INTRODUCTION TO CHEMDRAW ULTRA 12.0

ITEC107 - Introduction to Computing for Pharmacy

Objectives

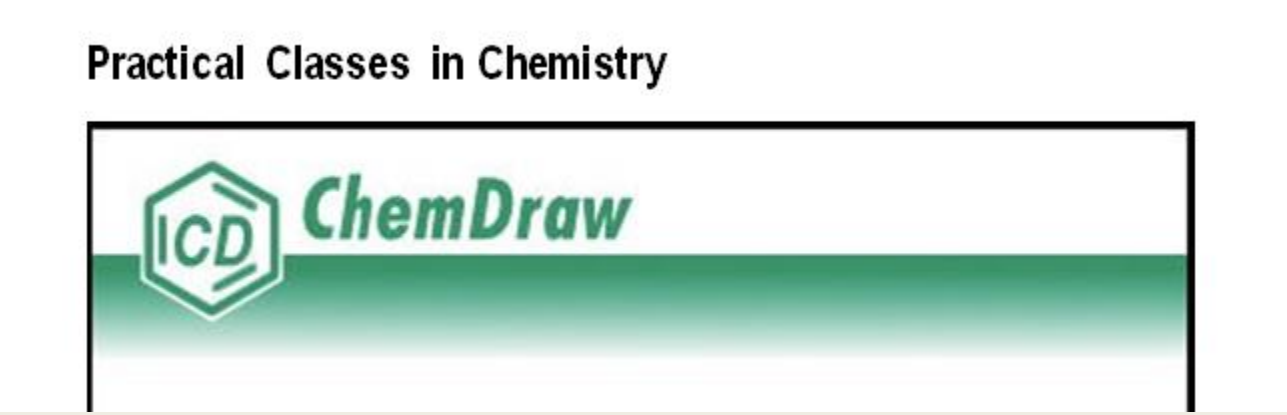
- Why use ChemDraw
- Open, view, save and close a document
- Exploring the user-interface and toolbars
- Analyzing the main toolbar
- Importing and Exporting from ChemDraw

Why ChemDraw?

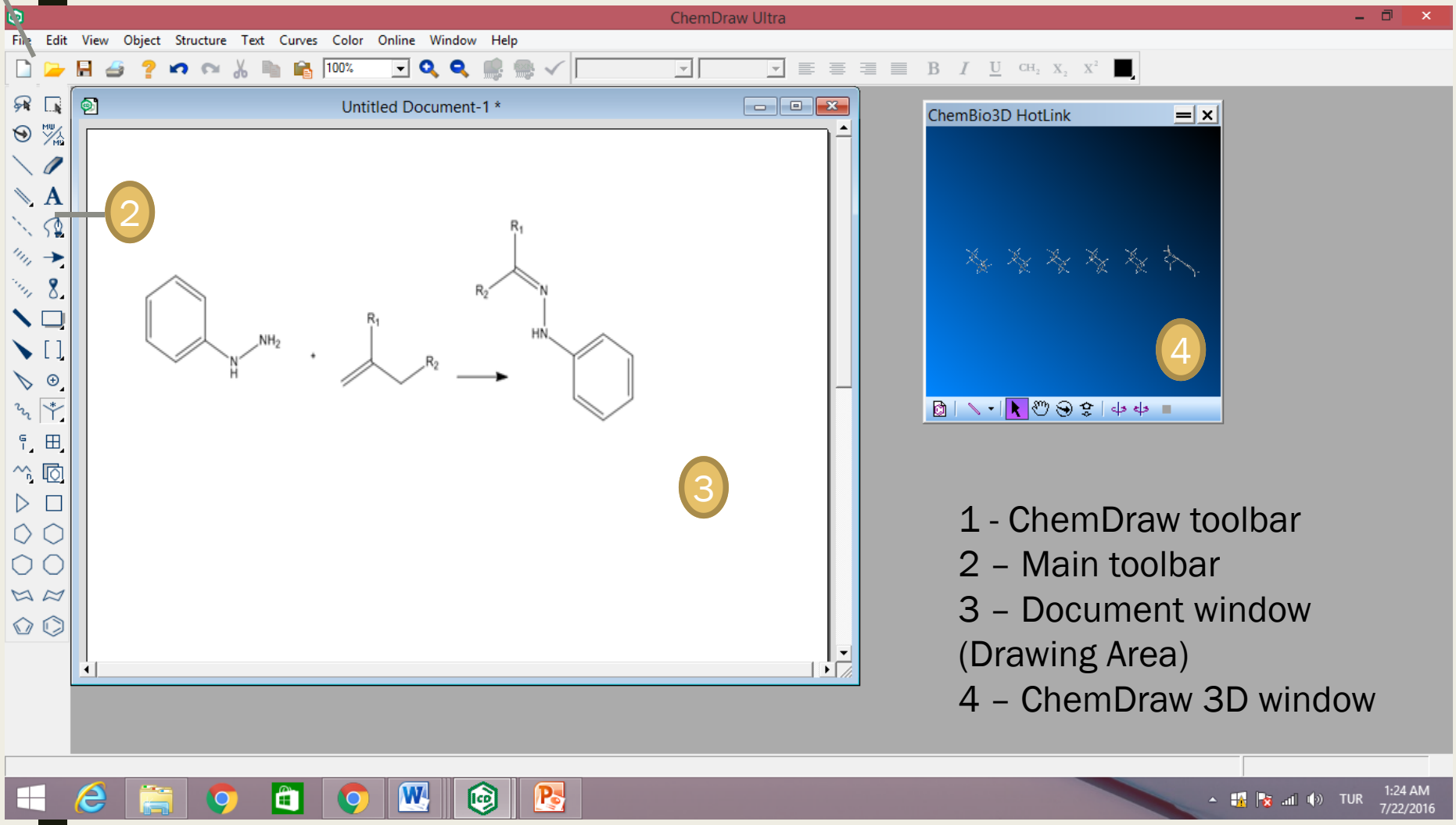
- The drawing of chemical formulae and reaction schemes is a repetitive task for chemists on all levels of their education. While hand-sketching is most efficiently used during discussions and learning, neat drawings are required for official reports, publications, and theses.
- Such drawings can be created with several computer programs, and one example is ChemDraw.

Why ChemDraw?

- ChemDraw is a simple-to-use program that allows to draw intuitively and efficiently simple two- dimensional representations of organic molecules. It is available for the PC as well as for the Mac platform



User Interface

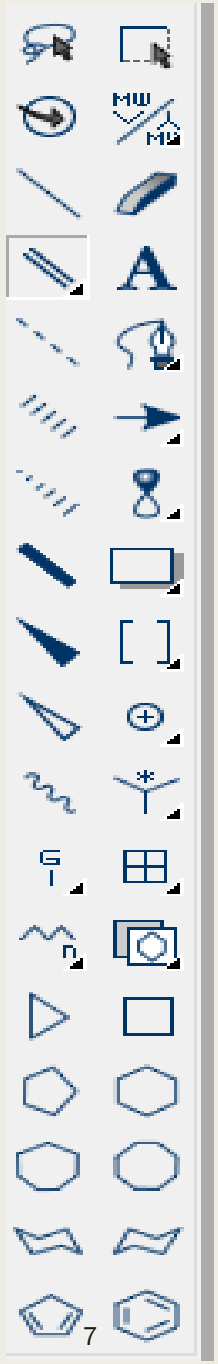


1 - ChemDraw toolbar
2 – Main toolbar
3 – Document window (Drawing Area)
4 – ChemDraw 3D window

ChemDraw Toolbars

- In ChemDraw, several new toolbars are introduced, such as Structure, Curves, Windows, and Biopolymer toolbars.
- To display or hide a toolbar, select it in the **View** menu. A check mark appears next to the toolbar name when it is visible. You can also hide the toolbar by clicking on the '**X**' icon on the upper-right corner of the toolbar.

ChemDraw Toolbars



The Main Toolbar

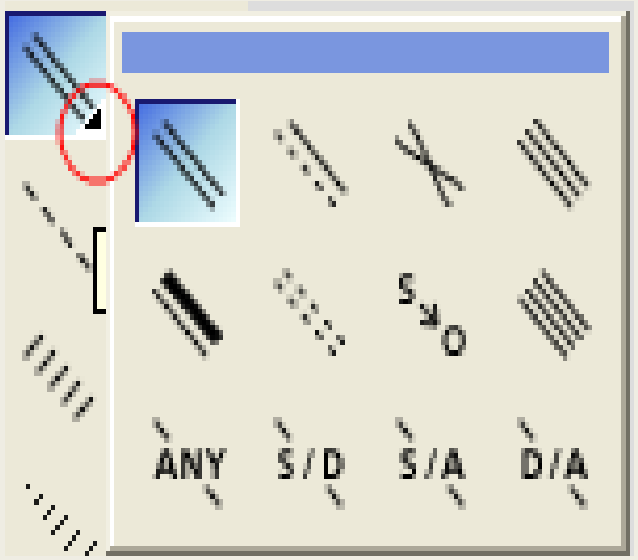
The main toolbar includes the tools most commonly used for drawing structures.

These include all selection and bond tools.

ChemDraw Toolbars

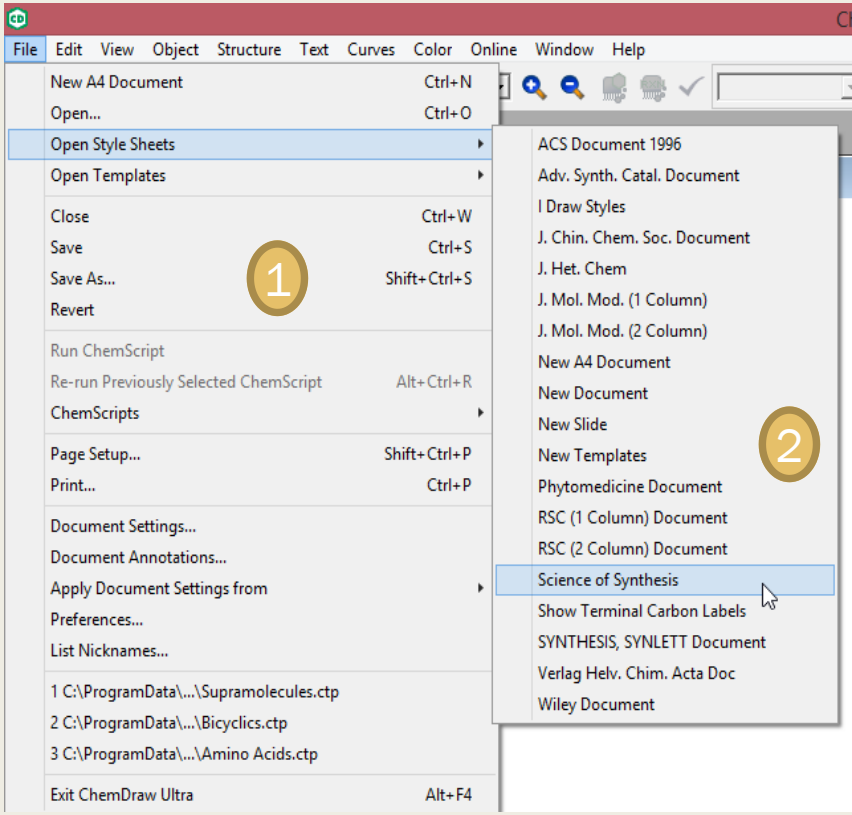
Tearing off Toolbars

Some tools on the main toolbar have other toolbars associated with them. These are indicated by a small black triangle in the lower right corner. For example:



Creating a New Document

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



Using Styles

- To create a new document using a different style sheet or stationery pad:
    1. Go to File>Open Style Sheets
    2. Choose a Style Sheet from the list.

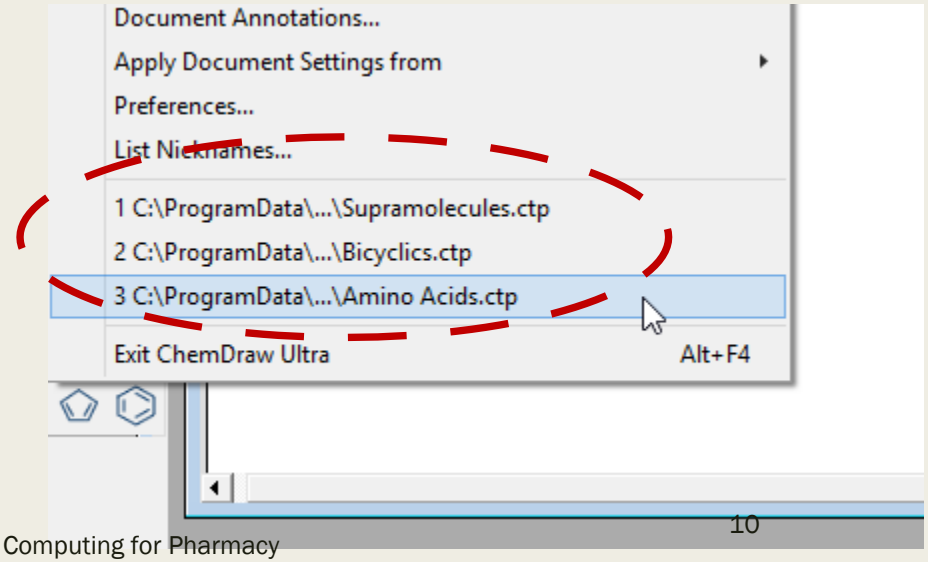
Opening a Document

To open a document, do one of the following:

a) Navigate to **File>Open**. From the Open dialog, select the file name and location of the file and click **Open**.

or

b) From the File menu, choose the document from the list at the bottom.



Saving a Document

To save a ChemDraw document in the default .cdx file format:

1. From the File menu, choose **Save** or **Save As.**

The save dialog box appears.

2. Choose a folder in which to store the file.
3. Type the filename and click **Save** or **OK** to create the file.

When Saving a Document

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.

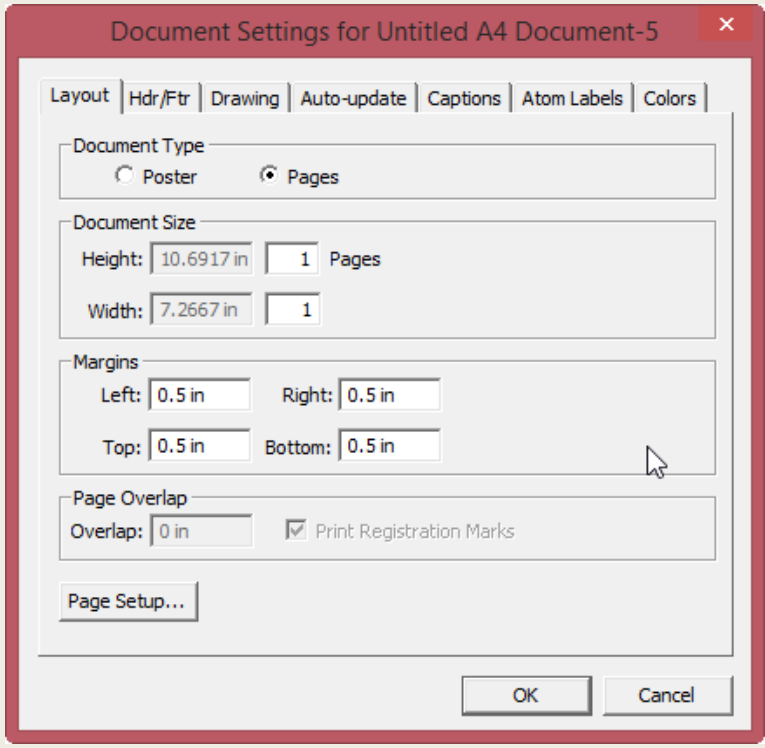
For example, if you save a ChemDraw drawing in the .eps file format, you will store only a picture of the structure without storing the chemical significance of the connections between atoms and bonds.

Page Layout

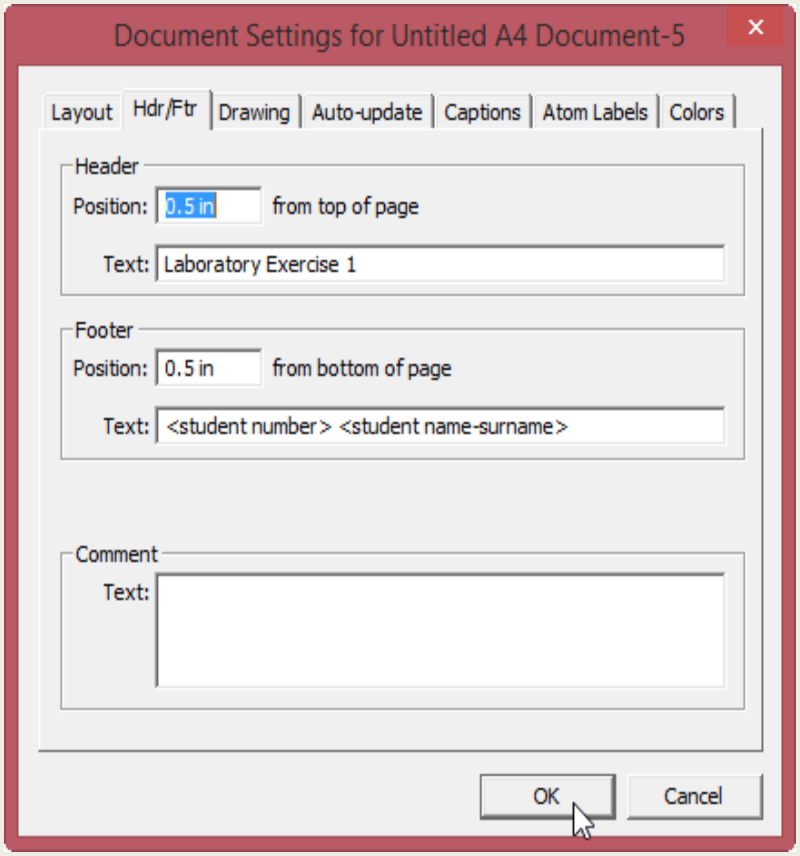
- Object alignment, page size, orientation, and other factors affect the presentation quality of your document.

The Document Window (Drawing Area)

- The document window may be dragged to enlarge the drawing area.
- Document Settings and Page Setup (**under File menu**) also let you modify the page, margins, headers, footers, document type, and size.



Header and Footer

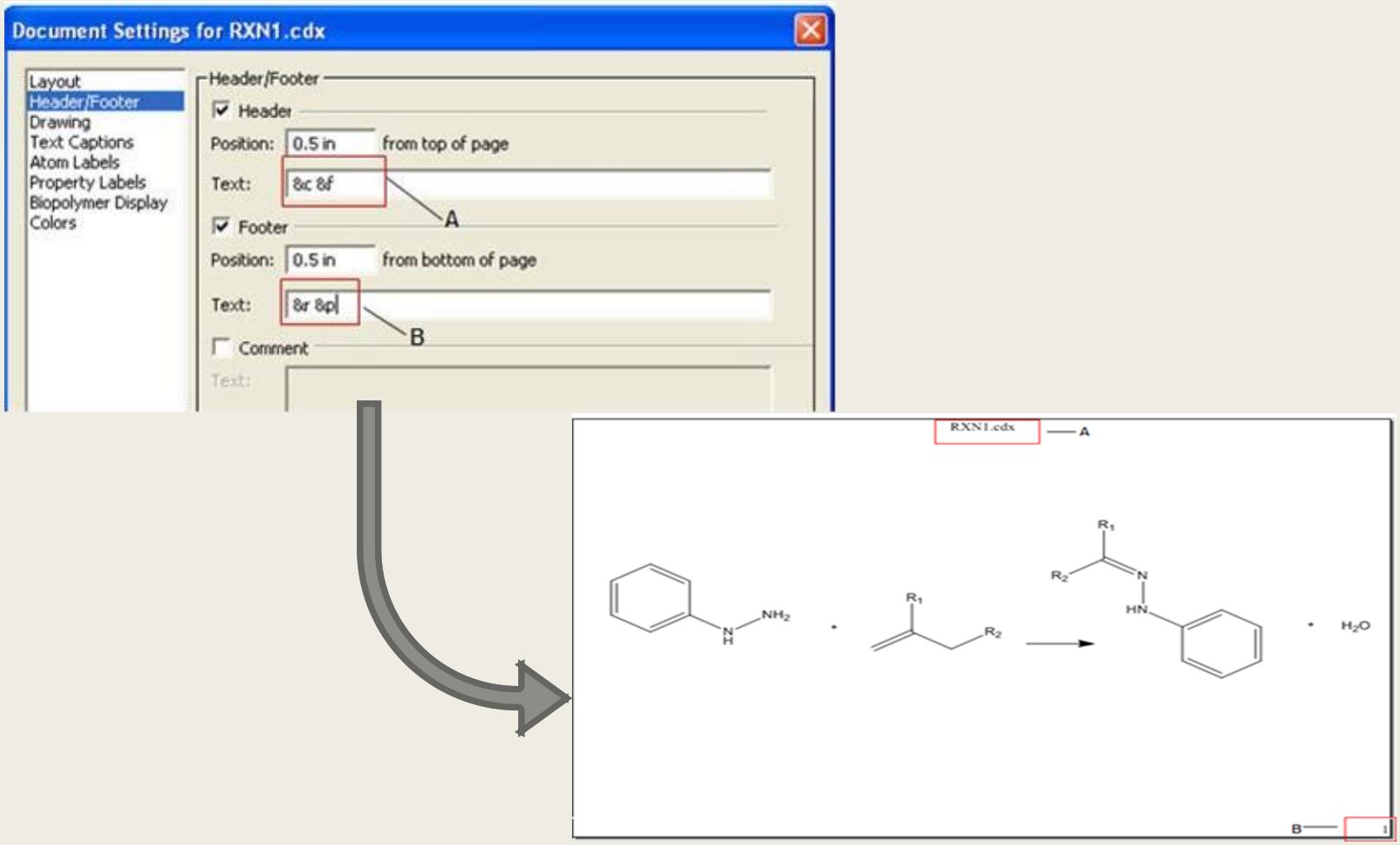


1. Open **File** menu
2. Select **Document Settings**
3. Select **Hdr/Ftr** tab
4. Enter the position from the edge of the page for the header or footer to appear.
5. Type the text to appear in the header or footer.

You may also type additional information in the Text box from the following:

- file name &f
- page number &p
- date printed &d
- time printed &t

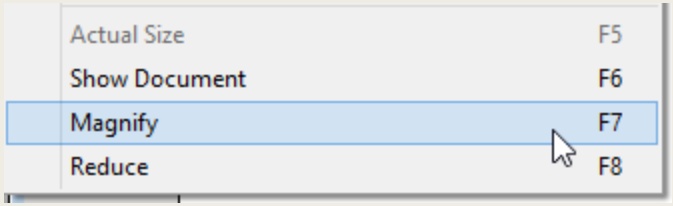
Header and Footer



Viewing Drawings

Magnify

Magnification changes how large or small your drawing appears without changing its dimensions. You can either select a value in the magnification drop down list or enter your own value between 1% and 999%.



1. Select an object to keep in view as you magnify the drawing.

Note: *If you do not select an object, the last object drawn is the center point of the magnification.*

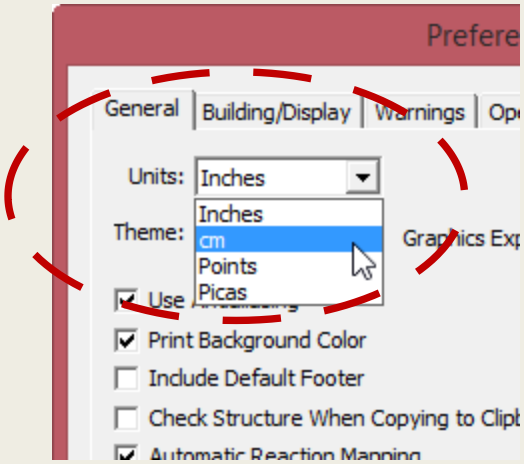
2. Select an option below:

- To increase the magnification, navigate to **View>Magnify**. To reduce the magnification, navigate to **View>Reduce**.
- To return the document to its actual size, navigate to **View>Actual**. To display the whole document, navigate to **View>Show Document**.
- To set the magnification to a specific value, select or enter a percentage in the General toolbar.

Viewing Drawings

Rulers

Use the rulers to position objects a measured distance from a reference point or create objects of an approximate size. To set the ruler units, go to **File>Preferences** and select the **General** tab.



Displaying Rulers

- To toggle rulers on and off, navigate to **View>Show Rulers.**
- As you move the pointer, guides appear on each ruler, indicating the position of the pointer

Viewing Drawings

Crosshairs

The crosshairs are helpful for positioning objects.

To toggle the crosshairs on and off, navigate to **View>Show Crosshair**.

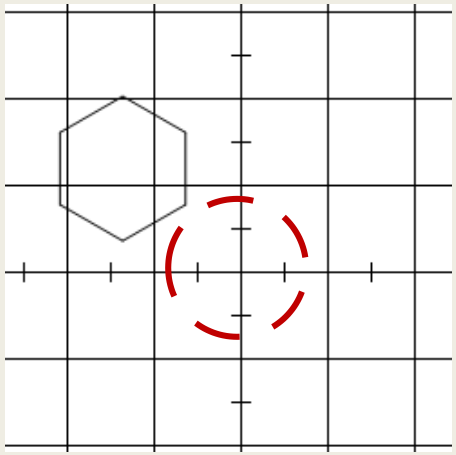
To assist you in aligning objects, the crosshairs include grid lines that extend from the major division marks on each axis.

Moving the Crosshair

1. Position the cursor where the Crosshair axes intersect.

- The cursor changes to an arrow near the center of the crosshair.

2. Click and drag the crosshair.



Viewing Drawings

Positioning Objects

To align two or more objects using the crosshairs, do the following:

1. Move the Crosshair axes and align it with the object.
2. Select an object and drag it until it is aligned with either axis of the crosshair or a grid line.
3. Select a second object.
4. Drag the second object to the crosshair axis or grid line and align it to the first.

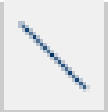
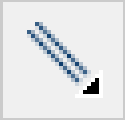
Main Toolbar

Main Toolbar

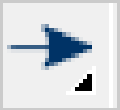
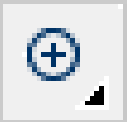
The table below describes the functions of the tools for all versions. Some of the tools have multiple options that can be selected from a tool palette.

TOOL	ICON	EXPLANATION
Selection		**Lasso**. Select objects by dragging around them. **Marquee**. 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
Frag-mentation toolbar		**Fragmentation tool**. Splits molecules across specific bonds. **Dissociation tool**. Breaks bonds and draws a reaction. **Retrosynthesis tool**. Breaks bonds and draws a reaction.

Main Toolbar

TOOL	ICON	EXPLANATION
Solid Bond		Draw bonds and set bond properties.
Eraser		Delete objects. Click on an object to delete; drag to delete multiple objects.
Multiple Bond toolbar		Draw multiple bonds and set bond properties. Bonds of different types can be selected from the Multiple Bonds tool palette.
Text		Create atom labels and captions.
Pen		Draw freehand shapes such as custom arrows and orbitals

Main Toolbar

TOOL	ICON	EXPLANATION
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. Different types of drawing elements can be selected from the Drawing Elements toolbar.
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.

Main Toolbar

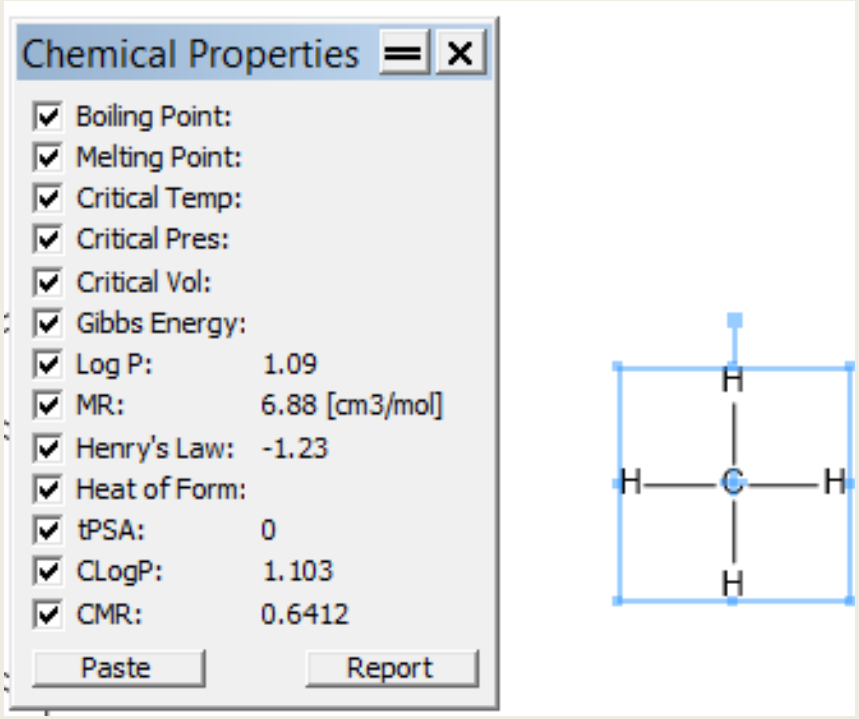
TOOL	ICON	EXPLANATION
Acyclic Chain		Draw chains of any length.
Query Tools toolbar		Draw stereochemical flags, indicate free sites, alternative groups and correspondences between atoms in query structures. Various options can be selected from the Query tool palette.
Templates toolbars		Draw structures with templates stored in template documents. Templates can be selected from the Templates toolbars.
Rings		Draw common structural components

Chemical Properties Window

The Chemical Properties window displays properties of the selected structure.

You can activate the window from the View menu.

- Chemical Properties view for Methane

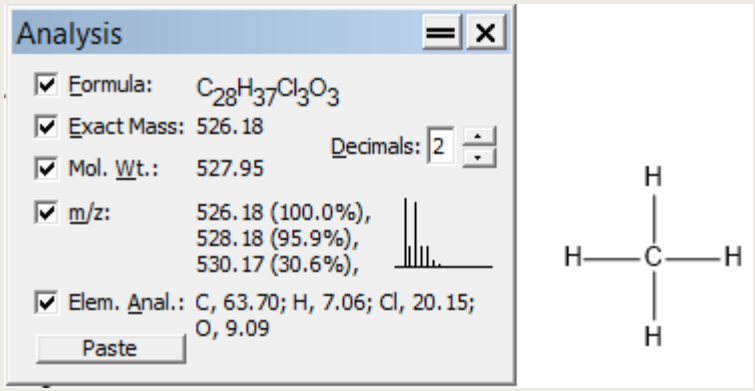


The Analysis Window

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

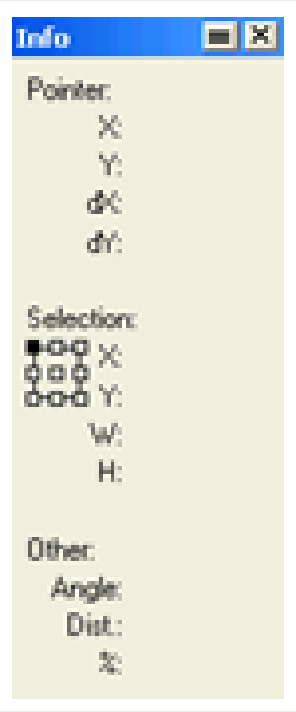
You can activate the window from the View menu.

- The analysis window view for Methane



The Info Window

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



The field shows the following:

- X/Y: current mouse coordinates
- dX/dY: change in X and Y coordinates of a moved selection.

Selection

- 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
- %: percentage of original size when resizing a selection

Printing a Document

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. From the File menu, choose **Page Setup**.
2. Make all appropriate selections for the printer you are using and click **OK**.
3. From the File menu, choose **Print**.
4. Make your selections in the Print dialog box and click **OK**.

To print a document from the Explorer or from the Finder:

1. Select the document you want to print.
2. From the File menu, choose **Print**.

The ChemDraw application is opened and the Print dialog box appears.

3. Make your selections in the Print dialog box and click **OK**.

Closing Options

To close a ChemDraw document:

- From the File menu, choose **Close**.

If the document contains unsaved information, you are prompted to save the file.

To close the ChemDraw application:

- From the File menu, choose **Exit ChemDraw** or **Quit ChemDraw.**

If you have unsaved document windows open, you are prompted to save them before you can close the application.

Importing and Exporting Data From ChemDraw

- Chemical drawing programs enable scientists to communicate chemical structures.
- ChemDraw includes many of the standard file formats for transferring information between ChemDraw and documents created using other applications.
- To enable viewing structures in a word processing document by someone who does not have ChemDraw, you must save the drawing as an image file. You may convert your drawing to bmp, gif, tiff, wmf and other readable image from **FILE > SAVE AS** menu.

Exporting Graphics from ChemDraw

Method 1:

- To insert your ChemDraw **.wmf** image file into a Microsoft Word document, position your cursor at the appropriate location on the page. Then use **INSERT > PICTURE > FROM FILE…**
- Select the file and click insert to insert the drawing to the document.

Exporting Graphics from ChemDraw

Method 2 (Direct Export Method):

- To export diagrams from ChemDraw into Word (or other programs): select the diagram, copy it to the clipboard (Edit-Copy or Command-C), go to Word and do Edit-Paste or Command-V to paste it into the document.

Importing Graphics to ChemDraw

- It is essential that the graphical chemistry content be just as editable as the text itself. To make this happen, the structure editor and word processor need to work together, despite not being specifically designed to do so. The process of moving a chemical structure or drawing from a structure editor to a word processor and back is called "round trip editing".

Importing Graphics to ChemDraw

- Diagrams that have been placed in a Word file can be edited where they are. If you double click on the diagram in the Word file, it will extract it into a little window in ChemDraw where you can edit it. Just close the window to put the edited diagram back into the Word file.
- If you right-click on the diagram in the Word file, you will see the **edit** and **open** options under the **CS ChemDraw Drawing Object** option.