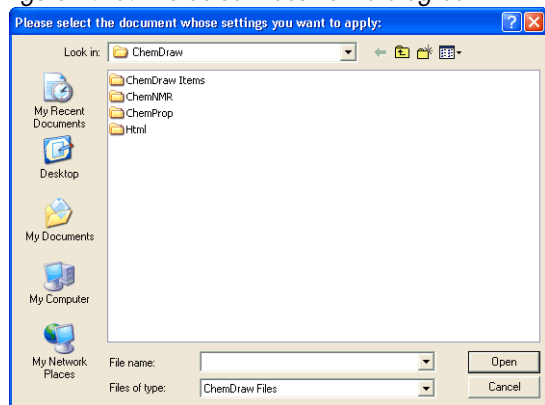
*NOTE: When you apply settings, they apply to the current document only and are not saved as the default for the next document. Use Open Special from the File menu if you want to change the default document settings.*

To apply the document settings from a document or style sheet not listed in the menu:

1. Click **Other** on the **Apply Document Settings from** submenu of the File menu.

The Select document dialog box appears.

Figure A.43: The Select Document dialog box



2. Open the appropriate folder and select a ChemDraw document or Style Sheet / Stationery Pad.
3. Click **Open**.

## Applying Object Settings from Other Documents

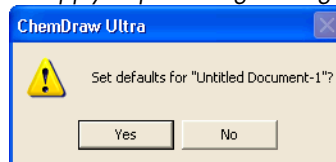
You can apply settings from another document to selected objects in the current document. You can apply the chosen settings to the selected objects only, or to all new objects drawn in the current document.

To apply object settings:

1. Select the object.
2. Point to **Apply Object Settings from...** on the Object menu, and choose the document from which to apply the settings.

A dialog box appears:

Figure A.44: Apply object settings dialog box



3. Take the appropriate action:

Table 19: Applying object settings from other documents

**If you want to apply the settings to the ...**      **Then click ...**

selected object only      **No**

selected object and any new objects you draw      **Yes**

The settings are applied.

## Drawing Settings

Drawing settings are document settings that affect how bonds and other objects are drawn. You can configure the drawing settings for an entire document or for a particular object as follows:

- For the entire document, use the Document Settings dialog box.



- For an object, use the **Object Settings** dialog box.

Changes made to the drawing settings affect the active document window only. Drawing settings can be saved in Style Sheets or Stationery Pads.

To apply settings from other documents to your document, select “Apply Document Settings from...” from the File menu.

The drawing settings are described in the following table:

Table 20: Drawing settings

<b>Adjust this...</b>	<b>If you want to ...</b>
Chain Angle	Set the angle (from 1 to 179 degrees) between bonds created by the Acyclic chain tool or modified by the Structure CleanUp command.  For more information see, “Drawing Acyclic Chains” on page 52 and “Structure CleanUp” on page 72.

Table 20: Drawing settings

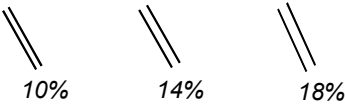
<b>Adjust this...</b>	<b>If you want to ...</b>
Bond Spacing	Set the distance between the lines in double or triple bonds. The distance is set either as: <ul style="list-style-type: none"> <li>The percent of the length of the bond (between 1 and 100). This allows for proportional spacing to be used if different bond lengths are used in the drawing.</li> </ul> <div style="text-align: center;">  </div> <p>An absolute value you choose in the units specified for your document.</p>
Fixed Length	Constrain the length of the bonds drawn to the length you specify when the Fixed Lengths command in the Object menu is selected (a check mark is next to it). This also adjusts the preferred bond length for structures modified by the Structure CleanUp command.  For more information see “Drawing with Fixed Lengths” on page 47 and “Structure CleanUp” on page 72.

Table 20: Drawing settings


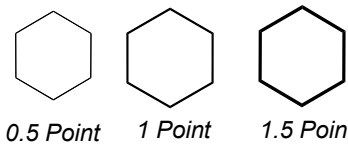


Adjust this...	If you want to ...
Bold Width	Set the width of the line used when bold and wedge bonds are drawn. The Bold Width setting must be greater than the Line Width setting. The end of a wedge is 1.5 times the bold width.
	
Line Width	Set the width of all bonds, lines, and arrowheads in the drawing.
	
Margin Width	Change the amount of space surrounding all atom labels that will erase portions of the bonds to which they are attached. The margin width also determines the amount of white space surrounding the front bonds in a bond crossing.
	For more information, see “Editing Atom Labels” on page 59 and “Changing Bond Crossings” on page 55.

Table 20: Drawing settings

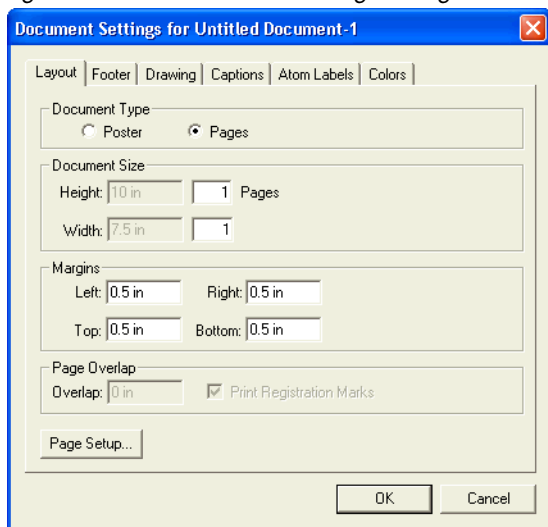
Adjust this...	If you want to ...
Hash Spacing	Set the spacing between the hashed lines used when wedged hashed bonds, hashed bonds, dashed bonds, dashed arrows, or dashed curves are drawn.
	
Color	Change the color in of selected objects. For more information, see “Customizing the Color Palette” on page 212.
	
Units	Set the units used in the Object Settings dialog box to centimeters, inches, points, or picas.
Atom and Bond Indicators	Set which indicators you want to display in your drawings. For more information about using indicators, see “Atom Numbering” on page 75 and “Showing Stereochemistry” on page 113.

## Configuring Settings for Documents

To configure the drawing settings for an entire document:

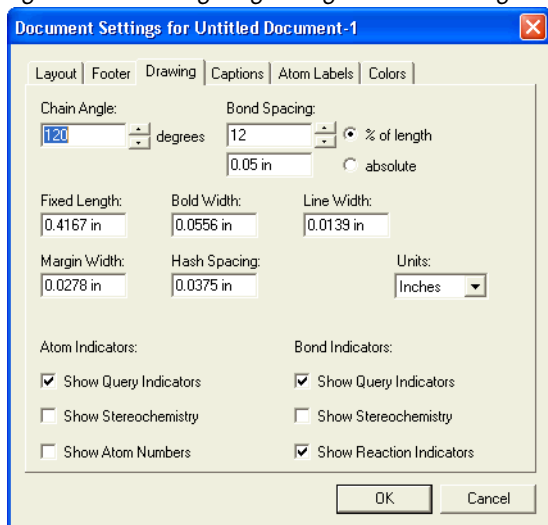
1. Click **Document Settings** on the File menu.

Figure A.45: The Document Settings dialog box



2. Click the **Drawing** tab and configure the settings.

Figure A.46: Configuring settings on the Drawing tab



3. Click **OK** when you are finished.

The settings you chose are applied to the entire document.

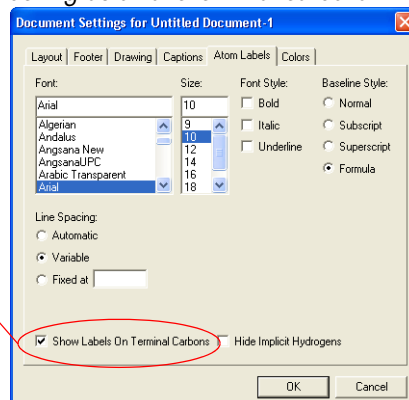
## Terminal Carbon Labels

There is a new Document Setting to automatically display terminal carbon labels. The default on installation is to not display terminal carbons.

If you prefer structures to display terminal carbons:

1. Click **Document Settings** on the File menu.
2. Select the **Atom Labels** tab.
3. Check the box next to **Show Labels On Terminal Carbons**.

Figure A.47: Setting automatic terminal carbons



Show labels on Terminal Carbons

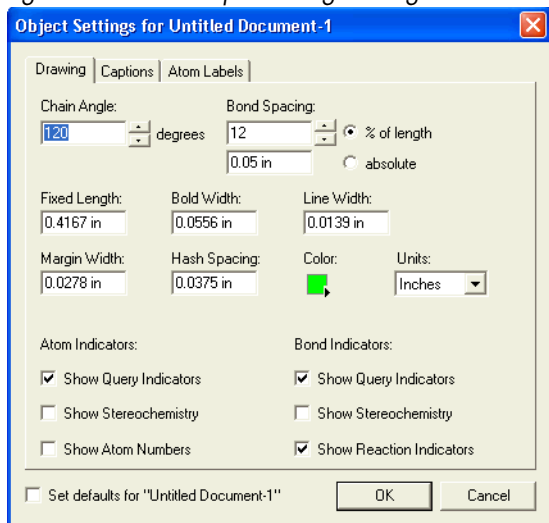
## Configuring Settings for Objects

To configure the drawing settings for a selected object:

1. Select the object.
2. Click **Object Settings** on the Object menu.

The Object Settings dialog box appears with the Drawing tab displayed.

Figure A.48: The Object Settings dialog box



3. Configure the settings and click **OK**.

The settings you chose are applied to the selected object only.

## Formatting Text

Text settings affect how captions and atom labels for the current document are drawn and formatted.

Formatting options include:

- Font (font type)
- Size (font size)
- Style (font and baseline style)
- Line spacing
- Alignment

These options are described in the following sections.

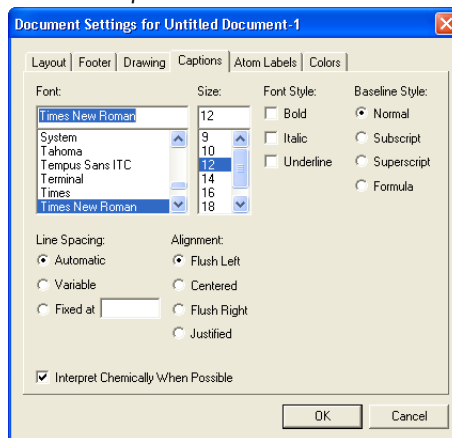
### Setting Font parameters

Changing text formats in the Document Settings dialog box affects the current document only. You can also change settings for individual objects by using the Object Settings dialog box, the Text menu, or the Style toolbar.

To edit the document text settings for captions and atom labels:

1. Click **Document Settings** on the File menu.
2. In the **Document Settings** dialog box, click **Captions** or **Atom Labels**.

Figure A.49: Captions tab



3. Change the settings if desired. The options are described in the following sections.
4. Click **OK**.

The formatting is applied to the current document.

### Setting the Baseline Style

You can specify the following baseline styles:

- **Normal**—Use this for standard text.
- **Superscript**—Reduces the text size by about 25 percent and raises its baseline.
- **Subscript**—Reduces the text by about 25 percent and lowers the baseline.
- **Formula**—Formats in a way that is appropriate for most chemical formulas, that is, numbers are automatically subscripted. You must, however, capitalize manually.

You can apply several styles to the same selected caption. You can also apply multiple styles to different portions of a single caption.

If the captions you select have more than one style, when you select the text with the Lasso or Marquee tool and select **Style** from the Text menu, a hyphen appears next to each style (other than Plain) that is applied to a portion of the selection. A check mark appears next to each style that applies to all of the selected text. Choosing a style other than “Plain” adds the new style to all of the selected captions. Previously applied styles are not affected—that is, for example, if you select Italic for a section that is Bold, it will be Bold Italic.

## Specifying Line Spacing

You can specify the three types of line spacing:

- **Automatic**—Consistently spaced lines of text based on the height of the tallest character in the entire caption. This is the default line spacing.
- **Variable**—Lines of text with different spacing based on the tallest character and the lowest descender in each line.
- **Fixed**—Consistently spaced lines using a spacing that you specify.

## Aligning Text

You can set the alignment of captions and atom labels to justify text to suit your needs. The options available depend on whether you are aligning captions or atom labels. Settings are made in the Object Settings dialog box.

To open the object settings dialog box, do the following:

1. Select a caption or atom label with the Lasso or Marquee tool.
2. Click **Object Settings** on the Object menu.

The Object Settings dialog box appears.

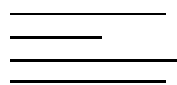
## Captions

You specify the caption justification and line spacing on the Captions tab of the Object Settings dia-

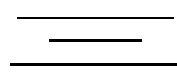
log box. All text in a single caption must have the same Justification and Line Spacing.

There are four available justifications:

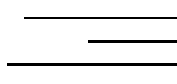
- **Flush Left**—creates left-justified caption text.



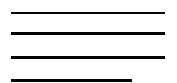
- **Centered**—creates centered caption text.



- **Flush Right**—creates right-justified caption text.



- **Justified**—creates right-left justified caption text.



## Atom Labels

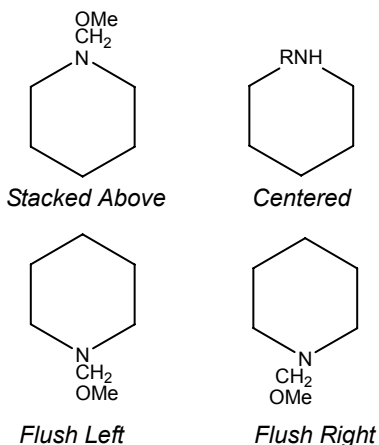
Use the **Centered**, **Flush Left**, **Flush Right**, **Stacked Above**, or **Automatic** justifications to create labels that identify atoms and functional groups in your chemical structure without obscuring any bonds or other atom labels.

*NOTE: When using Stacked Above justification, enter the tokens from top to bottom using Alt+Enter or Option+Return to go to a new line. For instance, in the example below, enter “OMe Alt+Enter [Option+Return] CH<sub>2</sub> Alt+Enter [Option+Return] N”.*

*If you change the justification after the label is entered, it will in most cases generate a warning.*

Examples of the atom label justifications are shown below.

Figure A.50: Atom label justification



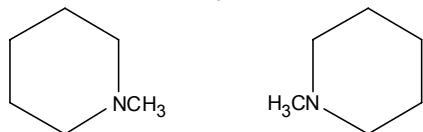
## Automatic Alignment

When you justify Atom labels automatically, ChemDraw breaks the label into tokens. A token consists of an uppercase letter followed by any numbers or lowercase letters. The first token is attached to the atom and the rest of the label appears without obscuring other parts of the chemical structure.

For example, to create N-methylpiperidine, label an atom in cyclohexane with the atom label **NCH<sub>3</sub>**, which contains the three tokens, **N** and **C** and **H<sub>3</sub>**. If you label **C3**, the tokens are placed from left to right because there are bonds to the left of the atom.

If you label **C5**, the tokens are placed from right to left because there are bonds to the right of the atom:

Figure A.51: Automatic alignment of atom labels



**Pro** In ChemDraw Pro, you can force an entire multi-atom label to be a token by defining it

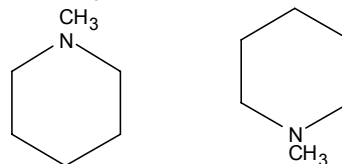
as a Nickname. This prevents the label from flipping when applied to the left side of a structure.

For example, if you define the Nickname **CH<sub>3</sub>**, and label **C5** with the combined label and nickname **NCH<sub>3</sub>**, the final orientation is **CH<sub>3</sub>N** instead of **H<sub>3</sub>CN**. In this case, the Nickname, **CH<sub>3</sub>**, is a token. For more examples, see “Using Nicknames” on page 81.

If you label **C1**, the second and third tokens are placed above the first token since there are bonds below the atom.

If you label **C4**, the second and third tokens are placed below the first token.

Figure A.52: Using a Nickname as a token



## Changing the Default Caption or Atom Label Text Format

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

You can change the format by:

- Changing the document settings for subsequent drawings in the current document.
- Choosing a new format for an individual caption or label from the Text menu or toolbar before you type.
- Selecting text and applying a new format to an individual label after you type.

## Specifying Document Settings for New Text

To specify the text settings for new captions and atom labels in the current document:

1. Click **Document Settings** on the File menu.

2. Click **Captions** or **Atom Labels** in the Document Settings dialog box.
3. Click the appropriate options.
4. Click **OK**.

These settings affect all new captions or atom labels in the current document. To use these settings in new documents save them in a Style Sheet or Stationery Pad. For more information, see “Saving Customized Settings as Style Sheets or Stationery Pads” on page 201.

## Setting an Individual Text Format Before Typing

You can set the text format for an individual caption or atom label before you type. The format change is applied to the current text only.

To set the text format before you type:

1. Click the Text tool and click in the document window.  
A text box appears.
2. Set the text format in one of the following ways:
  - Set **Font**, **Style** and **Size** options on the Text menu.
  - Set the format options from the Style toolbar.
3. Type the text in the text box.

The format is applied to the typed text. Any subsequent text you type is formatted according to the default document settings for the current document.

## Changing the Spacing of Individual Text Objects

You can change the text settings for a specific caption or atom. The setting change is applied to the selected object only. You can also choose whether to have the settings applied to the selected text and to all subsequent text you type.

To change the text settings for a specific caption or atom label:

1. Select the text to change with a selection tool.
2. Set the appropriate options on the Text menu.

To change only a part of a single caption, select part of the caption with the Text tool.

To specify a font and size for selected text, do one of the following:

- Choose the font and size from the Text menu.
- Right-click and choose the font and size from the right-click menu.
- Select the font and size from the drop-down menus on the Style Toolbar.

## Fractional Character Widths (Macintosh)

On the Macintosh, you can choose to have the spacing between characters as close to proportional as possible. If you are printing to a PostScript printer, this option improves the font appearance.

To set fractional widths:

1. Click **Document Settings** on the File menu.
2. Click the **Footer** tab in the Document Settings dialog box.
3. Click **Fractional Widths**.

## Specifying the Margin Width

You can adjust the white space surrounding the atom label so that some of the attached bond is hidden.

Figure A.53: Adjusting white space in atom labels



To adjust the white space:

1. Click **Document Settings** on the File menu.  
The Document Settings dialog box appears.

2. Click the **Drawing** tab.
3. Type a new **Margin Width** value.
4. Click **OK**.

The margin width is applied to all subsequent drawings in the current document.

## Creating HotKeys

To add or edit ChemDraw HotKeys, use a text editor (Notepad etc.) to open the **CS ChemDraw Hotkeys** file in the ChemDraw Items folder.

You can use any uppercase or lowercase alphanumeric key as a Hotkey with the exception of the hard coded HotKeys listed previously. If a capital and lowercase Hotkey do not exist, the Hotkey is assigned to both. If a key is used more than once in the file, the one closer to the end of the file takes precedence.

To add a Hotkey:

1. Add a new line and type the key you want to use.
2. Type a space.
3. Type the letters to associate with the Hotkey.  
HotKeys defined for single elements always result in the adding of the appropriate number of hydrogen atoms.
4. Save and close the HotKeys file.

To create a new HotKeys file:

1. Create a text file named **CS ChemDraw Hotkeys**.
2. Save the file in the ChemDraw Items folder.
3. Click **OK** or **Save**.

## Hard-Coded HotKeys

You cannot edit hard-coded HotKeys. *Table 21* contains a list of hard-coded HotKeys:

*Table 21: Hard-coded HotKeys*

<b>Hotkey</b>	<b>Function</b>
<b>Enter</b> or <b>return</b>	Opens the atom label text box.
<b>space</b>	Removes an atom label.
<b>Delete</b> or <b>Backspace</b>	Deletes objects.

*NOTE: In earlier versions of ChemDraw, quite a few more keys were hard-coded. In ChemDraw 10.0 any key not listed above can be customized.*

## Working with Color

With the color capabilities of ChemDraw, you can create full color presentations of your chemical drawings to appear on your monitor, print on a color printer, or create 35mm slides using a film printer.

Most computers can display any of 16 million colors, but the number of colors that can appear at any one time may be limited by the particular monitor and display card installed in your computer.

In ChemDraw, you can choose from a palette consisting of a Background Color, a Foreground Color, and up to twenty additional colors for any given drawing. A palette is stored in every document and Style Sheet or Stationery Pad. You can use Style Sheets or Stationery Pads to create a series of documents with the same color scheme.

Using color you can:



- Color atoms and bonds in a mostly black-on-white drawing to highlight areas of interest.
- Color parts of a structure in a reaction scheme to indicate where starting materials end up in the products of a complicated mechanism.
- Use colored boxes and circles to highlight atoms or molecules.
- Create slides that are easier to view by using light objects on a dark background.

## Coloring Objects

Any object that you can select with a selection tool can be colored. You can color individual bonds, part or all of a chemical structure, or objects such as boxes, curves, arrows, orbitals and reaction mechanism symbols.

The border of objects that are shaded or filled, such as white filled s-orbitals in the Orbitals palette, are the same color as the shading or fill. The border of objects that are hollow, such as circles and hollow boxes in the Drawing Elements palette can be colored, but the inside of the object cannot.

To color an object:

1. Select the object in a document window with a selection tool.
2. Do one of the following:
  - Click the Color button on the Style toolbar, and select the color from the menu that appears.
  - Choose a color from the Color menu.
  - Click the **Color** button on the **Drawing** tab of the Object Settings dialog box, and select the color from the menu that appears.

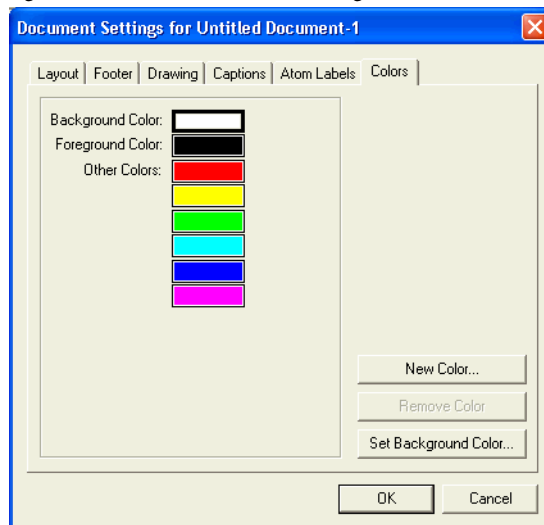
## Displaying the Color Palette

You can use the color palette to specify the color of objects and text in the document within the active window.

To view the Color palette:

1. Click **Document Settings** on the File menu.
2. Click the **Colors** tab.

Figure A.54: The Document settings colors tab



Use the Color tab to specify the following colors:

- **Background Color**—Fills the background of the current document in the active window.
- **Foreground Color**—Default color used when you draw a new object.
- **Other Colors**—Colors available in the Color Menu for changing the color of individual objects. The colors are represented in the same order that they appear in the Color menu.

You can customize the Color menu. Colors can be added, or existing colors can be changed. Changing a color, for example Other #2, changes all objects that are using the color.

*NOTE: If you select an individual or grouped object that contains multiple colors, there is a check mark next to each of the colors in the Color menu. The purpose of the check marks is to alert you that a change would affect more than one color.*

## Customizing the Color Palette

You can add, remove, or change the default foreground and background color and specify the other colors available for coloring objects.

Changes made to the color palette affect the current document only. You can save Color Palette settings (foreground, background, and up to 20 other colors) in a Style Sheet or Stationery Pad. For more information, see “Saving Customized Settings as Style Sheets or Stationery Pads” on page 201.

A summary of each of the options is described in the following table.

Table 22: Color palette options

Option	Description
<b>New Color</b>	Add a new color box and set its color using the Color Picker or Color Wheel dialog box.
<b>Remove Color</b>	Delete a color box that you have selected in the left side of the dialog box. Any objects using the removed color are changed to the Foreground color.
<b>Set Color</b>	Change the color associated with a color box that you have selected in the left side of the dialog box. Any objects using the old color are changed to the new color.

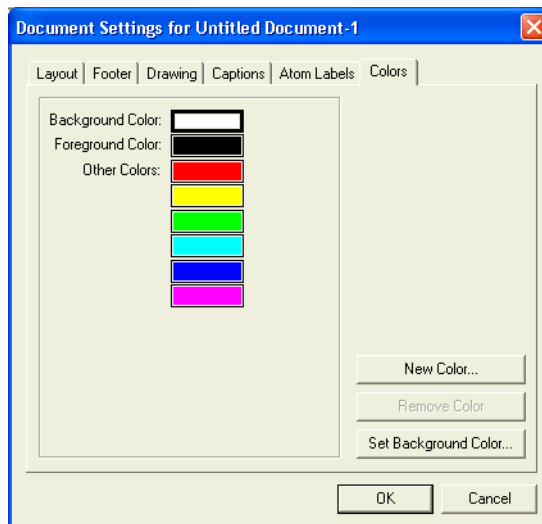
## Windows Color Settings

To change the palette of colors used in the current document:

1. Click **Document Settings** on the File menu.  
The Document Settings dialog box appears.

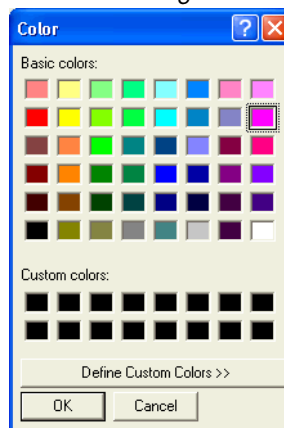
2. Click the **Colors** tab.

Figure A.55: Document settings Colors tab



3. Double-click the color to change.

Figure A.56: The Color dialog box



4. Click a color box in the Basic Colors or the Custom Colors section.

A highlighted border appears around the color you select.

5. Click **OK**.

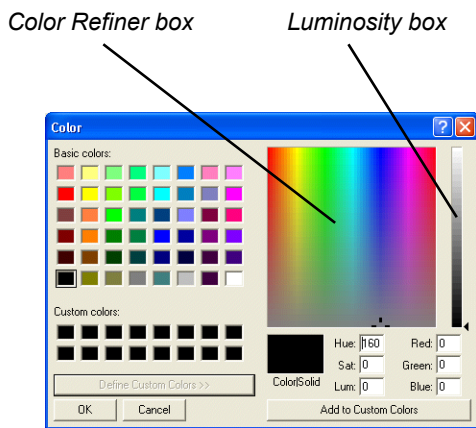
The color is changed to the new color and added to the Color menu.

## Adding or Customizing Windows Colors

To add colors or create customized colors:

1. Click **Define Custom Colors** in the Color dialog box.

Figure A.57: Setting custom colors



2. Click a color in the Color Refiner box to set the hue and saturation.

The pointer turns into a Crosshair when you click. You can drag to a different region to change the hue and saturation.

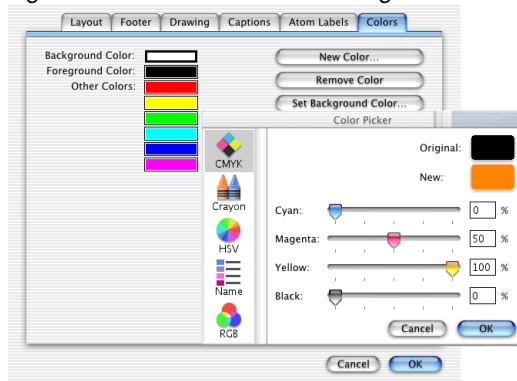
3. Click in the Luminosity box to set the brightness of the color.
4. If necessary, change the hue, saturation, luminosity, and RGB components by typing the values in the text boxes.
5. Click the **Add to Custom Colors** button.

## Macintosh Color Settings

To change the palette of colors used in the current document:

1. Click **Document Settings** on the File menu.  
The Document Settings dialog box appears.
2. Click the **Colors** tab.
3. Click **New Color**.

Figure A.58: The Color Picker dialog box



4. Use one of the icons on the left to select a method of defining your color, then select a color.

For more information about the Macintosh color options, refer to your System documentation.

5. Click **OK**.

The new color appears in the Colors tab in place of the original color and is added to the color menu.

## Adding or Customizing Macintosh Colors

To add a new color to the Color menu:

1. Click **New Color** or **Set Other Color** on the Color tab.  
The Color Picker dialog box appears.
2. Click a color in the Color Wheel.
3. If necessary, adjust the hue, saturation, brightness, and RGB components by typing in the values.
4. Click **OK**.

The new color is added to the list of Other Colors.

## Removing Colors

To remove a color from the Color menu:

1. Click the color you want to remove.  
A highlight box appears around the color.
2. Click **Remove Color**.  
The color disappears from the list of other colors. Objects that were drawn in the removed color are changed to the Foreground color

## Templates and Color

The background and foreground colors used in a template from the template pop-up palette are not used when the template is drawn in a document window. However, any other colors used in the template are added to the color palette of the current document if they are not already present. This is part of the autoscale feature. For more information, see “Autoscaling” on page 165.

## Saving Color Palette Settings

You can save the Color Palette in a Style Sheet or Stationery Pad. The Color Palette is saved in addition to other document settings such as Page Setup settings, Text settings, and Drawing settings.

## Printing

ChemDraw uses the standard system commands to print ChemDraw documents. The options that you have available to you depend on the printer that you are using. Refer to your printer’s documentation for more information.

In general, to print a ChemDraw document:

1. Click **Page Setup** on the File menu.
2. Make all appropriate selections for the printer you are using and click **OK**.
3. Click the **Print** command on the File menu.
4. Make your selections in the Print dialog box and click **OK**.

To print a document:

1. Select the document you want to print.
2. Click **Print** on the File menu.

The ChemDraw application is opened and the Print dialog box appears.

3. Make your selections in the Print dialog box and click **OK**.

## Printing Background Color

Print Background Color controls whether the Background Color contained in your ChemDraw document is printed.

To change whether the Background color is printed:

1. Click **Preferences** on the File menu.
2. Click **Print Background Color**.
3. Click **OK**.

## Macintosh Print Preferences

When you print a document, ChemDraw creates both a QuickDraw representation and a PostScript representation of the document’s contents.

QuickDraw is the graphical format that is supported by the Macintosh Operating System. Every printer that supports the MacOS can convert QuickDraw representations into printed output. However, QuickDraw does not support some features (for example, high-resolution printing) that are available only on some printers.

If you are transferring information to another application from which you print ChemDraw pictures, you should consider including PostScript commands and the ChemDraw LaserPrep File with the pictures. For information about special situations to consider, see “Transferring PostScript (Macintosh)” on page 167.

## Optimize Pictures for High-Resolution Non-PostScript Printing

The Macintosh High Resolution Clipboard supports high-resolution printers. Most applications support the High Resolution Clipboard. Because this was not always the case in the past, this preference continues to be available for users to turn off

if an application being used does not support the High Resolution Clipboard.

If you are unsure if the application uses a High Resolution Clipboard, try transferring pictures with this check box selected and deselected, and see which picture prints with higher quality.

If you are printing to a non-PostScript printer, deselect **Include ChemDraw LaserPrep** and **Include PostScript** to reduce the size of each picture. Do not deselect this option if the document will ever be printed to a PostScript printer.

Printers that use the PostScript page definition language use the PostScript representation. The PostScript representation describes objects by using mathematical shapes that can be precisely imaged at whatever resolution is used by your printer. The PostScript representation created by ChemDraw is composed of two parts, the PostScript commands and the ChemDraw Laser Prep. The ChemDraw Laser Prep contains specific instructions that enable the printer to interpret the PostScript commands contained in a ChemDraw document.

## Include PostScript

To transfer ChemDraw pictures to another document that will be printed on a PostScript printer:

1. Click **Preferences** on the File menu.
2. Click **Include PostScript**.

3. Click **OK**.

When Include PostScript is deselected, no PostScript commands are generated. This usually results in lower quality printing, particularly of drawings cut and pasted into other applications. However, because the representation used for printing when Include PostScript is not selected is the same as that used for drawing to the screen, better correspondence between the screen and printed output may be observed.

For more information, see “Transferring PostScript (Macintosh)” on page 167.

## Include ChemDraw Laser Prep

Selecting the include ChemDraw Laser Prep allows you to print to a printer that cannot be initialized using ChemDraw. If you create drawings with this option off, they will not print on PostScript printers without the use of ChemDraw.

To Include ChemDraw Laser Prep:

1. Click **Preferences** on the File menu.
2. Click **Include ChemDraw Laser Prep**.
3. Click **OK**.

*NOTE: When you select Include ChemDraw Laser Prep, you should also select Include PostScript.*

For more information, see “Transferring PostScript (Macintosh)” on page 167.



# Appendix B: Document Settings

## Creating Style Sheets or Stationery Pads

To create your own Style Sheet or Stationery Pad:

1. Create a new document.
2. Enter the settings in the Page Setup, Drawing, Text Settings, and Color Palette dialog boxes.
3. Click **Save As** on the File menu.
4. In the Save As dialog box:
  - d. Select the CD Style Sheet or Stationery Pad file format.

- e. Type a name for the document.
  - f. Select the ChemDraw Items folder as the location for saving the template.
5. Click **OK** or **Save**.

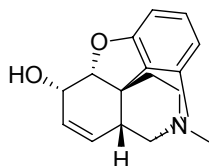
## ChemDraw Style Sheets or Stationery Pads

This following table contains drawing settings and a sample structure for each of the Style Sheets or Stationery Pads ChemDraw provides.

### Drawing, Atom Label, and Caption Text Settings in Journal Style Sheets or Stationery Pads

ACS 1996

**ACS 1996**



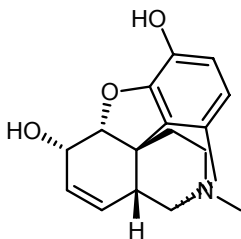
Morphine

- Fixed Length: **14.4 pt**
- Bold Width: **2 pt**
- Line Width: **0.6 pt**
- Margin Width: **1.6 pt**
- Hash Spacing: **2.5 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **18**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **10 pt**
- Drawing Area (Width x Height): **540 pt x 720 pt**
- Page Size: **US Letter**
- Reduction (%): **100**

## Drawing, Atom Label, and Caption Text Settings in Journal Style Sheets or Stationery Pads

Adv.Synth Catal.

### Adv. Synth. Catal.

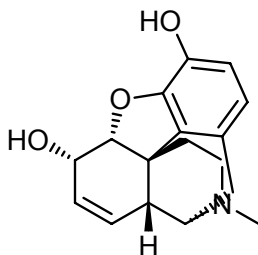


Morphine

- Fixed Length: 17 pt
- Bold Width: 2 pt
- Line Width: 1 pt
- Margin Width: 1.6 pt
- Hash Spacing: 2.5 pt
- Chain Angle (degrees): 120
- Bond Spacing (% of length): 18
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): **Times New Roman/Times**
- Caption Size: **12 pt**
- Drawing Area (Width x Height): **540 pt x 720 pt**
- Page Size: **US Letter**
- Reduction (%): **100**

J.Chin. Chem. Soc.

### J. Chin. Chem. Soc.



Morphine

- Fixed Length: 18 pt
- Bold Width: 2.5 pt
- Line Width: 1 pt
- Margin Width: 2 pt
- Hash Spacing: 2.5 pt
- Chain Angle (degrees): 120
- Bond Spacing (% of length): 20
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **12 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **12 pt**
- Drawing Area (Width x Height): **693 pt x 918 pt**
- Page Size: **US Letter**
- Reduction (%): **80**

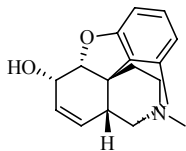


## Drawing, Atom Label, and Caption Text Settings in Journal Style Sheets or Stationery Pads

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J. Mol. Mod.

**J. Mol. Mod.**

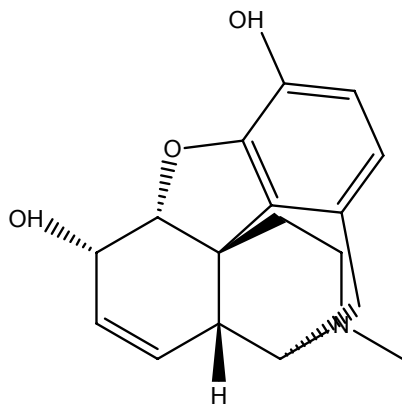


Morphine

- Fixed Length: **14.4 pt**
- Bold Width: **2 pt**
- Line Width: **0.6 pt**
- Margin Width: **1.6 pt**
- Hash Spacing: **2.5 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **18**
- Atom Label Font (Win/Mac): **Times New Roman/Times**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): Times New Roman/Times
- Caption Size: **10 pt**
- Drawing Area (Width x Height): **8.5 cm x 25.4 cm** (1 column); **17 cm x 25.4 cm** (2 column)
- Page Size: **US Letter**
- Reduction (%): **100**

New Document

# New Document



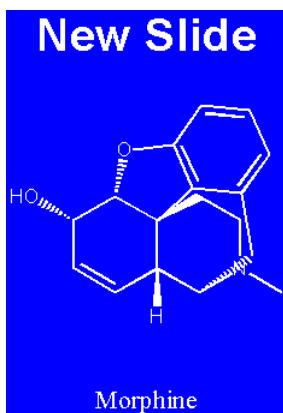
Morphine

- Fixed Length: **30 pt**
- Bold Width: **2 pt**
- Line Width: **1 pt**
- Margin Width: **2 pt**
- Hash Spacing: **2.7 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **12**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): **Times New Roman/Times**
- Caption Size: **12 pt**
- Drawing Area (Width x Height): **7.5 in x 10 in**
- Page Size: **US Letter** or **A4** (as selected)
- Reduction (%): **100**

## Drawing, Atom Label, and Caption Text Settings in Journal Style Sheets or Stationery Pads

---

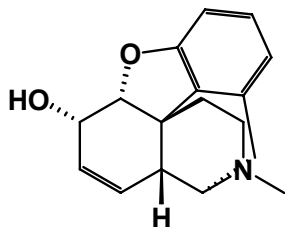
### New Slide



- Fixed Length: **30 pt**
- Bold Width: **4 pt**
- Line Width: **1.6 pt**
- Margin Width: **2 pt**
- Hash Spacing: **2.7 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **15**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **12 pt**
- Caption Font (Win/Mac): **Times New Roman/Times**
- Caption Size: **16 pt**
- Drawing Area (Width x Height): **7.5 in x 10 in**
- Page Size: **US Letter**
- Reduction (%): **100**

Phytomedicine

## Phytomedicine

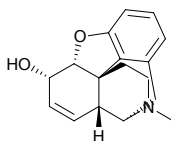


Morphine

- Fixed Length: **20 pt**
- Bold Width: **1.33 pt**
- Line Width: **1pt**
- Margin Width: **1.25 pt**
- Hash Spacing: **3 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **8**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **12 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **12 pt**
- Drawing Area (Width x Height): **540 pt x 720 pt**
- Page Size: **US Letter**
- Reduction (%): **100**

RSC

## RSC (1 and 2 column)

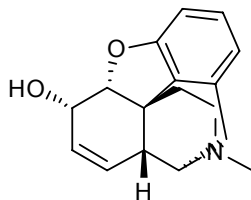


Morphine

- Fixed Length: **0.43 cm**
- Bold Width: **0.056 cm**
- Line Width: **0.016 cm**
- Margin Width: **0.044 cm**
- Hash Spacing: **0.062 cm**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **20**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **9 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **9 pt**
- Drawing Area (Width x Height): **8.9 cm x 25.4 cm (1 column); 19 cm x 27.7 cm**
- Page Size: **US Letter**
- Reduction (%): **100**

Science of Synthesis

Science of Synthesis

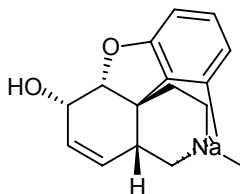


Morphine

- Fixed Length: **17 pt**
- Bold Width: **2 pt**
- Line Width: **0.8 pt**
- Margin Width: **2.25 pt**
- Hash Spacing: **2.5 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **18**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **10 pt**
- Drawing Area (Width x Height): **19.79 cm x 27.15 cm**
- Page Size: **A4**
- Reduction (%): **100**

Synthesis, Synlett

**SYNTHESIS, SYNLETT**



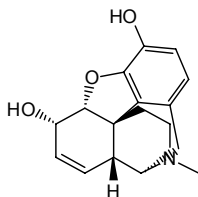
Morphine

- Fixed Length: **17 pt**
- Bold Width: **2 pt**
- Line Width: **0.8 pt**
- Margin Width: **1.3 pt**
- Hash Spacing: **2.5 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **18**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **10 pt**
- Drawing Area (Width x Height): **12 cm x 26.7 cm**
- Page Size: **A4**
- Reduction (%): **100**

## Drawing, Atom Label, and Caption Text Settings in Journal Style Sheets or Stationery Pads

Verlag Helvetica Chimica Acta

### Verlag Helvetica Chimica Acta

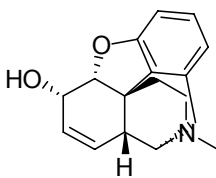


Morphine

- Fixed Length: **17 pt**
- Bold Width: **2.9 pt**
- Line Width: **0.54 pt**
- Margin Width: **2 pt**
- Hash Spacing: **2 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **14**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **10 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **12 pt**
- Drawing Area (Width x Height): **368 x 720 pts**
- Page Size: **US Letter**
- Reduction (%): **100**

Wiley Document

Wiley Document



Morphine

- Fixed Length: **17 pt**
- Bold Width: **2.6 pt**
- Line Width: **0.75 pt**
- Margin Width: **2 pt**
- Hash Spacing: **2.6 pt**
- Chain Angle (degrees): **120**
- Bond Spacing (% of length): **18**
- Atom Label Font (Win/Mac): **Arial/Helvetica**
- Atom Label Size: **12 pt**
- Caption Font (Win/Mac): **Arial/Helvetica**
- Caption Size: **12 pt**
- Drawing Area (Width x Height): **19.79 x 27.15 cm**
- Page Size: **A4**
- Reduction (%): **100**

# Appendix C: Chemistry File Formats

File formats other than ChemDraw may not preserve all of your data. ChemDraw can create many types of items—particularly graphical objects such as boxes and curves—that cannot be saved into chemical file formats.

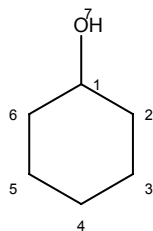
Other file formats sometimes contain data that cannot be interpreted by ChemDraw. ChemDraw always tries to interpret other file formats so that as much chemically-relevant data is preserved as possible, even if that causes the actual appearance of the file to change when it is saved and reopened.

Most file formats supported by ChemDraw are proprietary or extremely complex and are documented more thoroughly elsewhere. For example, you can find more information about CambridgeSoft's CDX file format at: [sdk.cambridgesoft.com](http://sdk.cambridgesoft.com)

## Connection Table File Format

The connection table format file described in this section is generated for the cyclohexanol structure shown below. All references to atom serial numbers are based on the Atom Numbering shown.

*Figure C.59: Atom numbering used in the following examples*



*Table 23* is a sample Connection Table file produced for cyclohexanol using ChemDraw. The line

numbers are added for purposes of discussion only.

*Table 23: Sample connection table for cyclohexanol*

Line 1	Cyclohexanol			
Line 2	7 7			
Line 3	0.0000	0.5000	0.0000	C
Line 4	-0.8667	0.0000	0.0000	C
Line 5	-0.8667	-1.0000	0.0000	C
Line 6	0.0000	-1.5000	0.0000	C
Line 7	0.8667	-1.0000	0.0000	C
Line 8	0.8667	0.0000	0.0000	C
Line 9	0.0000	1.5000	0.0000	O
Line 10	1 2 1 1			
Line 11	2 3 1 1			
Line 12	3 4 1 1			
Line 13	4 5 1 1			
Line 14	5 6 1 1			
Line 15	1 6 1 1			
Line 16	6 7 1 1			

Each line represents a data record containing one or more fields of information about the structure. Individual fields are delimited by space(s) or a tab. The fields in the Connection Table format file used by ChemDraw are discussed below. The field value for Carbon 6 from the example file is included in parentheses for reference.

- Line 1 is the molecule name. The molecule name is the file name when the file was created using ChemDraw.
- Line 2 contains two fields: the first field is the number of atom labels, and the second field is the number of bonds. These fields must be separated by at least one space.

- Lines 3. 9 each contain 4 fields describing information about the individual atoms: the first field is the X Cartesian coordinate (0.8667), the second field is the Y Cartesian coordinate (0.0000), the third field is the Z Cartesian coordinate (0.0000), and the fourth field is the atom label (C).

The spacing of these fields is very important. Any data outside the following columns (especially data overlapping the ranges) may render a file unreadable.

- Field 1: Columns 0. 9
- Field 2: Columns 10. 19
- Field 3: Columns 20. 29
- Field 4: Columns 31. end
- Lines 10. 16 each contain four fields describing information about the individual bonds between the atoms: the first two fields represent the serial numbers of the atoms that are connected by this bond (atom 1 and atom 6), the third field is the bond order (1) and the fourth field is the bond type (1).

The bond types for the Connection Table format are listed in *Table 24*:

*Table 24: Encoding for bond types*

value	bond type
1	Single.
2	Dashed.
3	Hashed.
4	Wedged hash with first atom at narrow end.
5	Wedged hash with second atom at narrow end.

*Table 24: Encoding for bond types*

value	bond type
6	Bold.
7	Wedged with first atom at narrow end.
8	Wedged with second atom at narrow end.
9	Wavy.
10	Hollow wedge with narrow end towards 1st atom.
11	Hollow wedge with narrow end towards 2nd atom.
12	Dative bond with arrow towards 2nd atom.
13	Dative bond with arrow towards 1st atom.
14	Any (bond property).
15	Single/Double (bond property).
16	Double/Aromatic (bond property).
17	Single/Aromatic (bond property).

**Double bonds** are bit encoded using a bitmask. The default value (0) indicates a normal (two solid lines) double bond, with the second line on the



right (looking from the first atom to the second). Other values are listed in *Table 25*:

*Table 25: Encoding of double bonds*

<b>value</b>	<b>bond type/position</b>
1	The second line is on the left (looking from the first atom to the second).
2	The two lines are centered.
4	A double bond with one dashed and one solid line.
8	A modifier to the previous two values, indicating that the user specifically set the positioning. If this bit is not present, ChemDraw calculated the positioning automatically.

*Table 25: Encoding of double bonds*

<b>value</b>	<b>bond type/position</b>
16	A double bond with one bold and one solid line.
32	A crossed bond.
64	A double bond with two dashed lines.

So, for example, a bitmask value of 13 (= 1 + 4 + 8) means a double bond with one dashed and one solid line (4), where the user specifically wants (8) the second line to be on the left (1).

*NOTE: This connection table format is obsolete, and is documented here for historical purposes only. This format should never be used for critical work where chemical information is important.*



# Appendix D: ChemDraw Chemistry

ChemDraw automatically converts lines, characters, and other symbols into chemically meaningful figures as you work. This work occurs in the background, but you can choose to view this chemical data using Check Structure, Analyze Structure, and Expand Atom Labels. ChemDraw also uses this chemical data when exporting to file formats that support only a subset of the notations that ChemDraw does.

This appendix describes how ChemDraw interprets what you draw and how you can help ChemDraw better interpret what you mean.

## Chemical Intelligence in ChemDraw

ChemDraw was designed as a tool to aid in chemical communication. Most chemists would understand  $\text{AcOo-C}_6\text{H}_4\text{COOH}$  immediately, whether or not they recognized it as aspirin. Most computer programs, however, require what is known as a “complete connection table,” in this case, a collection of 21 atoms connected by 5 double bonds and 16 single bonds in a specific pattern. ChemDraw takes what makes sense to a chemist and converts it into what makes sense to another application.

This chemical intelligence can be used as a sophisticated “spelling” checker for chemical compounds. For example, if you’re investigating organic acids, a compound with the structural formula  $\text{CH}_3\text{COO}$  would probably represent acetic acid. Present the same formula in a paper on transition metal chemistry, and you might be describing a novel methylated cobalt oxide. If you had asked ChemDraw to interpret it beforehand, you would have received a message reporting a valence

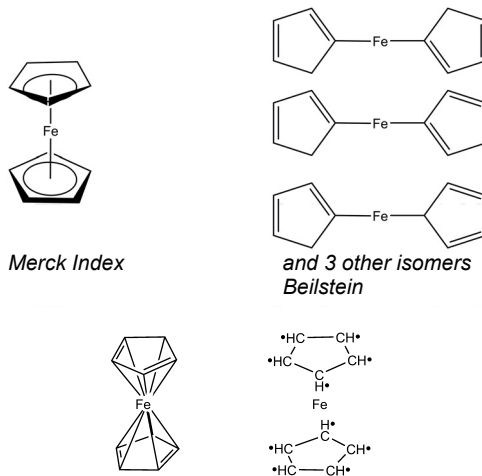
error, and you might have been prompted either to add a negative charge or to change the capitalization.

ChemDraw can offer only suggestions. If you and your audience understand what you are trying to depict, then you can ignore these suggestions. In many cases, you can teach ChemDraw to understand the notation you’re using. For more information, see “Applying Nicknames” on page 82.

## Database Conventions

Most databases require not only that you draw a structure in a way that makes sense, but that you draw it in the way that the database expects it. Consider ferrocene, which is represented in at least four different ways in major databases:

Figure D.60: Representations of ferrocene



















A successful search in one database might not produce any hits in another. When in doubt, consult the documentation for your database, and see if it offers any clues to the conventions used.

# Chemical Conventions

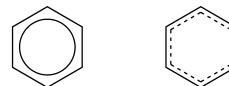
The following table describes the chemical conventions understood by ChemDraw.

Table 26: Bond conventions in ChemDraw

Bond	Description
	Single bond, unspecified stereochemistry.
  	Single bond, “down” stereochemistry (into the plane of the paper, away from the viewer), <i>from</i> the first drawn atom <i>to</i> the second drawn atom.
  	Single bond, “up” stereochemistry (out of the plane of the paper, toward the viewer), <i>from</i> the first drawn atom <i>to</i> the second drawn atom.
	Single bond, mixture of “up” and “down” stereochemistries in some unspecified proportion.
	Dative bond. Often used to indicate polar bonds, such as the N-O bond in pyridine N-oxide.
 	Double bond, with <i>cis/trans</i> stereochemistry as drawn.
	Double bond, with <i>cis/trans</i> stereochemistry unknown.
	Tautomeric bond, either single or double according to rules of tautomerism.
	Aromatic bond, part of a delocalized resonance system.
	Triple bond.
	Quadruple Bond.

A single bond near a closed circle is recognized as aromatic:


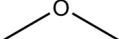

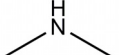

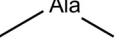



Figure D.61: Aromatic examples



## Atom Labels

A simple atom label may contain any of the following:

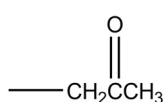
Table 27: Atom label examples

	A single element.
	An element and some number of hydrogen atoms.
 	A nickname.
 	Repeating units within parentheses.
  	A series of any combination of the above.

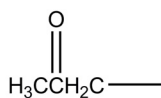
When analyzing an atom label, ChemDraw starts at the left and continues to the right, applying standard rules of valence to determine which atoms are bound to which. The exception is with an atom label in Automatic alignment on the left side of a compound. This sort of atom label is displayed “backwards” (H<sub>3</sub>CO instead OCH<sub>3</sub>) and is there-

fore parsed from right to left. Standard valences for each atom are defined in the Isotopes Table. By definition, a “simple” atom label has all bonds attached to the first (or last) character. A multi-attached atom label has bonds connected to more than one character, or has all of its bonds attached to a specific character in the middle of the atom label. Multi-attached atom labels are always parsed from beginning to end, but again the beginning might be on the right if the atom label was in Automatic style and on the left side of the original structure:

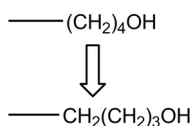
Table 28: Multi-attached labels



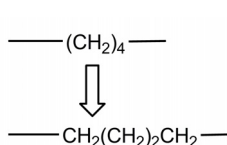
A multi-attached label that is parsed from left to right.



A multi-attached label that is parsed from right to left.



A bond attached to the open parenthesis of a repeating group is treated as if bonded to the first of those groups.



A bond attached to the close parenthesis or repeat count of a repeating group is treated as if bonded to the last of those groups.

Multiple fragments within a single label can be specified in the following ways:

Table 29: Multiple fragments



Implicitly, using standard valence rules.

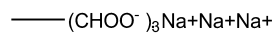
Table 29: Multiple fragments



Explicitly, using a space, period (unsubscripted or unsubscripted), bullet, or combination.



An unsubscripted, unsubscripted integer at the start of a fragment is recognized as a stoichiometric multiplier and is treated as if the appropriate number of fragments were drawn explicitly.



## Chemically Significant Text

Often it is simpler to write a chemical formula like MeOH or H<sub>2</sub>O than it is to draw out an entire atoms-and-bonds structure. ChemDraw correctly interprets any *unambiguous* structural formula. For example, CH<sub>3</sub>COCH<sub>2</sub>CH<sub>3</sub> is recognized as methyl ethyl ketone and MeOH is recognized as methanol. On the other hand, C<sub>6</sub>H<sub>6</sub> might mean benzene, or it might mean one of over 200 other isomers. C<sub>6</sub>H<sub>6</sub> is not recognized by ChemDraw, and generates an error message if you try to analyze it. Generally, empirical formulas (C<sub>2</sub>H<sub>6</sub> and H<sub>2</sub>SO<sub>4</sub>) are not recognized, but structural formulas (CH<sub>3</sub>CH<sub>3</sub> and HOSO<sub>2</sub>OH) are.

Molecular weight and elemental analyses of empirical structures is possible, but the Expand Label command does not work with them. Empirical structures are discarded when they are transferred to other applications that require unambiguous structures.

Chemically-significant text must be entirely in Formula or, for isotopes and charges, Superscript style. ChemDraw does not recognize a chemical formula embedded within a larger block of text.

Table 30: Chemically significant text

$\text{NH}_4^+$  If you draw a bond, add an atom label, and then delete the bond, you have a chemically meaningful text block whose font, size, and style match other atom labels.

$\text{H}_2\text{O}$  If you create a caption with the text tool and set it to Formula style, you have a chemically meaningful text block whose font, size, and style match other captions.

## Charges

Charges may be created as part of a textual atom label or with the appropriate symbol from the Chemical Symbols Palette. Charges are always assigned to a specific element in the atom label, whose acceptable valences become those of the similar isoelectronic neutral element.

Table 31: Charge examples

$\text{—O}^-$  A charge following an element is assigned to that element.

$\text{—}^+\text{NH}_3$   
↓  
 $\text{—(N}^+)\text{H}_3$  A charge that does not follow an element is assigned to the next element.

$\text{—NH}_3^+$   
↓  
 $\text{—(N}^+)\text{H}_3$  Charges that follow a monovalent element with a repeat count are assigned to the element before that element.

Table 31: Charge examples

$\text{—CO}_2^-$   
↓  
 $\text{—CO(O}^-)$  Charges that follow other repeating units are distributed among those units.

$\text{—NH}_3^+$  Charges may be superscripted.

$\text{—Fe}^{++}$  Multiple charges are recognized appropriately.

$\text{—Fe}^{+2}$   
 $\text{—Fe}^{2+}$  Charges may have repeat counts as long as both the charge and the repeat count are superscripted.

$\text{—NH}_3^+$   
↓  
 $\text{—(N}^+)\text{H}_3$  A “floating” charge placed with the Chemical Symbols Tool is assigned to the nearest atom. If no atom is within the distance set as the Fixed Length, the charge is ignored and not assigned to any atom.



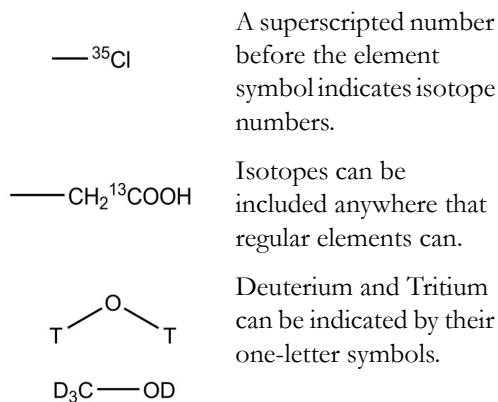
A “floating” charge placed within a delocalized system is recognized by the Analyze Structure function, but is discarded when saved to formats that require all charges to be associated with specific atoms.

## Isotopes and Elements

By default, ChemDraw correctly recognizes all isotopes in the full Table of the Elements. This data is provided by CRC Press, Inc. Isotopes are defined

in the Isotopes Table file. You can edit this file to add new isotopes in any text editor.

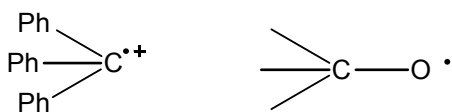
Table 32: Isotope examples



## Radicals

Radicals are indicated with the appropriate symbol from the Chemical Symbols Palette. As with charges, they are assigned to the nearest atom. Radicals always occupy one free valence, in addition to any charge effects.

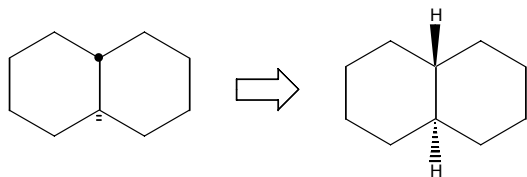
Figure D.62: Radical examples



## H-Dot/H-Dash

H-Dot and H-Dash symbols from the Chemical Symbols Palette indicate the stereochemistry of a single hydrogen atom. These symbols are most commonly used in fused systems.

Figure D.63: H-dot example



## Complexes

Compounds with electron pairs can act as Lewis bases, bonding with Lewis acids that are electron-deficient. Similar behavior can be seen between lone pairs and metals.

The best representation of these types of interaction is with a dative bond from the electron-pair donor to the acceptor. With a plain bond instead of the dative bond, ChemDraw would report a valence error. The dative bond more accurately represents the electron donation.

Complexes may also be represented with explicit lone pairs and without any bonds.

If you use a plain bond to indicate a complex, you may want to set Abnormal Valence to Allowed in the Atom Properties dialog.

Table 33: Complexes

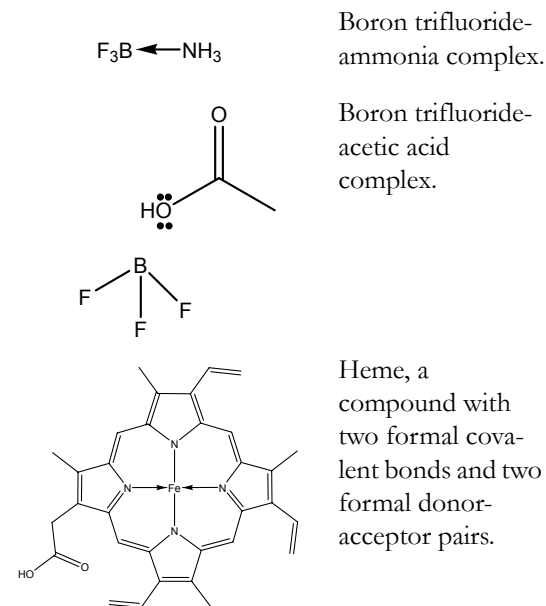
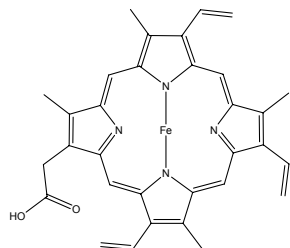


Table 33: Complexes



Another representation of heme.

## Multi-center Attachments

Multi-center attachments are meaningful only when created using Add Multi-Center Attachment from the Structure Menu. This command creates a pseudo-atom that is disregarded during chemical calculations, but still allows you to create diagrams that look meaningful to an experienced chemist.

Figure D.64:  $\eta^3$  or  $\pi$ -Allyl complex



Figure D.65: Ferrocene, a  $\pi$ -Aryl complex

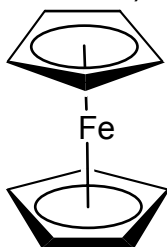


Figure D.66:  $Cp_2TiCl_2$ , another  $\pi$ -Aryl complex

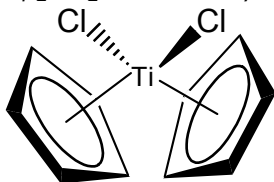
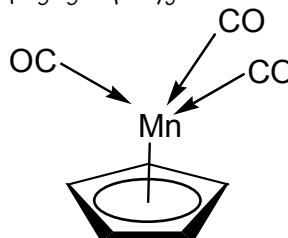


Figure D.67  $\eta^5-C_5H_5Mn(CO)_3$



## Stereochemistry

Absolute stereochemistry is calculated for tetrahedral atoms and double bonds according to the Cahn-Ingold-Prelog (CIP) priority rules. The CIP rules are designed to order ligands by their priority and determine a descriptor based on the orientation of the ordered ligands in space.

A ligand is an entity attached to a stereocenter. For example, a tetrahedral carbon has four ligands corresponding to its four substituents. When a tetrahedral carbon is in a ring, it still has four ligands: the two ligands outside the ring, a third consisting of the ring “unpeeled” clockwise, and a fourth consisting of the ring “unpeeled” counterclockwise.

Five rules are used to determine the priority of ligands are summarized below in simplified form. For more detailed information, see the references. They are checked sequentially as follows:

- **Rule 1**—Higher atomic number precedes lower
- **Rule 2**—Higher atomic mass precedes lower
- **Rule 3**—*cis* precedes *trans*
- **Rule 4**—Like pairs of descriptors precede unlike pairs
- **Rule 5**—R precedes S

ChemDraw checks differences up to 15 atoms distant from the stereocenter.



## Stereochemical Indicators

After the ligands are ranked, an indicator is assigned as shown in the following table.<sup>1</sup>

Table 34: Ligand ranking in stereochemistry

Stereocenter	Indicator
Double bond	Z if the highest ranking ligand of each pair are on the same side of the bond; otherwise E.
Tetrahedral atom	When the lowest-ranking ligand is located behind the central atom: <ul style="list-style-type: none"><li>• R when remaining 3 ligands are arranged clockwise in descending order</li><li>• S when remaining 3 ligands are arranged counterclockwise in descending order</li><li>• r or s is used for pseudo asymmetric atoms</li></ul>

## Stereochemical Flags

While the chirality of a specific stereocenter can be indicated with the appropriate wedged, hashed, or plain bond, sometimes it is useful to indicate the relative stereochemistry of a molecule as a whole, considering the relationship between all stereo-

1. R.S. Cahn, C.K. Ingold, and V. Prelog, "Specification of Molecular Chirality", *Angew. Chem., Int. Ed. Engl.* 1966, 5, 385-414 (errata: 1966, 5, 511); *Angew. Chem.* 1966, 78, 413-447.

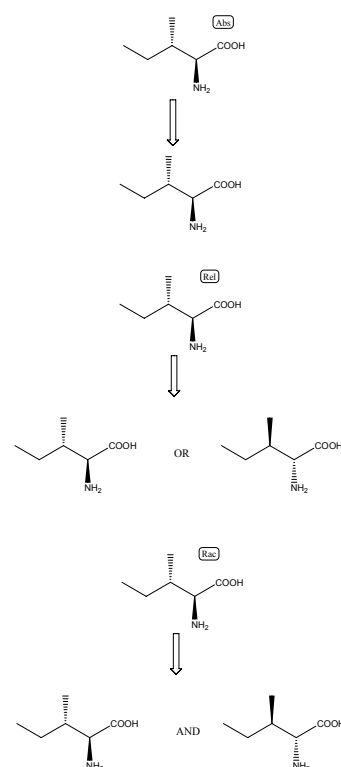
V. Prelog and G. Helmchen, "Basic Principles of the CIP-System and Proposals for a Revision", *Angew. Chem.* 1982, 94, 614-631; *Angew. Chem., Int. Ed. Engl.* 1982, 21, 567-583.

P. Mata, A.M. Lobo, C. Marshall, and A.P.

Johnson, "The CIP Sequence Rules: Analysis and Proposal for a Revision." *Tetrahedron:Asymmetry.* 1993, 4, 657-668.

centers. Stereochemical flags apply to the nearest structure; if no structure is within the distance specified by the Fixed Length value, the stereochemical flag is not assigned to any structure.

Table 35: Stereochemical flags



The Absolute flag indicates the exact stereoisomer as drawn.

The Relative flag indicates the exact stereoisomer as drawn, or its enantiomer.

The Racemic flag indicates a mixture of the exact stereoisomer as drawn and its enantiomer.

## Polymer Representations

Brackets are used to enclose repeated structures or structural fragments. ChemDraw provides bracket properties to specify the orientation and context of the repeating units. An explanation of the bracket properties is given in "Representing Polymers and Other Repeating Units" on page 99.

## References

"Graphic Representations (Chemical Formulae) of Macromolecules (Recommendations 1994)" *Pure Appl. Chem.*, **66**, 2469-2482 (1994).

“Source-Based Nomenclature for Copolymers (Recommendations 1985)” *Pure Appl. Chem.*, **57**, 1427-1440 (1985). Also available at: <http://www.iupac.org/publications/books/pbook/PurpleBook-C7.pdf>.

“Basic Definitions of Terms Relating to Polymers (1974)” *Pure Appl. Chem.*, **40**, 479-491 (1974) Also available at: <http://www.iupac.org/reports/1996/6812jenkins/index.html>).

Also see the Guide for the authors of papers and reports in polymer science and technology from IUPAC.

## Query Properties

By their nature, query properties do not represent actual chemical features, but describe broad classes or groups of features. For information on using query properties, see Chapter 5: Query Structures.

## Analysis Messages

When ChemDraw is unable to analyze your structure fully, two general types of messages are displayed:

- Status messages that report a problem that may not affect the final analysis

- Critical messages that may affect the final analysis

Table 36: Analysis messages

Message	Description
There are too many bonds to this unlabeled Carbon.	Displayed for every unlabeled atom with more than 4 filled valences. Filled valences include sum of bond orders, charge, radicals, and free sites. Aromatic bonds count 1.5 each, rounded down unless it is the only bond to the atom. Charge is signed and includes charge implied by dative bonds. The Substituents query property treats Free Sites, Up to and Exactly the same way: an atom with 2 explicit bonds and “Substituents: Up To 3” or “Substituents: Exactly 3” or “Substituents: Free Sites 1” has three filled valences.
An atom in this label has an invalid valence.	Displayed in a variety of cases where ChemDraw cannot find a place to put a bond or cannot find a bond to put on an atom. Valid valences for each element are listed in the Isotopes Table file.
ChemDraw can't interpret this label.	Displayed when ChemDraw finds text that it cannot identify as an element, nickname, generic nickname, or alternative group name.

Table 36: Analysis messages

Message	Description
Parentheses don't match.	Displayed when parentheses cannot be matched into nested open-close pairs.
This label has conflicting or unassignable charges.	Displayed when a plus and minus charge 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.
Formula cannot be computed for queries.	Displayed for every label that contains a generic nickname, an element list or an alternative group. This is a status message only; analysis continues as if the problematic label were not selected.
Text not in Formula style won't be interpreted.	Displayed for the first caption that is not an atom label or Alternative Group name, and which contains any text not in Formula, Subscript, or Superscript style. This is a status message only, and appears only once regardless of how many captions are in the selection.
This named alternative group contains no attachment point.	Displayed for any structure within an Alternative Group Box where the structure lacks an attachment point. This is a status message only.

Table 36: Analysis messages

Message	Description
This named alternative group contains fragments with inconsistent valences.	Displayed for any Alternative Group Box whose contained structures have varying numbers of attachment points. Since all structures within an Alternative Group Box are to be used interchangeably, they must have the same number of attachments. This is a status message only.
This named alternative group contains no fragment.	Displayed for any Alternative Group Box that is empty. This is a status message only.
Part of a molecule is outside of the alternative group definition.	Displayed for any Alternative Group Box whose border crosses part of a structure. This is a status message only.
This isolated bond is probably not intended to have chemical significance.	Displayed for unlabeled single bonds unattached to other bonds. All bonds are interpreted chemically, usually as $C_2H_6$ , and may cause unexpected results if intended as a graphical line only. This is a status message only.
The atom is very close to another atom or bond.	Displayed for any atom that is nearly touching another atom or bond but not bound to it. If a bond really was intended, the analysis of the structure produces incorrect results. This is a status message only.

Table 36: Analysis messages

Message	Description
The stereocenter has no stereo-bonds specified.	Displayed for any asymmetric center without attached wedged, hashed, dashed, or bold bonds. This is a status message only, and appears only when Show Stereochemistry is tuned on and there is at least one other wedged, hashed, dashed, or bold bond in the structure.
There is a valence and charge error somewhere in this aromatic system.	Displayed for any odd-membered ring drawn as a delocalized system (with a circle in the middle), where there is no corresponding associated charge. For example, a delocalized representation of cyclopentadiene must include either a negative charge or a multicenter attachment.
The stereocenter has conflicting or ambiguous stereo-bonds specified.	Displayed for any stereocenter (tetrahedral atom, asymmetric double bond, etc.) where the absolute stereochemistry cannot be determined from the structure as drawn. For example, this message would be shown for a carbon atom attached by bold bonds to four different ligands. This message is displayed only when Show Stereochemistry is also turned on.

Table 36: Analysis messages

Message	Description
This label has an unrecognized isotopic mass.	Displayed 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, $^{24}\text{CH}_3$ .

# Appendix E: How ChemProp Works

## ChemProp Values

ChemProp enables you to calculate predicted values of selected physical and thermodynamic properties for structures of up to 100 atoms. The following topics describe how ChemProp obtains its values.

### LogP

**LogP** (partition coefficient for *n*-octanol/water)—three fragmentation methods are used to predict the logP values.

Method one is based on 94 atomic contributions evaluated from 830 molecules by least squares analysis. This method works with a standard deviation of 0.47 logP units and can handle molecules containing hydrogen, oxygen, nitrogen, sulfur and halogens.

6. Method two is an extension of method one that is based on 120 atomic contributions evaluated from 893 molecules by least squares analysis. In addition to the atoms introduced for method one, it can handle molecules that contain phosphorus and selenium atoms. This method works with a standard deviation of 0.50 logP units.
7. Method three is based on 222 atomic contributions calculated from 1868 molecules by least squares analysis. This method allows a calculation of logP with a standard deviation of 0.43 logP units and can handle molecules containing hydrogen, oxygen, nitrogen, sulfur, halogens and phosphorus atoms. If this method is applied to molecules with internal hydrogen bonds, the standard deviation is 0.83 logP units.

## Henry's Law

**Henry's Law Constant**—The air to water partition coefficient that is expressed as ratio of vapor pressure to water solubility or as a unitless distribution coefficient that can be evaluated as a ratio of the concentration in air to the concentration in water.

Two methods are used to predict Henry's Law constant.

1. The first is an approach based on the bond contribution method. This method uses 59 bond contribution values and 15 correction factors. The contributions were calculated by least squares analysis using a data set of 345 chemicals. This method estimates with a mean error of 0.30 units and a standard deviation of 0.45 units and can handle molecules containing carbon, hydrogen, oxygen, nitrogen, sulfur, phosphorus and halogens.
2. In the second method, Henry's Law constant is estimated from an equation found using linear regression. Multifunctional compounds were omitted from this study. This method should not be used for compounds where distant polar interaction is present.

## Molar Refractivity

**Molar refractivity**—Two fragmentation methods are used to estimate the molar refractivity value.

1. Method one includes 93 atomic contributions evaluated from 504 molecules by using a constrained least squares technique. This method works with a standard deviation 1.27 cm<sup>3</sup>/mol and can handle molecules containing hydrogen, oxygen, nitrogen, sulfur and halogens.

2. The second method is an extension of method one that includes 120 atomic contributions evaluated from 538 molecules by using a constrained least squares analysis technique. In addition to the atoms introduced for method one, this method can handle molecules with phosphorus and selenium atoms. This method works with a standard deviation of 0.77 cm<sup>3</sup>/mol.

**Ultra**

## **ClogP and CMR**

Specific algorithms for calculating LogP and molar refractivity from fragment-based methods developed by the Medicinal Chemistry Project and Bio-Byte.

For more information, see: <http://www.biobyte.com>

## **Topological Polar Surface Area**

The polar surface area of a molecule (measured in square Angstroms) is an important property that can be used for the prediction of pharmaceutical transport properties in the body. Historically, this property has been calculated using time-consuming

3D techniques, but a recent paper<sup>1</sup> has provided a remarkably accurate way of predicting it very rapidly. ChemDraw implements this algorithm, and displays it on the Chemical Properties window.

## **Other Properties**

**Heat of Formation, Gibbs Free Energy, Ideal Gas Thermal Capacity, Freezing Point, Critical Temperature, Critical Pressure, and Critical Volume** are estimated using Joback's fragmentation method.

### **Normal Boiling Point and Melting Point—**

Estimated in K using two methods.

1. Joback's fragmentation method.
2. The Joback method as modified by Stein. All boiling points are estimated at a pressure of 1 atm.

1. Ertl, P., Rohde, B., and Selzer, P., 2000. Fast Calculation of Molecular Polar Surface Area as a Sum of Fragment Based Contributions and Its Application to the Prediction of Drug Transport Properties. *J.Med. Chem.*43: 3714-3717.

# Appendix F: How ChemNMR Works

ChemNMR estimates chemical shifts for all hydrogen or carbon atoms for which additivity rules are available. Following a hierarchical list, it first identifies key substructures of a molecule. A substructure provides the base value for the estimated shift. For example, benzene would be identified as the key substructure of trinitrotoluene.

When a substructure happens to be a ring system not available in the data, ChemNMR approximates its base shift using embedded rings and, if necessary, it will even disassemble the ring into acyclic substructures.

ChemNMR views remaining parts of the molecule as substituents of a substructure. Each substituent adds to or subtracts from the base shift of the substructure to which it is attached. Additivity rules determine the increment of each contribution. If an increment for a substituent cannot be determined, ChemNMR uses embedded substituents—smaller structural units with the same neighboring atoms. Or, it will use increments of identical or embedded substituents of a corresponding substructure by assuming that the effects of the substituents are of the same magnitude.

ChemNMR provides a detailed protocol of the estimation process applied. It gives substructures as names, compound classes in most cases, substituents in form of a linear code, respectively.

The data set for the  $^1\text{H}$  NMR Shift tool currently contains 700 base values and about 2000 increments. The  $^{13}\text{C}$  NMR Shift tool is based on 4000 parameters. It also implements models for ethylenes (cis/trans) and cyclohexanes (equatorial/axial).

## ChemNMR Limitations

The program handles the following elements:

H, D, He, Li, Be, B, C, N, O, F, Ne, Na, Mg, Al, Si, P, S, Cl, Ar, K, Ca, Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Ga, Ge, As, Se, Br, Kr, Rb, Sr, Y, Zr, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Cd, In, Sn, Sb, Te, I, Xe, Cs, Ba, La, Ce, Pr, Nd, Pm, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu, Hf, Ta, W, Re, Os, Ir, Pt, Au, Hg, Tl, Pb, Bi, Po, At, Rn, Fr, Ra, Ac, Th, Pa, U, Np, Pu, Am, Cm, Bk, Cf, Es, Fm, Md, No, Lr. Functional groups are expanded automatically.

In case of  $^1\text{H}$  NMR, it estimates shifts of about 90% of all  $\text{CH}_x$ -groups with a standard deviation of 0.2–0.3 ppm. The use of polar solvents may strongly increase these deviations. It does not estimate shifts of hydrogen atoms bonded to heteroatoms because they are significantly affected by solvents, concentration, impurities, and steric effects.

In case of  $^{13}\text{C}$  NMR, it estimates over 95% of the shifts with a mean deviation of -0.29 ppm and standard deviation of 2.8 ppm.

For more information see:

Fürst, A.; Pretsch, E. *Anal. Chim. Acta* **1990**, *229*, 17.

Pretsch, E.; Fürst, A.; Badertscher M.; Bürgin, R.; Munk, M. E. *J. Chem. Inf. Comp. Sci.* **1992**, *32*, 291–295.

Bürgin Schaller, R.; Pretsch, E. *Anal. Chim. Acta* **1994**, *290*, 295.

Bürgin Schaller, R.; Arnold, C.; Pretsch, E. *Anal. Chim. Acta* **1995**, *312*, 95–105.

Bürgin Schaller, R.; Munk, M. E.; Pretsch, E. *J. Chem. Inf. Comput. Sci.* **1996**, *36*, 239–243.





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# Appendix CS-1: Technical Support

## Overview

CambridgeSoft Corporation (CS) provides technical support to all registered users of this software through the internet, and through our Technical Support department.

Our Technical Support webpages contain answers to frequently asked questions (FAQs) and general information about our software. You can access our Technical Support page using the following address: <http://www.cambridgesoft.com/services/>

If you don't find the answers you need on our website, please do the following before contacting Technical Support.

1. Check the ReadMe file for known limitations or conflicts.
2. Check the system requirements for the software at the beginning of this User's Guide.
3. Read the Troubleshooting section of this appendix and follow the possible resolution tactics outlined there.
4. If all your attempts to resolve a problem fail, fill out a copy of the CS Software Problem Report Form at the back of this User's Guide. This form is also available on-line at:  
<http://www.cambridgesoft.com/services/mail>
  - Try to reproduce the problem before contacting us. If you can reproduce the problem, please record the exact steps that you took to do so.
  - Record the exact wording of any error messages that appear.
  - Record anything that you have tried to correct the problem.

You can deliver your CS Software Problem Report Form to Technical Support by the following methods:

**Internet:** <http://www.cambridgesoft.com/services/mail>

**Email:** [support@camsoft.com](mailto:support@camsoft.com)

**Fax:** 617 588-9360

**Mail:** CambridgeSoft Corporation

ATTN: Technical Support

100 CambridgePark Drive

Cambridge, MA 02140 USA

## Serial Numbers

When contacting Technical Support, you must *always* provide your serial number. This serial number was on the outside of the original application box, and is the number that you entered when you launched your CambridgeSoft application for the first time. If you have thrown away your box and lost your installation instructions, you can find the serial number in the following way:

- Choose About CS <application name> from the Help menu. The serial number appears at the bottom left of the About box.

For more information on obtaining serial numbers and registration codes see: <http://www.cambridgesoft.com/services/codes.cfm>

## Troubleshooting

This section describes steps you can take that affect the overall performance of s Desktop Applications, as well as steps to follow if your computer crashes when using a CS software product.

## Performance

Below are some ways you can optimize the performance of CambridgeSoft Desktop Applications:

- In the Performance tab in the System control panel, allocate more processor time to the application.
- Install more physical RAM. The more you have, the less ChemOffice Desktop Applications will have to access your hard disk to use Virtual Memory.
- Increase the Virtual Memory (VM). Virtual memory extends RAM by allowing space on your hard disk to be used as RAM. However, the time for swapping between the application and the hard disk is slower than swapping with physical RAM.

Change the VM as follows:

- System control panel, Performance tab.

## System Crashes

CambridgeSoft Desktop Applications should never crash, but below are the steps you should go through to try to resolve issues that cause computer crashes while using a CS software product.

1. Restart Windows and try to reproduce the problem. If the problem recurs, continue with the following steps.
2. The most common conflicts concern Video Drivers, Printer Drivers, screen savers, and virus protection. If you do need to contact us, be sure to determine what type and version of drivers you are using.

- **Video Driver related problems:** If you are having problems with the display of any CambridgeSoft Desktop Application, try switching to the VGA video driver in the display Control Panel (or System Setup, and then retest the problems. If using a different driver helps, your original driver may need to be updated—contact the maker of the driver and obtain the most up-to-date driver. If you still have trouble contact us with the relevant details about the original driver and the resulting problem.
  - **Printer Driver related problems:** Try using a different printer driver. If using a different driver helps, your original driver may need to be updated—contact the maker of the driver and obtain the most up-to-date driver. If you still have trouble contact us with the relevant details about the original driver and the resulting problem.
3. Try reinstalling the software. Before you reinstall, uninstall the software and disable all background applications, including screen savers and virus protection. See the complete uninstall instructions on the CambridgeSoft Technical Support web page.
  4. If the problem still occurs, use our contact form at: <http://www.cambridgesoft.com/services/mail> and provide the details of the problem to Technical Support.

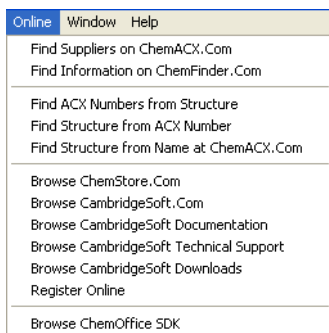
# Appendix CS-2: Accessing the CambridgeSoft Web Site

## Online Menu Overview

The ChemFinder Online menu gives you quick access to the CambridgeSoft web site from within ChemFinder. With the Online menu, you can:

- Register your software.
- Search for compounds by name or ACX number and insert the structure in a worksheet
- Use ACX numbers, or names or structures in the worksheet, to search for chemical information
- Browse the CambridgeSoft website for technical support, documentation, software updates, and more

To use the Online menu, you must have internet access.



## Registering Online

ChemOffice 2006 applications utilize a new security scheme. In order to activate any ChemOffice application, you must register with the CambridgeSoft website to receive a registration code. Upon filling out a registration form, the registration code is sent to you by email. This registration scheme does not apply to site licenses.

If your serial number is invalid for any reason, or if you do not have an internet connection, you will have to contact CambridgeSoft Support to receive a registration code.

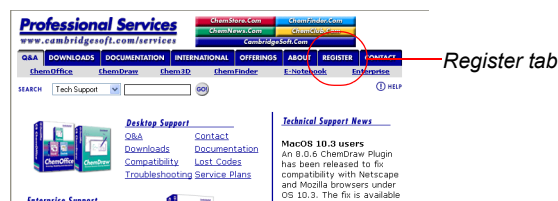
You may use your ChemOffice application a limited number of times while waiting for the registration process to be completed. Once the application times out, you must register to activate the software.

In addition to registering your software, you can request literature, or register for limited free access to ChemFinder.com, ChemACX.com, ChemClub.com, and the email edition of ChemNews from the Register Online link of the Online menu. This link connects you to the CambridgeSoft Professional Services page. From this page you can link to a registration form.

To register online:

1. From the Online menu, choose Register Online.

The CambridgeSoft Professional Services page opens in your browser.



2. Select the Register tab.

## Accessing the Online ChemDraw User's Guide

The Online menu link Browse CS ChemDraw Documentation opens the CambridgeSoft Desktop Manuals page, where you can access current and

previous versions of the ChemFinder User's Guide.

To access the CambridgeSoft Manuals page:

1. From the Online menu, choose **Browse CS ChemDraw Documentation**.



The Desktop Manuals page appears. PDF versions of the CambridgeSoft manuals can be accessed from this page.

**NOTE:** *If you do not have a CambridgeSoft User account, you will be directed to a sign-up page first.*

2. Click version of the manual to view.

## Accessing CambridgeSoft Technical Support

The Online menu link **Browse CS ChemFinder Technical Support** also opens the CambridgeSoft Professional Services page. There are a number of links on this page for Troubleshooting, Downloads, Q&A (the ChemOffice FAQ), Contact, and so forth.

## Finding Information on ChemFinder.com

The Find Information on ChemFinder.com menu item links your browser to the ChemFinder database record of the compound you have selected.

ChemFinder is the public-access database on the ChemFinder.com website. It contains physical, regulatory, and reference data for organic and inorganic compounds.

To access ChemFinder.com:

1. In ChemFinder, select a structure you want to look up.
2. From the Online menu, choose **Find Information on ChemFinder.com**.

The ChemFinder.com page opens in your browser with information on the selected structure.

In ChemFinder.com you can search for chemical information by name (including trade names), CAS number, molecular formula, or molecular weight. Follow the links to do substructure queries. The following illustration shows part of the page for Benzene.

**ChemFinder.com**  
Database © Internet Searching

Enter a Chemical Name, CAS Number, Molecular Formula or Weight.  
Use \* for partial names (e.g. ben\*).  
Search here for free. For professional searching, use ChemINDEX.

**Benzene [71-43-2]**  
**Synonyms:** (6)annulene; Benzene; Benzene ; benzine; Benzol; Benzolene; bicarburet of hydrogen; carbon oil; Coal naphtha; cyclohexatriene; mineral naphtha; motor benzol; nitration benzene; Phenia; Phenyl hydride; pyrobenzol;

**Tools**  
BUY AT CHEMACK.COM  
VIEW CHEMRAW STRUCT  
VIEW CHEM3D MODEL  
CAS RN Lookup  
THE MEECK INDEX  
NCI DATABASE

**OpenChem**  
VIEW LINKS  
ADD COMPOUND  
ADD/CHANGE PROPERTY  
ADD LINK

**Formula** C<sub>6</sub>H<sub>6</sub>      **Molecular Weight** 78.1134  
**CAS RN** 71-43-2      **Melting Point (°C)** 5.5  
**ACX Number** X1001498-9      **Boiling Point (°C)** 80.1  
**Density** 0.8786      **Vapor Pressure** 2.77  
**Refractive Index** 1.5011      **Vapor Pressure** 12.7 kPa @ 25 C  
**Evaporation Rate**      **Water Solubility** Slightly sol. (0.18 g/100 mL).  
**Fish Point (°C)** -11      **EPA Code** K040; K049; K051; K052; K056; K083; K085; K087; K103; K104; K105; K141; K142; K143; K144; K145; K147; K151; U019; D018  
**DOT Number** UN 1114 Flammable liquid; UN 1115 Flammable liquid  
**Comments** Colorless liquid with a paint-thinner-like odor detectable at 12 ppm.      **ITECS** CV1400000

**More information about the chemical is available in these categories:**  
Biochemistry      Health      Misc      MSDS  
Pesticides/Herbicides      Physical Properties      Regulations      Structures  
Trading      Usage

## Finding Chemical Suppliers on ACX.com

The Find Suppliers on ChemStore.Com menu item links your browser to the chemacx.com database record of suppliers of the compound you have selected.

ChemACX (Available Chemicals Exchange) is a Webserver application that accesses a database of commercially available chemicals. The database contains catalogs from research and industrial chemical vendors.

ChemACX allows the user to search for particular chemicals and view a list of vendors providing those chemicals.

To use Find Suppliers on ChemStore.Com menu access:

1. In ChemFinder, select a structure you want to look up.
2. From the Online menu, choose Find Suppliers on ChemStore.com.

The ChemACX.Com page opens in your browser with information on the selected structure.

For example the ChemACX.com page for Benzene is shown below.

The screenshot shows the ChemACX website interface. At the top left is the ChemACX CambridgeSoft logo. On the top right are links for SHOPPING CART, LOGIN, YOUR ACCOUNT, and HELP. Below these are navigation buttons: Print, Preferences, Help, About, and Log Off. A search bar contains 'New Query', 'Edit Query', 'Refine', 'Mark All Records', and 'Export Hits'. Below the search bar, it says 'Substances matching your query: 2' and 'Record 1-2 of 2 hits'. Two records are displayed side-by-side, each with a chemical structure of benzene and its CAS number: Record #1 (CAS#: 71-43-2) and Record #2 (CAS#: 27271-55-2). Each record has 'NAMES', 'DETAILS', and 'MARK' buttons above it.

For more information on using the ChemACX website, see the ChemOffice Enterprise Workgroup & Databases Manual.

## Finding ACX Structures and Numbers

ChemFinder searches ACX and returns information about related structures and numbers. You can place the returned information in your document.

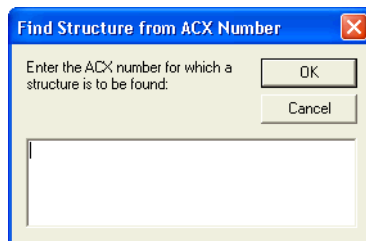
### ACX Structures

There are two ways to find ACX structures: by ACX number or by name.

To find a structure that corresponds to an ACX number:

1. From the Online menu, choose Find Structure from ACX Number.

The Find Structure from ACX number dialog box appears.



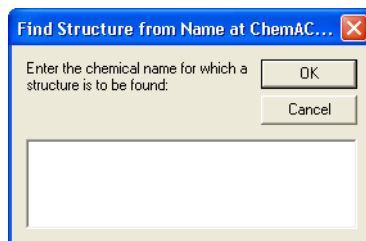
2. Type the ACX registry number.
3. Click the OK button.

The Structure appears in your document.

To find a structure from a name

1. From the Online menu, choose Find Structure from Name at ChemACX.com.

The Find Structure from Name dialog box appears.



2. Type in a name. As with ChemFinder.com, you can use a chemical name or a trade name.
3. Click the OK button.

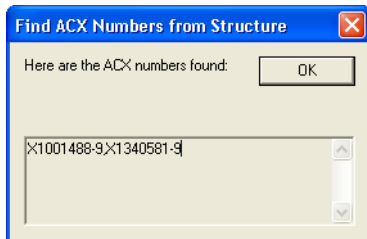
The Structure appears in your document.

## ACX Numbers

To Find an ACX number for a structure:

1. In a ChemFinder document, select the structure for which you want to find an ACX number.
2. From the Online menu, choose Find ACX Numbers from Structure.

The ACX number appears in the Find ACX Numbers from Structure dialog box.



## Browsing ChemStore.com

Browse ChemStore.com opens the ChemStore page of the CambridgeSoft web site.

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### CS ChemOffice Software Developer's Kit

Welcome to the CS ChemOffice software developer's kit (SDK) web site that provides documentation, sample code, and other resources for the ChemOffice component Application Programming Interfaces (APIs). You can use these APIs to create custom add-ons that enhance ChemOffice functionality or to add ChemOffice functionality to your programs. If you cannot find the code or samples on this site you are looking for, we may be able to provide you with what you need. Please contact [consulting](#) with the details of your code request.

Unless otherwise indicated, the information present on this site applies to the [latest versions](#) of our software.

APIs are available for the following ChemOffice components:

- ChemDraw

The ChemOffice SDK page contains documentation, sample code, and other resources for the Application Programming Interfaces (APIs).





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# CambridgeSoft Solutions

DESKTOP SOFTWARE  
ENTERPRISE SOLUTIONS

CHEMICAL INFORMATICS  
BIOLOGICAL INFORMATICS

KNOWLEDGE MANAGEMENT  
SCIENTIFIC DATABASES



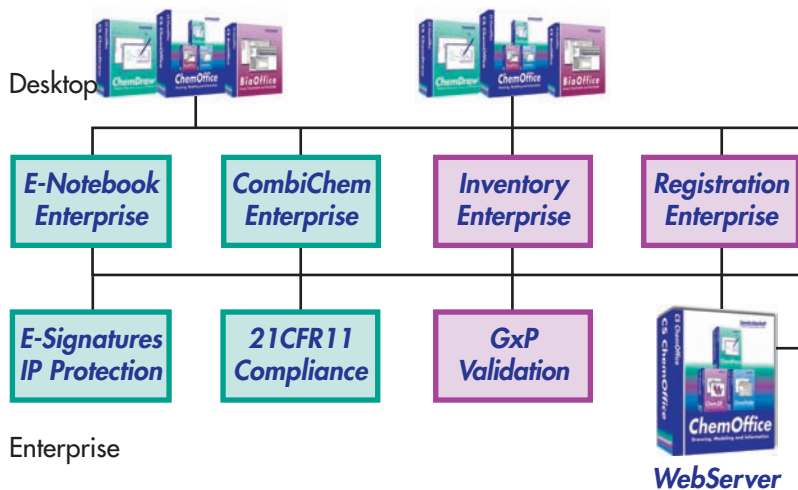
**CambridgeSoft®**

Life Science Enterprise Solutions  
Lösungen für biowissenschaftliche Unternehmen  
Solutions d'entreprise Life Science  
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# CAMBRIDGESOFT ChemOffice Desktop to

## KNOWLEDGE MANAGEMENT

## CHEMICAL INFORMATICS



## DESKTOP TO ENTERPRISE

Chem & Bio Office  
ChemOffice Workgroup  
ChemOffice Enterprise

Just as Chem & Bio Office supports the daily work of the individual scientist, ChemOffice Enterprise, with Oracle Cartridge, and ChemOffice Workgroup, based on SQL Server, help organizations from small workgroups to large enterprises collaborate and share information more effectively.

## KNOWLEDGE MANAGEMENT

E-Notebook Enterprise  
Reaction Explorer  
CombiChem Enterprise  
E-Signatures  
21CFR11 Compliance

Research organizations thrive when information is easily captured, well organized, and readily available. E-Notebook Enterprise streamlines record keeping with rigorous security and efficient archiving, and facilitates text and structure searching. Reaction Explorer can display the ancestors and descendants of a particular batch in seconds, while CombiChem Enterprise provides the power of combinatorial chemistry. E-Signatures provides intellectual property protection and 21CFR11 Compliance implements an organization's regulatory compliance process.

## CHEMICAL INFORMATICS

Inventory Enterprise  
GxP Validation  
Registration Enterprise  
DocManager Enterprise  
Oracle Cartridge

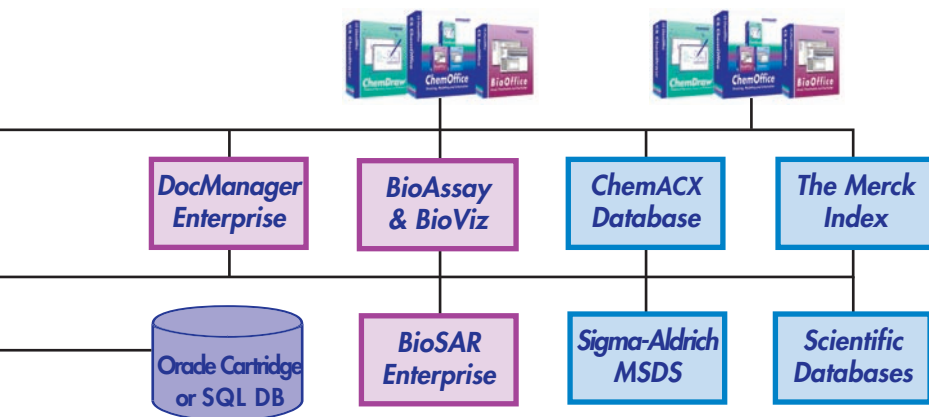
Managing huge data streams is a key challenge. Registration Enterprise organizes information about new compounds according to an organization's business rules, while Inventory Enterprise provides complete management of chemical and biological inventories, including GxP validation. DocManager Enterprise is an important part of collaborative research data management. Oracle Cartridge adds chemically intelligent searching to Oracle, integrating with ChemOffice Enterprise applications.

## SOLUTIONS

# Enterprise Solutions

### BIOLOGICAL INFORMATICS

### SCIENTIFIC DATABASES



*BioAssay Enterprise*  
*BioViz*  
*BioSAR Enterprise*  
*BioDraw*

*ChemDraw & Chem3D*  
*ChemFinder & ChemInfo*  
*BioAssay & BioViz*  
*BioDraw*  
*Inventory & E-Notebook*

*The Merck Index*  
*Scientific Databases*  
*ChemACX Database*  
*Sigma-Aldrich MSDS*

*Development*  
*Training & Support*

## BIOLOGICAL INFORMATICS

Finding structural determinants of biological activity requires processing masses of biological assay data. Scientists use *BioAssay Enterprise* and *BioSAR Enterprise* to set up biological models and visualize information, to generate spreadsheets correlating structure and activity, and to search by structure. The *BioViz* application allows you to create graphical representations of data.

## DESKTOP SOFTWARE

Success begins at the desktop, where scientists use *ChemDraw*, *ChemOffice*, and *BioOffice* to pursue ideas and communicate with the natural language of chemical structures, biological pathways, and models. Scientists organize information and manage data with *E-Notebook* and *Inventory*. *Chem3D* provides modeling, *ChemFinder* aids searching, while *BioOffice* adds *BioAssay*, *BioViz* and *BioDraw*. Integrated with Microsoft Office to speed research tasks.

## SCIENTIFIC DATABASES

Good research depends on reference information, starting with the structure-searchable *ChemACX Database* of commercially available chemicals and *Sigma-Aldrich MSDS*. *The Merck Index* and other scientific databases provide necessary background about chemicals, their properties, and reactions.

## PROFESSIONAL SERVICES

CambridgeSoft's scientific staff has the industry experience, and chemical and biological knowledge to maximize the effectiveness of your information systems.

Includes		Available Suites	ChemOffice Ultra	ChemOffice Pro	ChemDraw Ultra	ChemDraw Pro	BioOffice Ultra	BioDraw Ultra	BioAssay Ultra	BioViz Ultra	Inventory Ultra	E-Notebook Ultra	The Merck Index	ChemACX Ultra	
Software	*ChemDraw Ultra	Win/Mac	■	■	■										
	*ChemDraw Pro	Win/Mac				■									
	*ChemDraw Std	Win/Mac					■	■	■	■	■			■	
	*ChemDraw ActiveX/Plugin Pro	Win/Mac	■	■	■	■	■	■				■		■	
	*Chem3D Ultra	Win	■	■			■	■							
	*Chem3D ActiveX Pro	Win	■	■	■		■	■						■	
	*Chem3D & E-Notebook Pro	Win			■										
	Chem3D & E-Notebook Std	Win			■		■							■	
	ChemFinder Pro	Win	■	■				■							
	ChemFinder Std	Win			■		■					■		■	
Applications & Features	*BioDraw Pro (Pathworks)	Win	■	■	■			■	■	■	■				
	*BioAssay Pro	Win	■					■		■					
	*Inventory Pro	Win	■					■				■			
	*E-Notebook Ultra	Win	■					■						■	
	BioViz/Chem & Bio Finder	Win	■					■		■	■			■	
	CombiChem/Excel	Win	■											■	
	ChemFinder/Oracle	Win	■												
	ChemFinder/Office	Win	■	■	■			■						■	
	ChemDraw/Excel	Win	■	■	■									■	
	Struct<=>Name	Win/Mac	■	■	■										
Databases	ChemNMR & ClogP	Win/Mac	■	■	■										
	Stoichiometry Grid	Win/Mac	■	■	■										
	TLC Plate Tool	Win/Mac	■	■	■	■									
	Mass Fragmentation Tool	Win/Mac	■	■	■	■									
	Structure Clean Up	Win/Mac	■	■	■	■									
	Polymer Draw	Win/Mac	■	■	■	■									
	LabArt & BioArt	Win/Mac	■	■	■	■	■	■	■	■	■			■	
	Tinker/Chem3D	Win	■	■			■	■							
	MOPAC Client	Win	■	■			■	■							
	GAMESS Client	Win	■	■			■	■							
Gaussian Client	Win	■	■			■	■								
Jaguar Client	Win	■	■			■	■								
The Merck Index	Win/Mac												■		
*ChemACX Ultra (1 Year)	Win	■									■			■	
*ChemINDEX Ultra	Win	■	■	■		■	■						■		
ChemRXN, NCI & AIDS	Win	■	■	■		■	■						■		

\*Available Separately



# Chem & Bio Office

## Software Standard for Scientists

*the ultimate software suite for scientists*

**ChemOffice** is a powerful suite of software, consisting of *ChemDraw*, *Chem3D*, *ChemFinder* and *ChemACX* for chemists, *BioOffice*, *BioAssay*, *BioViz*, and *BioDraw* for biologists, and *Inventory*, *E-Notebook* and *The Merck Index* for scientists. *ChemOffice* and *BioOffice* are available for Microsoft Windows.

*the standard achieves the ultimate*

**ChemDraw** includes *Struct <=> Name*, *ChemDraw/Excel* and *ChemNMR*. Create stereochemically correct structures from chemical names, and get accurate IUPAC names for structures. Estimate NMR spectra from a *ChemDraw* structure with direct atom to spectral correlation. The *ChemDraw ActiveX/Plugin* adds chemical intelligence to your browser for querying databases and displaying information.

*computational chemistry made easy*

**Chem3D** provides visualization and display of molecular surfaces, orbitals, electrostatic potentials, charge densities and spin densities. *Chem3D* utilizes MOPAC, Gaussian, GAMESS and extended Hückel to compute molecular properties. *ChemProp* computes Connolly surface areas, molecular volumes and properties, including Tinker, ClogP, molar refractivity, critical temperature & pressure.

*desktop to enterprise searching*

**ChemFinder** is a chemically intelligent database manager and search engine. *ChemDraw/Excel* creates searchable spreadsheets. *ChemFinder/Word* searches documents, spreadsheets, and files for chemical structures and references. *ChemFinder* includes *CombiChem/Excel* for combinatorial library generation in chemical spreadsheets. *ChemFinder/Oracle* provides enterprise solution integration.

*ultimate suite for biologists*

**BioOffice** is the ultimate suite for management, analysis and visualization of biological data using *BioAssay* and *BioViz*. Use *BioDraw* for drawing pathways. Includes *Chem3D*, *Inventory* and *E-Notebook*.

*draw pathways*

**BioDraw**, formerly called Pathworks, makes drawing and annotating your biological pathways straight-forward and quick, adding a level of uniformity and detail which is unmatched.

*screening data*

**BioAssay** manages both high and low throughput biological screening data. Designed for complex lead optimization experiments, the software supports the quick set-up of biological models.

*visualize data*

**BioViz** offers automated calculations, curve fitting, and customized structure activity reports, including a user friendly interface for importing, viewing, validating & plotting biological assay data.

*handle reagent tracking*

**Inventory** manages your reagent and biological tracking needs. Using MSDE as the desktop database, you organize, store and search over your inventory. *Inventory* integrates with the *ChemACX* database of available chemicals and *ChemMSDX* safety data providing chemical sourcing and purchasing.

*efficient notebook keeping*

**E-Notebook** is the efficient, accurate way to write lab notebooks. It stores MS Office documents, *ChemDraw* structures and reaction drawings, and related data in a notebook searchable by text or chemical structure. Organize pages by project, experiment, or in your own style. Use *CombiChem/Excel* to build libraries.

*access info with ease*

**Databases** include *The Merck Index* and *ChemINDEX*, including the NCI and AIDS databases. The *ChemACX Database* contains nearly 400 catalogs from leading suppliers and *ChemMSDX Database* contains over 20,000 material safety data sheets for commonly used laboratory chemicals.

# Chem & Bio Office Workgroup

## Integrated Research, Discovery, Development,

### Research & Discovery - Search for Products

Since the company's founding, CambridgeSoft's desktop software, starting with its industry-leading *ChemDraw*, has been the cornerstone application for scientists who draw and annotate molecules, reactions, and pathways. The suite of applications has developed and CambridgeSoft now provides solutions in virtually all areas of discovery. Researchers can record and share their experimental information using *E-Notebook*, while protecting intellectual property with digital signatures and 21CFR11 compliance. They can design both single experiments or design combinatorial libraries of compounds. They find and purchase reagents in *ChemACX* database, store

and use them from *Inventory*, record newly made compounds within a proprietary *Registration* system, record the results from biological testing in *BioAssay*, analyze the results with *BioViz*, and generate reports linking activity and structure with *BioSAR*.

Virtually every aspect of discovery—from synthesis planning, library enumeration, reagent selection, primary and secondary screening, *in vivo* testing, through to analysis of results and reporting is covered by this integrated application suite.

### Development - Converting Leads into Testing

Building on productivity software, CambridgeSoft created enterprise applications to meet the needs of an

ChemOffice	Enterprise Ultra	Enterprise Pro	Enterprise Std	Workgroup Ultra	Workgroup Pro	Workgroup Std
Includes						
E-Notebook Enterprise or Workgroup	■			■		
BioAssay Enterprise or Workgroup	■			■		
BioSAR Enterprise	■					
BioViz Desktop				■		
Registration Enterprise	■	■				
Inventory Enterprise or Workgroup	■	■		■	■	
ChemACX Database	■	■		■	■	
ChemINDEX Database	■	■	■	■	■	■
Oracle Cartridge	■	■	■			
SQL Server Compatible				■	■	
ChemFinder Ultra				■	■	■

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## and Enterprise Solutions Trials and Manufacturing Workflow

ever expanding research and development community that relies on data sharing across scientific disciplines, research campuses, and even oceans as globalization has increased demands. Since it is web-based, the software is deployed readily throughout a research and development organization. Using *Registration*, *E-Notebook*, *BioAssay*, and *BioViz*, in conjunction with *DocManager* and *DrugDeg*, scientific teams are well armed to solve the daily challenges of development. These teams include scientists who scale up and design manufacturing procedures, toxicologists who determine the metabolic fate of drug candidates, formulation scientists who determine drug dosing and delivery systems, as well as many others.

### **Trials & Manufacturing - Last Steps to Success**

A suitable drug candidate is one that has the desired activity to provide disease therapy while still meeting drug safety requirements, can be manufactured in a cost effective and reproducible fashion under 21CFR11 and GMP guidelines, and is stable under normal formulation and storage conditions. With a drug candidate in hand, the final challenge is to determine safety and efficacy, beyond the laboratory, in a patient population.

Manufacturing requires the hand off of data and batch process records from the pilot plant studies using *Inventory*, *E-Notebook*, and *Registration* systems under Good Laboratory and Manufacturing Processes (GxP).

The handling of materials, including chain of custody requirements, material documentation, material workflow, such as availability states and recertification dates, are tracked and handling by the system. The systems meet these requirements and provide the basis to manage materials and records during clinical trials. Clinicians can design and record results from protocols, and all of these web based software systems provide the access required by clinicians who are removed from the sponsoring company.

**ChemOffice Enterprise** is a comprehensive knowledge management and informatics solution, covering electronic notebooks, biological screening, chemical registration and more over your intranet. *Enterprise Ultra* includes *E-Notebook* for record keeping, *BioAssay* for low and high throughput screening with integrated plate inventory, *BioSAR* for SAR reports, *Registration* system, *Inventory* for reagents and *ChemACX* database of available chemicals. Technologies include *ChemDraw ActiveX* and *Oracle Cartridge*.

**ChemOffice Workgroup** is a comprehensive knowledge management and informatics solution, covering electronic notebooks, biological screening and more over your intranet. *Workgroup Ultra* includes *E-Notebook* for record keeping, *BioAssay* for low and high-throughput screening, *BioViz* for visualization, *Inventory* for reagents and *ChemACX* database of available chemicals. Technologies include SQL Server for affordability and ease of administration.

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# E-Notebook, Reaction Explorer, Electronic Journal and Record Keeping

## E-Notebook

*E-Notebook* provides a smooth web-based interface designed to replace paper laboratory notebooks, with a fully configurable, secure system for organizing the flow of information generated by your organization. You can enter reactions, Microsoft Word documents, spectra and other types of data, and search this data by text, substructure or meta data. You can organize your electronic pages by projects, experiments or any other classification that conforms to your workflow.

## E-Notebook Enterprise

*E-Notebook Enterprise* edition integrates notebook keeping at group and enterprise levels to promote lab productivity and information sharing. Oracle Cartridge manages chemical structures in a common data repository with detailed security and 21CFR11 Compliance. The enterprise edition also works with procurement and inventory management systems to save time locating chemicals and entering structures.

## E-Notebook Workgroup

*E-Notebook Workgroup*, intended for use with a medium number of users, offers much of the functionality delivered in *E-Notebook Enterprise* while using SQL Server as the database. Learning to use and administer the application is quick and straightforward. *E-Notebook* applies various data types to suit different disciplines with an unlimited number of workflows.

- *E-Notebook* offers custom organization of notebook pages at personal or enterprise levels
- Quick access to important data by searching on keywords, dates, chemical structures and more
- *Reaction Explorer* can display the ancestors and descendants of a batch in seconds

## E-Notebook Ultra

*E-Notebook Ultra* is the efficient, accurate way to write lab notebooks entries as you work. It stores Microsoft Office documents, *ChemDraw* structures and reaction drawings, and related data in an electronic notebook you can search by text or chemical structure. Organize pages by project, experiment or your own style with the MSDE database. *CombiChem/Excel* builds combinatorial libraries.

## Reaction Explorer

*Reaction Explorer* is a powerful application that assembles a vast amount of information into a lucid synthesis map. The map provides reaction information, as well as quick access to experiments. *Reaction Explorer* displays two types of relationships between compounds: relationships grouped by batch and those grouped by compound. Both types of displays are configurable, allowing scientists to create a look and feel that they are comfortable with.

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## E-Signatures & 21CFR11 Compliance

### Property Protection and Regulatory Compliance

The batch display tracks the history of a particular entity through several subsequent reactions and experiments. This might be of interest to a chemical auditor or patent attorney needing to track down the original source of material.

The compound display is more general, and shows all possible pathways to and from a compound. This is ideal for chemists working to optimize a process, or a patent attorney trying to link a product to discovery, or a scientist trying to compile work done by several other scientists.

### Process Chemistry

The objective of process research is to identify efficient processes for the synthesis of active pharmaceutical agents at the scale required for clinical trials and commercial use. It is necessary to provide precise descriptions of these processes so that they can be executed by different groups in different locations. *E-Notebook's* process chemistry modules are designed to support these dual workflow and regulatory-compliance needs of process chemists. After the steps in a synthesis have been optimized, either individual steps or the entire synthesis must be scaled.

*E-Notebook* also provides the capability to scale reactions by virtually any parameter from reagent amount to vessel size. Individual reactions may be scaled as well as total syntheses. Batch procedures created with *E-Notebook* can be used to produce automatically batch record worksheets.

The screenshot displays the 'page "NotebookC-001"' window. At the top, it shows the reaction: c1ccccc1C=O + CC(=O)O → c1ccccc1C(=O)O. Below the reaction, there is a table for 'Reaction Conditions' and a 'Reaction' table with columns for 'Step', 'Date', 'Time', 'Location', 'Scale', 'Yield', 'Notes', and 'Status'. The 'Reaction' table contains several rows of data. At the bottom of the window, there is a 'Comment' field with the text 'Reviewed and approved', a 'User ID' field with 'A1q', and a 'Password' field. A 'Sign and Store' button is visible. To the right, a 'Display Ancestors' window is open, showing a hierarchical tree of chemical structures connected by arrows, representing the synthesis pathway. The structures include 'Cat', 'CH2=CH2', 'CH2=CH2', 'CH2=CH2', and 'CH2=CH2'. A green arrow points to the 'Display Ancestors' window with the text '▼ Display Ancestors'. A green arrow points to the 'Sign and Store' button with the text '▲ Authenticate Work'.

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# E-Notebook, Reaction Explorer, Electronic Journal and Record Keeping

## CombiChem Enterprise

Combinatorial chemistry, in particular the technique of parallel synthesis, has become an essential element of the drug discovery process. By using parallel synthesis techniques, chemists are able to multiply their productivity by a factor of between 5 and 100. *CombiChem Enterprise* has been developed to provide the tools required by the combinatorial chemist to manage and document parallel synthesis experiments.

Flexibility is the key when dealing with databases of chemical compounds. *CombiChem Enterprise* can use reagent lists from a variety of different sources: SD files, *ChemFinder* databases, *ChemFinder* hit lists, *ChemACX Database*, or directly from the user via *ChemDraw*. Regardless of the source, *CombiChem* produces a list of reagents which match a particular generic reactant.

## E-Signatures IP Protection

*E-Signatures* provides data storage and access functions for electronic records. It is used in conjunction with *E-Notebook* as a long-term storage system. While *E-Notebook* is intended to capture and record data as the experiments are carried out, *E-Signatures* serves as the repository for finished experiments and other documents. Electronic records must be available indefinitely, and their authenticity must be verifiable independently of the *E-Notebook* system. In addition to the record, *E-Signatures'* long-term archive includes a digital signature, a timestamp, and

- Highly flexible and configurable to match an organization's workflow
- Consulting teams analyze and adapt existing procedures to comply with new regulations
- Systems include authentication and digital signatures and adapt to changing regulations and demands for intellectual property protection

associated metadata. Managers, patent attorneys, and scientists can retrieve records based on searches over the metadata.

*E-Signatures* also manages the signature workflow for electronic records and documents in process. Digital signatures are captured at the time of record creation, which can later serve to prove the authenticity of the stored electronic records. Reviewers, witnesses, and other individuals can countersign records for various business purposes, including witness records necessary to meet the needs of 37 CFR and similar regulations worldwide.

## 21CFR11 Compliance

Large and growing enterprises are facing a challenge to their core missions of developing and producing new products including food, therapeutic pharmaceuticals, medical devices, cosmetics or other health

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## **E-Signatures & 21CFR11 Compliance** *Property Protection and Regulatory Compliance*

enhancing items. The complexity lies in complying with government regulations designed to protect public health and safety. The most notable of these is Title 21 of the Code of Federal Regulations governing Electronic Records and Signatures (21CFR11).

Once you have determined how your enterprise will comply with these new regulations, implementing those decisions needs to be done quickly, efficiently and with the understanding that the rules for compliance are in flux. In order to succeed, you must be able to respond to change. CambridgeSoft's *21CFR11 Compliance* consulting has both the tools and the expertise to provide complete solutions, carry out integration with existing systems, and help execute the process as quickly as your organization demands.

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# Inventory, Registration, Chem and Bio Inventory and Registration

## Chem & Bio Inventory

*Inventory* is an application designed to manage the chemical and reagent tracking needs of laboratories and research centers. The system manages data associated with both commercially procured and internally produced chemical substances from procurement or initial production through depletion and disposal. To meet the needs of institutions of all sizes, *Inventory* comes in an Enterprise edition, a Workgroup edition and two Desktop editions.

*Inventory Enterprise* is an Oracle-based, *ChemOffice Enterprise* product. Designed for large organizations, it comprises a number of features not included in the desktop or workgroup versions. *Inventory Enterprise* conveniently manages plate information. In addition to storing, moving, and deleting plates, the application allows users to create daughter plates and reformat plates. *Inventory Enterprise* can be tightly integrated with *Registration Enterprise* and *ChemACX Database*.

*Inventory Workgroup* is a thick-client SQL Server-based product. This version is suitable for larger organizations that do not have the interest or desire to maintain an Oracle server.

*Inventory Ultra* is the same MSDE based product, while also including the *ChemACX Database*, CambridgeSoft's collection of nearly 400 catalogs from suppliers of chemical reagents.

- *Inventory* offers plate handling for high-throughput experimentation
- *Inventory* is GxP Compliant with validated audit trails
- *Registration* has flexible business rules for registration, salt handling, and batch fields with chemical intelligence that includes advanced stereochemistry

*Inventory Pro* is an all-inclusive desktop product. It includes Microsoft SQL Server Desktop Edition (MSDE), the re-distributable database for SQL Server. No additional licensing is required.

## Registration Enterprise

*Registration Enterprise* includes a robust data model for pure compounds, batches, salt management, automatic duplicate checking and unique ID assignments. Compounds may be entered individually or through the use of a batch loader. The data model resides entirely in Oracle and uses Oracle's security and transaction framework. *Registration* is easily adapted to any workflow.

New compound chemical and non-chemical data is entered into a temporary storage area through a web form. When the compound is registered, it is compared for uniqueness via a configurable, stereo-selective duplicate check, and assigned a registry

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## DocManager & Oracle Cartridge

### Document Searching and Enterprise Infrastructure

number. All information about the compound, including its test data and other syntheses, is tracked by the registry number. When a compound is registered, the structure is checked for novelty. If a duplicate already exists in the database, the user can elect to register the information as a new batch of the existing compound, or assign it a unique registry number.

*Registration Enterprise* is the only true n-tiered application of its kind that is designed around thin clients and thin servers. This translates into ultimate flexibility on both the client and server side. Oracle is supported on a variety of platforms and operating systems. Using Oracle keeps your proprietary data secure through the use of Oracle's role based security and allows all chemical and non-chemical data to be stored directly in the Oracle tables.

### Formulations & Mixtures

Formulation scientists face different challenges from those working with individual molecules, yet many of the tools they are forced to use emerge from the drug-discovery world, where single-molecule research is the norm. Take an essential task such as compound registration and you will find that most

systems are designed for registration of single molecules, with little thought for the world of formulations and mixtures. CambridgeSoft has developed a system specifically designed for this registration need called *Formulations & Mixtures*.

Found ID container(s)

Container ID	Name	CAS	Substance	Barcode	Expires On	Entered On
6	Water			95		
280	H <sub>2</sub>		HYDROFLUORIC ACID	280	31/12/2004	21/10/2002
239	Fluorobenzene	462-56-6	Fluorobenzene	239	31/12/2004	
388	Tetraethyl ammonium hydro	76-69-2	TETRAETHYLAMMONIUM BROMIDE	388	30/03/2002	31/12/2002
457	dibromomethane	76-69-2	dibromomethane	457	31/12/2004	
719	1,4-DIOXANE	123-91-8	1,4-DIOXANE	719	31/12/2004	31/10/2002
541	Sodium iodide	7681-95-2	Sodium iodide	541	31/12/2004	
557	Pentaerythritol Tetrahydrate	78-11-5	Pentaerythritol Tetrahydrate	557	31/12/2004	
632	+OCTINE	1940-45-8	+OCTINE	632	31/12/2004	
730	Dimethylglycine, diiodum s	6908-54-5	Dimethylglycine, diiodum s	730	31/12/2004	

Summary | Substance | Supplier | Quantities | Comments | EHS | Custom

**LABDOWN**

Container Size:  Container Type:  Distilled

Dry-Weight:  Location:  Distilled

Purity:  CAS Number:  Distilled

Concentration:  Container ID:  Distilled

Density:  Date Created:  Distilled

Solvent:  Created by:  Distilled

Expiration Date:  Status:  Distilled

Owner:  Current User:  Distilled

Batch ID:

### ▲ Manage your Inventory

### H412 Assay Procedure

• **Preparation:** Room-temperature tablets from 95% alcohol, mp 220-224° (some decompose) when heated in vacuo.  $\text{C}_{20}\text{H}_{32}\text{O}_4$   $\text{M} = 320.48$  ( $\rho = 1.2$  in 95% alcohol),  $\text{H}^{\text{NMR}}$   $\delta$  2.0pp ( $\text{c} = 0.125$  in benzene),  $\text{H}^{\text{IR}}$   $\nu_{\text{max}}$  2940 ( $\text{c} = 0.1$  in 0.2 in alcohol),  $\text{IR}$  max: 297 cm ( $\nu$  1.4  $\times 10^3$ ), see Mann et al., J. Biol. Chem. 186, 247 (1956), Waterhouse, 1958a, ibid. 211. Fluffy solid in cold methanol, ethanol, acetone, much less so in ether, benzene, chloroform, slightly so in water (25 mg/100 ml at 25°). The water soln is neutral. Gives conjugated vils with intense green fluorescence in usual  $\text{H}_2\text{SO}_4$ . Reduces Benedict's soln on heating.

### ▼ Index Documents

Add Document Details

Next Step:

You are logged in as **doc\_admin**

(41 kb last modified at 11/5/2003 3:03:00 PM) shows below

of the document. Make changes if necessary before submission.

Procedure

Category

Use the WYSIWYG assay Procedure

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# Inventory, Registration, Chem and Bio Inventory and Registration

## DocManager Enterprise

Web browser based, *DocManager Enterprise* extends the capability of standard search engines to include full free text searching and chemically intelligent structure searching of electronic documents including Text, Microsoft Word, Excel, PowerPoint, and Adobe PDF.

The *DocManager Enterprise* interface allows users to easily submit documents through a series of simple to navigate web forms. When a new document is submitted, *DocManager* builds a free-text index of the document, and extracts chemical information into a chemically-aware, substructure searchable database. Chemical information can originate from either *ChemDraw* or ISIS Draw.

*DocManager Enterprise* includes a batch loading utility for administration level users to load multiple documents at one time. The system can be configured to submit a batch of documents as one event, or as a reoccurring submission to be executed daily. The administrator simply specifies a time for the submission to take place and the location of the files.

*DocManager Enterprise* utilizes the searching intelligence of the *ChemOffice Enterprise* suite. In addition to standard textual and numerical searching, *DocManager* searches the submitted documents for chemical structure or reaction.

- *DocManager* parses Word, Excel and PowerPoint documents, including free text
- *DocManager* has a web based interface and a file drop folder for quick submissions
- *Oracle Cartridge* is compatible with Linux, Solaris, AIX and Windows and includes structure searching, property predictions and nomenclature

## Oracle Cartridge

The CambridgeSoft *Oracle Cartridge* is used by all *ChemOffice Enterprise* applications for storing, searching over, and analyzing chemical data. It can also be used in the development of your custom Oracle applications. Chemical structure information is difficult to manipulate without utilizing special software. Oracle data cartridges define new, recognized datatypes. CambridgeSoft's *Oracle Cartridge* utilizes this technology making it possible to manipulate chemical structure and reaction data from within Oracle, improving portability and consistency in applications. Since the *Oracle Cartridge* is accessed through Oracle, this allows the programmer to interact with chemical structure data directly in Oracle. The CambridgeSoft *Oracle Cartridge* supports CDX, CDXML, MolFile, RXN, and SMILES formats making it flexible enough to be included with both new and legacy data, without the need for conversion.

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## **DocManager & Oracle Cartridge** *Document Searching and Enterprise Infrastructure*

### **ChemFinder Enterprise**

*ChemFinder Enterprise* is a multiple-user system designed for sites with heavy-duty chemical and biological data needs. *ChemFinder Enterprise* contains its own engine for working with local and shared databases and it is also delivered with the CambridgeSoft *Oracle Cartridge*, the powerful Oracle-hosted structure engine based on *ChemFinder* search technology. So, the face of *ChemFinder Enterprise* is the same friendly form-oriented interface as the desktop version, but underneath is a fast direct connection to Oracle and the robust, scalable *Oracle Cartridge* running on the server.

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# BioAssay, BioViz, Assay Screening and Visualization

## BioAssay

Biological assay data comes in many forms, from a scientist's observations to output from a plate reader. Software designed to store and analyze this data must provide a solution for both the ultra-high volume laboratories, including laboratory automation, calculation, and statistics, as well as the very complicated low and medium throughput assays such as animal models and *in vivo* experiments. Organizing, analyzing, and sharing data can be a challenge for screening biologists, regardless of the amount of automation or manual data manipulation employed.

*BioAssay* was designed to tackle the needs of high and low throughput screening biologists alike by providing an application flexible enough to model any assay, regardless of complexity, while robust enough to provide an easy to use interface for importing, storing and analyzing the data. The software supports the quick set-up of biological models, automated calculations and curve fitting, data validation, and the creation of customized structure activity reports.

*BioAssay Enterprise* offers a scalable, flexible biological screening solution utilizing Oracle's role based security and the *Oracle Cartridge*. As part of *ChemOffice Enterprise*, *BioAssay* is easily integrated with *Inventory Enterprise* for plate tracking and management, *Registration Enterprise* for the registration of new compounds and *BioSAR Enterprise* for customized reporting.

- *BioAssay* effectively manages data from complex biological assays involved with lead optimization
- *BioViz* provides a flexible reporting and plotting engine for your scientific data
- *BioViz* integrates with *BioSAR* for one step in-depth data analysis from a *BioSAR* report

*BioAssay Workgroup*, intended for single site deployment, uses SQL Server as a database, instead of Oracle. This solution offers affordability and ease of maintenance, but still remains a robust solution suitable for a smaller group's needs. Organize and share your biological screening data with minimal administrative costs.

*BioAssay Ultra* is designed to deliver much of the functionality of our enterprise level applications, without a widespread roll out. MSDE database compatible, *BioAssay Ultra*, coupled with *BioViz*, offers a user friendly interface for importing, viewing, validating, and plotting your biological assay data from your desktop.

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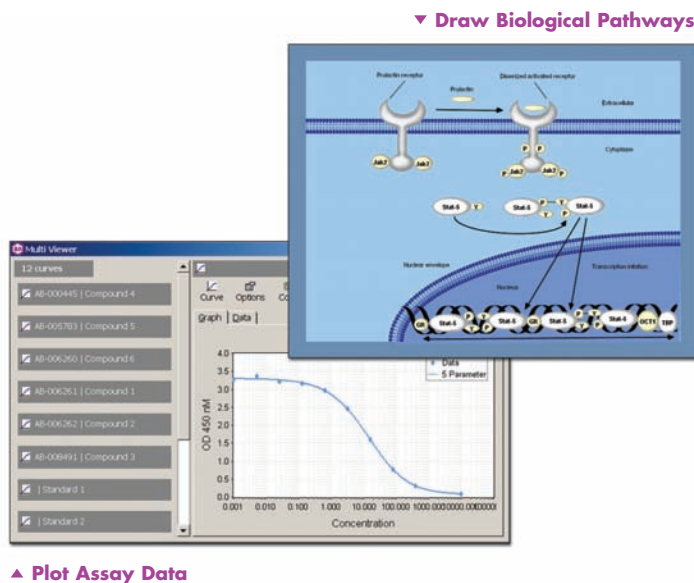
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## BioSAR & BioDraw Data Mining and Pathway Drawing

### BioViz

*BioViz*, with *ChemFinder*, transforms the numbers in your database into graphics on your screen. Retrieve or search for a set of compounds, choose the data you want to see, whether it is biological test results in Oracle tables, physical property values calculated automatically or prices in a catalog, and *BioViz* will generate an interactive window showing a scatterplot, histogram, or other useful data graphic.

The Plot Window, the key to data visualization in *BioViz*, shows two variables plotted against each other in a scatterplot with each point representing a structure from the current hit list. If you modify the list, for example by performing a search, the plot updates to show the new set of points. You can drag a rectangle around a set of points to select them, or zoom in to see them more closely.



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# BioAssay, BioViz, Assay Screening and Visualization

## BioSAR

*BioSAR Enterprise*, a strategic must for any discovery organization interested in serious data mining, is a data-dictionary driven structure-activity analysis program. Users may choose among assays registered in the dictionary or search for assays of interest. The power of *BioSAR* lies in the researcher's freedom from dependence on IT support. Once an assay is registered into the data-dictionary, it is automatically included in the powerful analysis framework. By reducing the time between question and answer, *BioSAR* gives researchers the ability to explore new ideas, the bottom line for discovery information systems. Systems that provide answers after questions have become irrelevant are of no use. *BioSAR* avoids this issue by placing application development in the researcher's control.

*BioSAR Enterprise* allows the researcher to create custom reports and views of their data. You decide what is displayed, and *BioSAR* takes care of the rest. While most SAR tools provide only a table-based interface, *BioSAR* provides a both a form view and table view. The form view provides highly detailed information about one compound, whereas the tabular view makes viewing comparisons between compounds more feasible. There is often a tradeoff between power and simplicity, and most SAR tools opt for the former at the expense of the latter. *BioSAR*, however, merges the sophistication of a powerful data catalog technique with knowledge gained through years of

- *BioSAR* is a catalog driven data mining and structure- activity analysis program
- *BioSAR* provides both form and table views within a simple and powerful web interface
- *BioDraw* makes it easy to draw and annotate biological pathways including common elements such as membranes, enzymes, receptors and DNA

working closely with users. The result is a SAR application that is as intuitive as it is powerful.

Security within *BioSAR Enterprise* is highly granular. Different roles exist for administrators, publishers, and browsers. Administrators may add assays to the data catalog engine, publishers may create reports and publish them, and browsers may use data query and analysis. Most data mining tools provide a mechanism to store queries, but the interface for creating queries is too complex. With *BioSAR*, each set of assays is a complete report with a query form, a view form, and a table view, combining the convenience of a *ChemFinder* or *ISIS* application with the power and flexibility of a data catalog-driven mining program.

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## **BioSAR & BioDraw** *Data Mining and Pathway Drawing*

### **BioDraw**

Reporting on and presenting findings is a task familiar to every biologist. Making this process easier and more effective benefits everyone involved. *BioDraw*, formerly called Pathworks, is doing for biologists what *ChemDraw* has done for chemists for years—saving time, and resulting in a more professional representation of the science at hand.

*BioDraw* makes drawing and annotating biological pathways quick and easy, adding a level of uniformity and detail which is unmatched. Typical drawings of biological pathways include many elements that are difficult to draw with the standard presentation and word processing software that is on the market. Common pathway elements such as membranes, enzymes, receptors, DNA and reaction arrows are built into the *BioDraw* toolbar. *BioDraw* also allows users to import images in GIF, PNG or JPEG format.

Keeping data organized is of utmost importance in any lab. *BioDraw* reflects that importance by allowing users to store annotations for each element in a drawing. Annotation data ranges from manually entered text to attached documents, restriction maps, microarrays, sequence information, literature references, or links. Any data, regardless of format, is stored side-by-side with the drawing for future retrieval.

The drawing and data organization offered by *BioDraw* gives any biologist an advantage. Sharing this advantage assists the community as a whole. *BioDraw* offers many ways to share your drawings and accompanying data. Users can export data to Microsoft Office applications for inclusion in presentations and grant proposals or save data as an image file for use in journal article submission.

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# ChemDraw, Chem3D, Structure Drawing and Molecular Modeling

**ChemDraw Ultra** adds *Struct<=>Name*, *ChemDraw/Excel*, *ChemNMR*, CLogP, tPSA and *ChemFinder/Word* to *ChemDraw Pro*. With rich polymer notation, atom numbering, *BioArt* templates, and modern user interface, *ChemDraw* is more powerful than ever before. Create tables of structures, identify and label stereochemistry, estimate NMR spectra from a *ChemDraw* structure with structure-to-spectrum correlation, obtain structures from chemical names, assign names from structures, and create multi-page documents and posters.

**ChemDraw Pro** will boost your productivity more than ever. Draw publication-quality structures and reactions. Publish on the web using the *ChemDraw Plugin*. Create precise database queries by specifying atom and bond properties and include stereochemistry. Display spectra, structures, and annotations on the same page. Use the *Online Menu* to query *ChemACX.Com* by structure and identify available vendors.

**Struct<=>Name** contains the leading comprehensive methods for converting chemical structures into chemical names and names to structures. It can be used for many types of compounds, including charged compounds and salts, highly symmetric structures and many other types of inorganic and organometallics. *Struct<=>Name* is available in two forms: a batch application, and an interactive version that is also available in *ChemDraw Ultra*.

- *ChemDraw's* improved *Struct<=>Name* feature produces names for more types of compounds
- Live *ChemDraw* window embedded in *Chem3D* application allows simultaneous 2D and 3D editing
- *Chem3D* brings workstation-quality molecular graphics and rigorous computational methods to your desktop

**ChemDraw/Excel** allows the user to create chemically knowledgeable spreadsheets within the familiar Microsoft Excel environment. You can build and manipulate chemical structures within Excel, compute chemical properties and perform database searches.

**ChemNMR** can be used to accurately estimate <sup>13</sup>C and <sup>1</sup>H (proton) chemical shifts. The molecule and the spectrum appear in a new window. The chemical shifts are displayed on the molecule and the spectrum is linked to the structure so that clicking on a peak in the spectrum highlights the related fragment on the molecule.

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# ChemFinder & ChemInfo

## Structure Searching and Scientific Databases

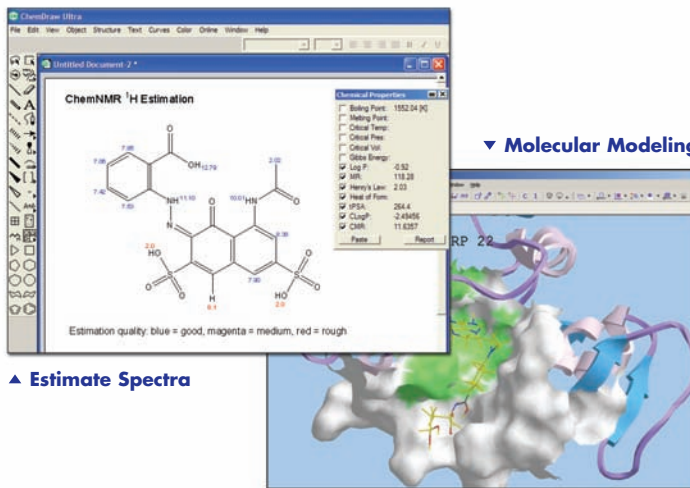
**Chem3D Ultra** includes a number of molecular modeling capabilities such as molecular overlay, conformational searching and dihedral driver support. It also includes interfaces for optional use of MOPAC, Gaussian and GAMESS. The user can also compute advanced physical properties such as *CLogP* and *ChemProp*. These properties can be used to create SAR tables. *ChemSAR/Excel* can then be used to explore structure activity relationships. High quality *Chem3D* graphics can be viewed on the web using the *Chem3D ActiveX*.

**Chem3D Pro** brings workstation quality molecular visualization and display to your desktop. Convert *ChemDraw* and ISIS/Draw sketches into 3D models. View molecular surfaces, orbitals, electrostatic potentials, charge densities and spin densities. Use built-in extended Hückel to compute partial atomic charges. Use MM2 to perform rapid energy minimizations and molecular dynamics simulations. *ChemProp* estimates physical properties such as logP, boiling point, melting point and more. Visualize Connolly surface areas and molecular volumes.

**MOPAC** is a semi-empirical quantum mechanics package which can be applied to the study of chemical properties and reactions.

It can also be used to predict a number of chemical and physical properties. *Chem3D* contains an interface to the MOPAC package.

**Gaussian** is a collection of semi-empirical and *ab initio* molecular orbital (MO) computational methods which can be used to predict energies, molecular structures, molecular properties, as well as molecular spectra. *Chem3D* enables the user to transparently create input and analyze output resulting from Gaussian.



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# ChemDraw, Chem3D, Structure Drawing and Molecular Modeling

**ChemFinder Enterprise** is a multiple-user system designed for chemical and biological data management. *ChemFinder Enterprise* contains its own engine for working with local and shared databases and it is also delivered with the CambridgeSoft *Oracle Cartridge*, the powerful Oracle-hosted structure engine based on *ChemFinder* search technology. So, the face of *ChemFinder Enterprise* is the same friendly form-oriented interface as the desktop version, but underneath is a fast direct connection to Oracle and the robust, scalable *Oracle Cartridge* running on the server.

*BioViz*, included in *ChemFinder Enterprise*, provides a new set of data visualization features. These features allow you to plot structural and biological data in a variety of styles, filter plots based on your criteria, highlight lists and intersecting sets on plots, generate histograms of data distributions, and more.

**ChemFinder Pro** is a fast, chemically intelligent, relational database search engine for desktop, workgroup or enterprise applications. Extended integration with Microsoft Excel and Word adds chemical searching and database capability to spreadsheets and documents.

Today, an ever-increasing number of chemical databases are available in *ChemFinder* format. Compatibility with MDL ISIS databases is provided by SDfile and RDfile import/export. *ChemFinder* provides network server workgroup functionality when used with *ChemOffice Workgroup* and *Enterprise*.

- *ChemFinder* offers improved searching and hitlist management, along with new property generation
- *ChemFinder* is tightly integrated with CambridgeSoft's *Oracle Cartridge*
- Search *ChemACX* and other CambridgeSoft databases for important chemical information

**The Merck Index** is an encyclopedia of chemicals, drugs and biologicals, with over 10,000 monographs covering names, synonyms, physical properties, preparations, patents, literature references, therapeutic uses and more.

**ChemACX Database** includes 500,000 chemical products from nearly 400 supplier catalogs, searchable with a single query by structure, substructure, name, synonym, partial name, and other text and numeric criteria. *ChemSCX* is a compilation of searchable catalogs from leading screening compound suppliers.

**ChemMSDX Database** provides material safety data sheets for 7,000 pure compounds.

**ChemINDEX Database** includes 100,000 chemicals, public NCI compounds, AIDS data, and more.

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# ChemFinder & ChemInfo

## Structure Searching and Scientific Databases

**NCI Database** contains over 200,000 compounds with anti-cancer drug dose-response data.

**AIDS Database** is an NCI compiled database for AIDS anti-viral compounds.

**ChemRXN Database** is a collection of 30,000 fully atom-mapped reactions selected and refined from the chemical literature. It includes reactions from InfoChem's ChemSelect database and ISI's ChemPrep database.

**ChemFinder.Com** is the award-winning web site with information and WWW links for over 100,000 chemicals. Users can search by name or partial name, view structure drawings, or use the *ChemDraw ActiveX/Plugin* for structure and substructure searches. In addition, users can view live *ChemDraw* files on Windows and Macintosh clients.

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# BioDraw, BioAssay, BioViz

## Pathways, Biological Assay and Visualization

### BioAssay Ultra

*BioAssay Ultra*, the cornerstone of *BioOffice*, provides flexible storage, retrieval, and analysis of biological data. *BioAssay* easily manages both high and low throughput biological screening data. Designed for complex lead optimization experiments, the software supports the quick set-up of biological models, automated calculations and curve fitting, and the creation of customized structure activity reports. *BioAssay* brings all of this functionality to your desktop. *BioAssay Ultra*, compatible with MSDE database, offers a user friendly interface for importing, viewing, validating and plotting your biological assay data.

### BioViz

Combining biological data with the chemical structure is of utmost importance in any drug discovery environment. *BioViz* allows you to analyze structure-related data combined with biological data visually. *BioViz*, within *ChemFinder*, provides a graphical representation of the data loaded into a *ChemFinder* form. Users can search over data and construct a scatterplot, histogram, or other useful data charts. Plots are interactive to allow you to select subsets of your data.

### BioDraw

*BioDraw*, formerly called Pathworks, makes drawing and annotating your biological pathways quick and easy, adding a level of uniformity and detail which is unmatched. Typical drawings of biological pathways include many elements that are difficult to draw with

- *BioAssay* offers flexible storage, retrieval and analysis of biological data
- *BioViz* provides a graphical representation of the data loaded into a *ChemFinder* form
- *BioDraw* allows for quick and easy drawing and annotating of biological pathways, including importing of images in GIF, PNG or JPEG format

the standard presentation and word processing software on the market. Common pathway elements such as membranes, enzymes, receptors, DNA and reaction arrows are built into the *BioDraw* toolbar and including them in your document is as easy as including a rectangle. Click on the toolbar shortcut and drop the element into your document. Resize and move elements by clicking and dragging and create an accurate and concise drawing in minutes.

*BioDraw* allows the import of images in GIF, PNG or JPEG format. *ChemDraw* users are also able to include *ChemDraw* structures in drawings without difficulty.

Keeping data organized is of utmost importance in any lab. The *BioDraw* application reflects that importance by allowing you to store annotations for each

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# Inventory & E-Notebook

## Materials Management and Electronic Journal

element in your drawing. Annotation data ranges from manually entered text to attached documents, literature references, or links. Any data, regardless of format, is stored side-by-side with the drawing for future retrieval.

The drawing and data organization offered by *BioDraw* gives any biologist an advantage. Sharing this advantage assists the community as a whole. *BioDraw* offers many ways to share your drawings and accompanying data.

### ▼ Notebook Pages

The screenshot displays the BioDraw software interface. At the top, a chemical reaction is shown: a bicyclic amine reacts with a carbonyl compound in the presence of MgEtO and Et<sub>2</sub>O to form a bicyclic amide. Below the reaction, a notebook page titled "Dyotropic Rearrangement Reaction" contains a detailed procedure for the preparation of gamma lactones. The procedure includes steps for the preparation of anhydrous magnesium bromide and the subsequent reaction of the lactone with the bicyclic amine. A table lists the reaction conditions and results, including the name of the product, its molecular weight, and the yield. The table is as follows:

Reaction	Name	Structure	Mol. Wt.	Yield
1	gamma-lactone	<chem>C1CCOC1</chem>	114.1	100%
2	gamma-lactone	<chem>C1CCOC1</chem>	114.1	100%
3	gamma-lactone	<chem>C1CCOC1</chem>	114.1	100%
4	gamma-lactone	<chem>C1CCOC1</chem>	114.1	100%
5	gamma-lactone	<chem>C1CCOC1</chem>	114.1	100%
6	gamma-lactone	<chem>C1CCOC1</chem>	114.1	100%
7	gamma-lactone	<chem>C1CCOC1</chem>	114.1	100%
8	gamma-lactone	<chem>C1CCOC1</chem>	114.1	100%
9	gamma-lactone	<chem>C1CCOC1</chem>	114.1	100%
10	gamma-lactone	<chem>C1CCOC1</chem>	114.1	100%

At the bottom left, a "Chemfinder" window shows a list of chemical structures. At the bottom right, a "Data Visualization" window displays a scatter plot of "CLOGP" (y-axis, ranging from -5 to 15) versus "MolWt" (x-axis, ranging from 0 to 1000). The plot shows a positive correlation between molecular weight and CLOGP, with data points clustered around a central value of approximately 400 for MolWt and 5 for CLOGP.

### ▲ Data Visualization

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# BioDraw, BioAssay, BioViz

## Pathways, Biological Assay and Visualization

### Inventory Ultra

*Inventory* is an application designed to manage the chemical and reagent tracking needs of laboratories and research centers. The system manages data associated with both commercially procured and internally produced chemical substances from their procurement or initial production through their depletion and disposal.

*Inventory Ultra* is an MSDE based product and includes the *ChemACX Database* with nearly 400 catalogs of chemical reagents. The three primary entities in an *Inventory* system are locations, containers, and substances. Users or administrators configure a network of locations, which represent locations within an organization.

Containers are created to represent actual containers in your facility. Each container is assigned a unique barcode, which can be printed, using a customized template, from the *Inventory* interface. Each container stores a substance. Additional text fields are available to track other chemical contents such as the solvent, and custom fields may also be defined. To keep track of substances, the system maintains its own internal chemical structure database containing unique substances that can be associated with inventory containers. Advanced duplicate checking is incorporated in the system.

Every field in a record, including chemical structure, molecular formula and molecular weight are search-

- *Inventory* manages the chemical and reagent tracking needs of laboratories and research centers
- *Inventory* maintains its own internal chemical structure database with advanced duplicate checking
- *E-Notebook* stores Microsoft Office documents, *ChemDraw* structures, reaction drawings and related data in a convenient, searchable format

able. The application includes a number of specially designed inventory search forms. Search results are returned in list form and can be exported into a document (PDF, RTF, HTML) using the report engine.

The *Inventory* interface allows for printing labels as well as generating elaborate reports. *Inventory* uses a report application that incorporates wizards that allow for the quick creation of simple report and label templates that can be shared across an organization.

### Inventory Pro

*Inventory Pro* contains the same features as *Inventory Ultra* without the *ChemACX Database*.

### E-Notebook Ultra

*E-Notebook Ultra* is the efficient, accurate way to write lab notebooks entries as you work. It stores

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# ***Inventory & E-Notebook*** ***Materials Management and Electronic Journal***

Microsoft Office documents, *ChemDraw* structures and reaction drawings, and related data in an electronic notebook that is searchable by text or chemical structure. You can organize pages by project, experiment, or in your own style with the MSDE database. *CombiChem/Excel* builds combinatorial libraries.

*E-Notebook* is configured exactly like a chemist would like his or her own notebook to be. Reactions can be easily drawn into the reaction template by either selecting from the generous list of preloaded reagents or by entering or drawing one's own chemicals. Commonly used reagents can be stored in a separate folder for easy access. Another fantastic feature is the procedural section. This section contains prewritten procedural sentences with the ability to easily drop in the specific names of reagent chemicals present in the reaction. One can also easily add other data to the notebook page such as spectra and Word or Excel documents.

## ***CombiChem/Excel***

CambridgeSoft provides you with the tools to effectively plan combinatorial chemistry experiments in Excel. The *CombiChem/Excel* add-in introduces additional functionality for handling combinatorial chemistry. Users can generate products from a reaction and lists of reagents, you can view all the products arising from a given reagent or all the reagents of a given product, and you can lay out reagent and reaction plates.

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# The Merck Index, NCI, AIDS, Scientific Reference, Chemical Reactions and Patents

## The Merck Index

Among printed chemical reference works, one that stands out for its integrity, detail and longevity is *The Merck Index*. *The Merck Index* database is a structure-searchable encyclopedia of chemicals, drugs, and biological agents which includes the complete 10,250 monographs of the 13th edition, 230 new monographs unavailable anywhere else, as well as 540 monographs retired from the 12th Edition.

*The Merck Index* is available in many forms to suit the various needs of both individuals and institutions. Personal subscriptions are available in one-year and one-month time periods. A stand-alone package, requiring no other applications, is also available for personal use.

The subjects covered include human and veterinary drugs, biological agents and natural products, industrial and laboratory chemicals, and environmentally significant compounds. In addition to the standard searches, compound monographs can be searched by *ChemDraw* structure as well as substructure.

## Traditional Chinese Medicines

Many of today's well-known drugs have their origins from natural sources. Access to this wealth of knowledge is now available with the *Traditional Chinese Medicines* database. The database consists of monographs for 10,458 chemicals isolated from 4,625 natural sources used in traditional Chinese remedies. The monographs feature bio-activity data for many

- *The Merck Index* offers encyclopedic reference for over 10,000 chemicals, drugs and biological agents
- *Traditional Chinese Medicines* provides chemical information and their biological effects of complex compounds isolated from natural sources
- All electronic databases are updated, contain information unavailable in print, and are searchable by structure, as well as text and numeric range

of the compounds, effects and indications of the medicines, English, Latin, and Chinese names for the natural sources, and over 2,000 references. This information is also available as an SD file to facilitate *in silico* research.

## ChemINDEX

The ability to quickly look up data such as chemical properties, biological assay results and toxicological information is no longer a luxury item, but instead a requirement. Scientists have used the award-winning *ChemFinder.Com* database since 1995. Now, the data on *ChemFinder.Com* is integrated into *ChemOffice* as *ChemINDEX*. *ChemINDEX* contains data on over 75,000 compounds including structures, names and synonyms, physical properties, and Internet links.

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## ChemACX & Sigma-Aldrich MSDS

### Available Chemicals and Material Safety Data Sheets

#### NCI, AIDS & Cancer

Three informative databases have been integrated into one powerful application with the NCI and AIDS database collections. The application starts with a collection of over 200,000 molecules collected by the National Cancer Institute. Searchable fields include structure, synonym, CAS RN, formula, and molecular weight.

#### ChemRXN

*ChemPrep* and *ChemSelect* are the two reactions databases that make up *ChemRXN*. *ChemPrep* is a reaction database assembled by the Institute for Scientific Information (ISI). This reaction database is designed to help organic chemists find reactions easily. It includes full literature citations. *ChemSelect*, licensed from InfoChem GmbH, is a reaction database containing 13,000 important organic reactions.

#### ChemSynth

*ChemSynth*, from InfoChem GmbH, is a database of sample reactions comprising essential information on 180,000 reactions. These reactions have been selected because they have greater than 50% yield and have been cited in leading journals more than once. The database consists of reaction information and literature reference.

#### ChemReact68

*ChemReact68*, from InfoChem GmbH, is a database of sample reactions comprising essential information on 68,000 reactions. These reactions have been selected because they have greater than 50% yield and have appeared in more than five example reactions. The database consists of reaction information and literature references.

#### Scientific Databases

REFERENCE DATA	
The Merck Index	11,000 monographs
Traditional Chinese Medicines	10,000 substances
ChemINDEX Database	75,000 substances
NCI, AIDS & Cancer	270,000 substances
Drugs: Synonyms & Properties	8,000 drugs
Medicinal Chemistry	540,000 substances
SOURCING & SAFETY DATA	
ChemACX Database	380 catalogs
ChemMSDX Database	23,000 MSDSs
Sigma-Aldrich MSDS	130,000 MSDSs
REACTION & SYNTHESIS DATA	
ChemRXN Database	28,000 reactions
ChemSynth	178,000 reactions
ChemReact68	68,000 reactions

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# Development, Deployment, Custom Development and System Deployment

In order to provide our customers with a total solution for scientific informatics, CambridgeSoft offers the following services to assist our clients in maximizing the productivity of their research and discovery organizations.

## Informatics Planning

### Strategic and Operational Planning

A formal analysis is conducted to provide a roadmap for successful technology utilization. This process includes:

- An analysis of the current state of the science technology environment, including architecture and operational processes
- A view of the strategic goals and the barriers to achievement
- The delivery of a phased technology transition plan

### Requirements Analysis & Proof of Concept

CambridgeSoft consultants can create or refine requirements to produce an environment that will ensure success. With years of experience meeting the needs of the scientific community, CambridgeSoft understands the user. The prototyping process allows definition and testing of the functional and technical feasibility of potential technology solutions. The process provides a baseline for the future development and deployment of a tailored solution. Users gain valuable first hand knowledge in experiencing how the system can help achieve individual and workgroup goals.

With custom development, CambridgeSoft works collaboratively with your team to create a system that meets your needs while executing our quality driven software development process. We deliver what you need, on time and within budget, without surprises.

### Project Readiness Assessment

Is your project set up for success? Is it well defined into measurable deliverables? Are the roles of project members clearly defined? CambridgeSoft's Project Readiness Assessment has one goal in mind—to create or assess current plans and make recommendations to ensure that results are achieved.

### 21CFR11 Compliance

Successfully implemented, a traceable and usable system is essential to any organization involved in the creation and management of data in a regulated environment. As an integral part in creating 21CFR11 and GxP validated applications, CambridgeSoft offers services to:

- Audit the software and process
- Create conforming systems design specifications
- Generate test plans and validation matrices
- Insure systems compliance with functional guidelines

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# Training & Support

## Educational Training and Technical Support

### Product Development

#### Data Conversion and Integration

When developing a new system, the process of converting existing data and creating interfaces with other data systems is an essential part of the process. CambridgeSoft's professional services staff is equipped to seamlessly incorporate existing data into the development of a new enterprise system. Organizations will be able to capitalize on historical scientific data while setting the platform for future success.

#### Custom Development

You have discovered a unique application need in your organization, but cannot find a solution that will meet your functionality or cost requirements. With custom development, CambridgeSoft works collaboratively with your team to create a system that meets your needs, while executing our quality driven software development process. We deliver what you need, on time and within budget, without surprises.

#### Systems Integration

The ability to integrate core applications with other systems in the technology environment is a competency required to deliver the functionality of a new application.

#### Product Tailoring

Your organization can see the benefit from implementing a CambridgeSoft application,

but would like to customize it for a unique environment. Our professional services teams can provide those specific features by making custom modifications that will be supported in the future.

### Systems Deployment

#### Installation and Configuration

CambridgeSoft will install and configure applications to meet the needs of your user community. For unique environments, we build custom installers that allow us to productively deploy software across an enterprise.



All specifications subject to change without notice.

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**MAIL** CambridgeSoft Corporation 100 CambridgePark Drive Cambridge, Massachusetts 02140 USA  
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# **Development, Deployment,** *Custom Development and System Deployment*

## **Systems Optimization**

CambridgeSoft's systems deployment team will work with you to make sure that your computing environment has been optimized for high performance. Your systems, networks, applications and databases are assessed and designed to deliver maximum achievement.

## **Beta and Pre-Release Programs**

CambridgeSoft is committed to maximizing your productivity through the use of our products, as well as exposing you to the newest technologies. Our beta and pre-release programs provide you with that knowledge, allowing CambridgeSoft to improve applications with your customer feedback.

## **Pilot Software Evaluations**

It often makes sense to pilot an application before a major commitment for an enterprise wide implementation is made. CambridgeSoft will work closely with you to plan the evaluation, deploy the application, and gather critical feedback regarding systems design, API's and technology specifications.

## **Training**

Effective user, administrator and help desk training is often an afterthought in many systems deployments. However, the productivity returns generated by an investment in systems training can provide dramatic returns. CambridgeSoft offers training in the following ways:

- On-site "real time" training through our profes-

Managed Informatics allows your organization to focus on science, allowing CambridgeSoft to plan, implement and manage your technology environment.

sional services staff supporting your systems environment

- On-site formal classroom training
- Webinars for multi-location instruction
- Off-site at CambridgeSoft facilities

## **Systems Management**

### **Managed Informatics**

There is no longer a need to worry about licensing fees, maintenance contracts, systems administration work or database support. Informatics Outsourcing provides the people, processes and technology to develop a unique level of service for your organization. For a monthly fee, CambridgeSoft will deliver the informatics applications and the technology staff required to maximize productivity. This service allows your organization to focus on science, while CambridgeSoft plans, implements and manages your technology environment.

### **Ultra Services**

The Ultra Services program is CambridgeSoft's personalized, premium service for supporting our

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# Training & Support

## *Educational Training and Technical Support*

customers. Organizations can take advantage of both telephone and electronic access to CambridgeSoft's support scientists who can address:

- Usage and installation questions
- Product compatibility and interoperability questions
- Diagnostic review to help isolate the cause of a problem
- Configuration assistance
- Planning information for software updates and upgrades
- Assistance with problem resolution

### **Technical Support & Remote DBA Services**

To complete our Management Services offerings, Technical Support and Remote DBA Services, for Oracle and SQL Server, are also available.

All specifications subject to change without notice.

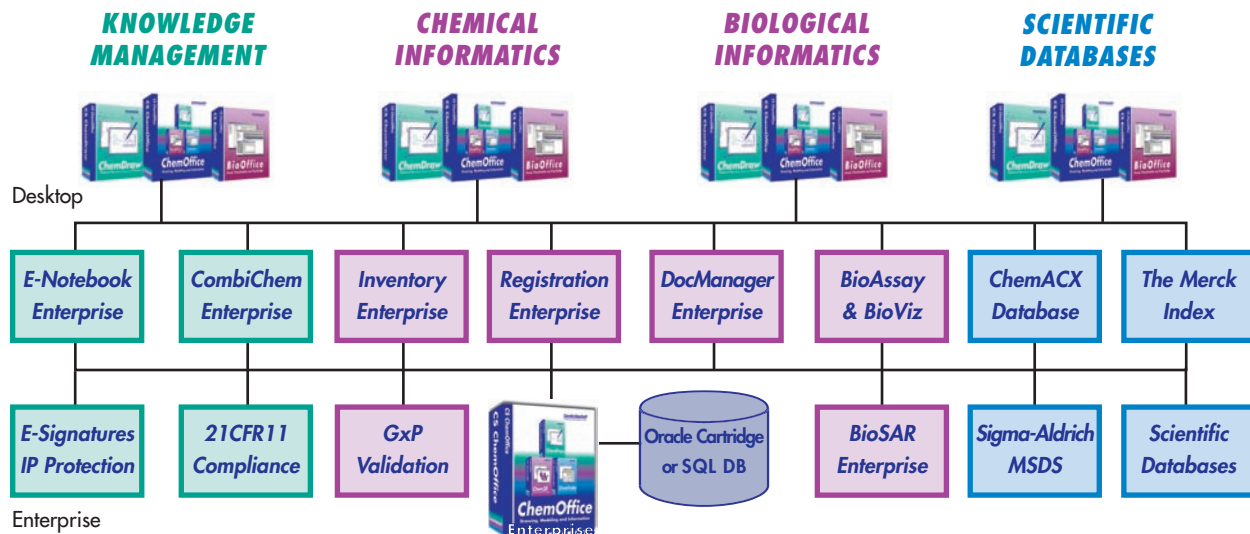
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# Chem & Bio Office

## Desktop Software to Enterprise Solutions



## Research, Discovery, Development, Trials & Manufacturing

**Enterprise Solutions** include *ChemOffice*, with *Oracle Cartridge*, and *ChemOffice Workgroup*, based on SQL Server to help organizations from small workgroups to large enterprises collaborate and share information more effectively.

**Desktop Software** includes *ChemOffice*, a powerful suite of software, consisting of *ChemDraw*, *Chem3D*, *ChemFinder* and *ChemACX* for chemists, *BioDraw*, *BioAssay* and *BioViz* for biologists, and *Inventory* and *E-Notebook*.

**Knowledge Management** with *E-Notebook*, including *Reaction Explorer*, *CombiChem*, *E-Signatures* for intellectual property protection and *21CFR11 Compliance*, streamlines daily record-keeping with rigorous security and efficient archiving.

**Chemical Informatics**, including *Registration*, organizes new compound information. *Inventory* provides complete management of chemical and biological inventories including *GxP Validation*. *DocManager* indexes chemical structures in documents.

**Biological Informatics** scientists use *BioAssay*, *BioViz*, *BioSAR* and *BioDraw* to set up biological models and visualize information, generate spreadsheets correlating structure and activity, search by structure, and draw and annotate pathways.

**Scientific Databases** include the *ChemACX Database* of commercially available chemicals and *Sigma-Aldrich MSDS*. *The Merck Index* and other scientific databases provide information about chemicals, their properties, and reactions.

**Professional Services** includes custom development, system deployment, educational training, and technical support for pharmaceutical, biotechnology, and chemical customers, including government and academia, by experienced staff.

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Lösungen für biowissenschaftliche Unternehmen  
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# CS Software Problem Report

For *faster* response and accuracy, use the Web:  
[www.cambridgesoft.com/services/mail](http://www.cambridgesoft.com/services/mail)

## USER INFORMATION (Please Print Legibly)

Name \_\_\_\_\_  
Title \_\_\_\_\_  
Firm \_\_\_\_\_  
Street \_\_\_\_\_  
City \_\_\_\_\_ State \_\_\_\_\_ Zip \_\_\_\_\_  
Country \_\_\_\_\_  
Tel \_\_\_\_\_ Fax \_\_\_\_\_  
Email \_\_\_\_\_

## Submit this form via...

WWW [www.cambridgesoft.com/services/mail](http://www.cambridgesoft.com/services/mail)  
EMAIL [support@cambridgesoft.com](mailto:support@cambridgesoft.com)  
FAX 1 617 588-9360  
MAIL CambridgeSoft, 100 CambridgePark Dr.  
Cambridge, MA 02140 USA

## DETAILS OF THE PROBLEM

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## SYSTEM CONFIGURATION

### SOFTWARE

Application Name \_\_\_\_\_  
Version Number \_\_\_\_\_  
Serial Number \_\_\_\_\_

### SYSTEM

Windows (version) \_\_\_\_\_  
MacOs (version) \_\_\_\_\_  
Web Browser(s) (version) \_\_\_\_\_

Please cut here or photocopy page.







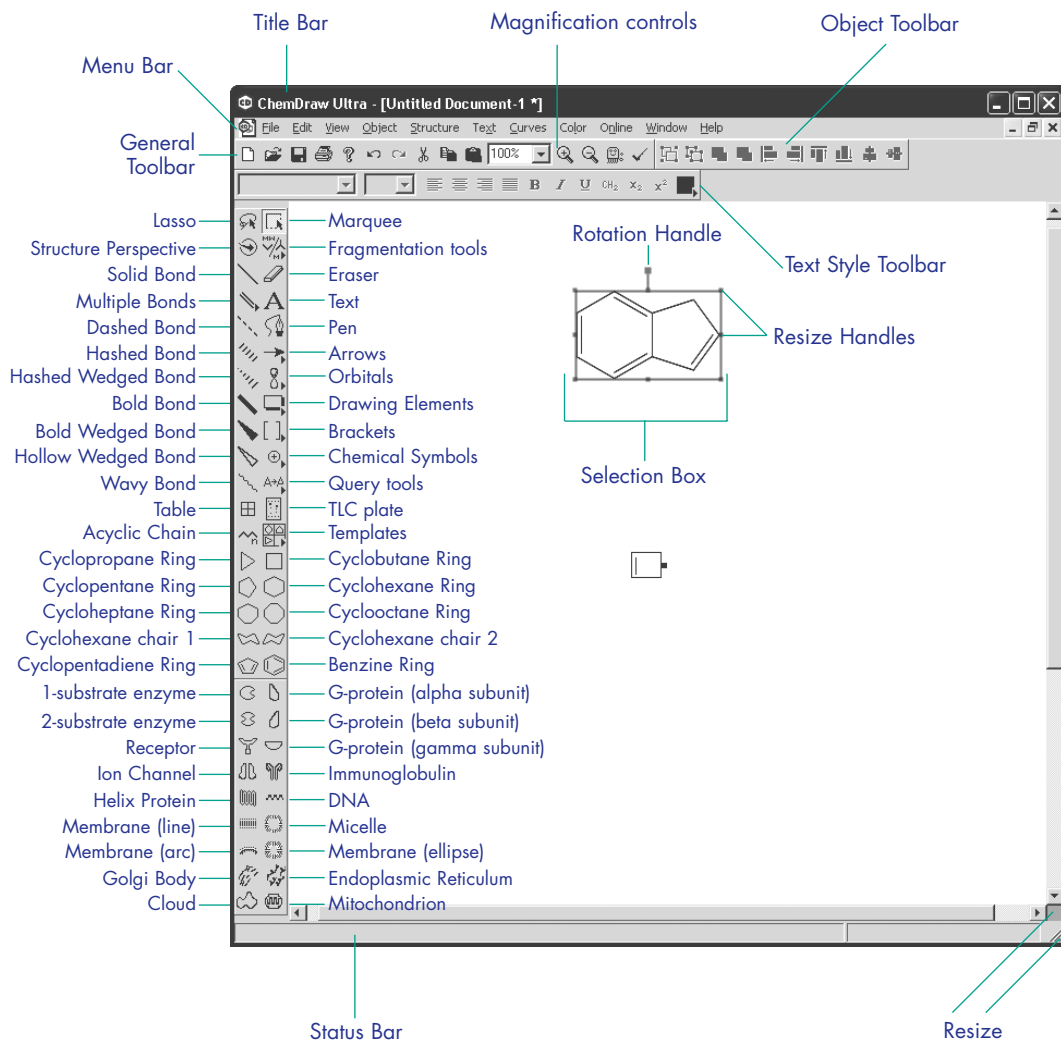
# CS ChemDraw<sup>®</sup>

## for Windows

CambridgeSoft<sup>®</sup>  
www.cambridgesoft.com

## Quick Reference

### SCREEN ELEMENTS



## WORKING WITH SELECTIONS

If you want to ...	Here's how ...
Add items to a selection	SHIFT+select items not currently selected
Remove items from a selection	SHIFT+select items currently selected
Duplicate a selection	CTRL+drag Selection Rectangle
Constrain dragging to X or Y direction	SHIFT+drag Selection Rectangle
Duplicate and constrain dragging	SHIFT+CTRL+drag Selection Rectangle
Switch between selection and another tool	CTRL+ALT+TAB
Resize selection excluding atom labels	Drag Resize handle of Selection Rectangle
Resize selection including atom labels	CTRL+drag Resize handle of Selection Rectangle
Rotate selection excluding atom labels	Drag Rotation handle of Selection Rectangle
Rotate selection including atom labels	CTRL+drag Rotation handle of Selection Rectangle
Distort aspect ratio of selection	Drag sides of the Selection Rectangle
Resize without distortion	Drag corners of the Selection Rectangle
Free Resize	SHIFT + drag corners of the Selection Rectangle
Open Rotate or Resize dialog box	Double-click Resize handle or Rotation handle

## DRAWING TECHNIQUES

Draw a first bond	Drag to draw the bond
Add a bond to a structure	Click an atom or drag from an atom
Label an atom using a bond or ring tool	Double-click an atom (triple-click to repeat last label)
Label an atom using the Text tool	Click an atom (double-click to repeat last label)
Label an atom using a HotKey	Point at an atom and press a HotKey (e.g., "c")
Draw a double bond (solid, dashed, bold only)	Select bond type from context menu
Draw a triple bond (solid only)	Select bond type from context menu
Reduce bond order using Eraser tool	Click once
Change double bond alignment	Click center of double bond using any bond tool
Change double bond type	Click center of double bond using different bond tool
Move an atom	SHIFT+drag an atom using a bond tool
Change bond type	Click center of bond using different bond tool
Change bond layering using bond tool	Double-click center of bond you want forward
Draw a ring	Click or drag using a Ring tool
Create a spiro-linkage	Click or drag from an atom using a Ring tool
Create a fused ring	Click a bond using a Ring tool
Change size of non-bond object	Drag starting point of object (e.g., arrowhead)

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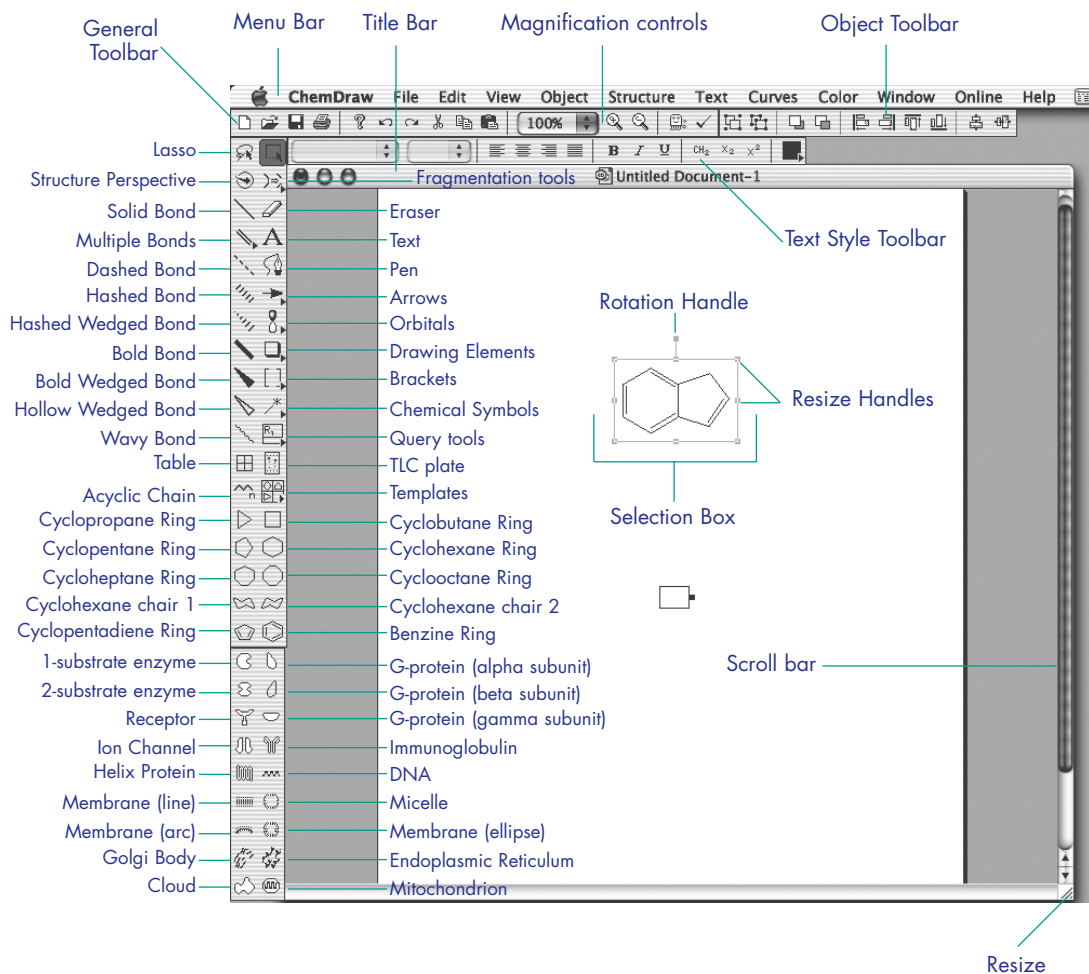
# CS ChemDraw<sup>®</sup>

## for Macintosh

CambridgeSoft<sup>®</sup>  
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## Quick Reference

### SCREEN ELEMENTS



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Remove items from a selection	SHIFT+select items currently selected
Duplicate a selection	APPLE+drag Selection Rectangle
Constrain dragging to X or Y direction	SHIFT+drag Selection Rectangle
Duplicate and constrain dragging	SHIFT+APPLE+drag Selection Rectangle
Switch between selection and another tool	CTRL+APPLE+TAB
Resize selection excluding atom labels	Drag Resize handle of Selection Rectangle
Resize selection including atom labels	APPLE+drag Resize handle of Selection Rectangle
Rotate selection excluding atom labels	Drag Rotation handle of Selection Rectangle
Rotate selection including atom labels	APPLE+drag Rotation handle of Selection Rectangle
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# CS ChemDraw® for Excel

for Windows

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www.cambridgesoft.com

## Quick Reference

### SCREEN ELEMENTS

The screenshot shows the ChemDraw for Excel interface. The title bar reads "ChemDraw for Excel - Book1". The menu bar includes File, Edit, View, Insert, Format, Tools, Data, ChemOffice10, Window, and Help. Below the menu bar is the Excel menu bar and the Excel toolbar. The ChemDraw toolbar is located below the Excel toolbar. The worksheet displays a chemical structure in cell A1 and a table in cells B1:D2.

	A	B	C	D
1		Name	Formula	MW
2	Structure1	cypermethrin	C <sub>22</sub> H <sub>19</sub> Cl <sub>2</sub> NO <sub>3</sub>	416.30

### TOOLBAR



1. New ChemDraw Worksheet — Create a new worksheet.
2. Import Table — Import an SDF file or a ChemFinder database.
3. Export Table — Export selected cells or the entire spreadsheet to an SDF file or ChemFinder database.
4. Import ChemFinder list — Import an open hitlist.
5. Load Molecule — Load a single molecule from a file.
6. Save Molecule — Save a single molecule to a file.
7. Cut Molecule — Remove a molecule and place it on the clipboard.
8. Copy Molecule — Copy a molecule and place it on the clipboard.
9. Paste Molecule — Paste a molecule from the clipboard.
10. Name Molecule — Name a molecule.
11. Show Pictures — Display molecules.
12. Hide Pictures — Hide molecules.
13. Resize Pictures — Resize molecules using the resize handles.
14. Align All Pictures — Enlarge cells or reposition the molecules within the cells.
15. Normal Search — Search for exact structures and substructure using the Search Query dialog box.
16. Similarity Search — Search for similar structures using the Similarity Query dialog box.
17. R-Group Analysis — Shows groups attached to the query structure.
18. Convert SMILES to Molecule — Convert a valid SMILES string to a molecule.
19. Convert Name to Molecule — Convert a name into a molecule.