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The Future of Scientific Software

ChemDoodle® v5.1 User Guide

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Introduction

This User Guide provides information on the iChemLabs product, ChemDoodle.

About ChemDoodle

ChemDoodle, in short, can create images of molecules. But it is much more than that. ChemDoodle can efficiently generate chemical documents and figures for use in publications, produces non-molecular objects such as spectra and TLC plates, is integrated with databases, can manipulate a large number of chemical files and formats, and in general, streamlines a lot of the tasks that one is confronted with when trying to do or explain chemistry in a digital medium. ChemDoodle isn't just another program for drawing molecules, it's a brand new application for interacting with chemical data and creating chemical art!

ChemDoodle is designed to be intuitive and easy to learn. ChemDoodle is used by a wide range of individuals, from high school students to accomplished professors and we have done our best to provide the most intuitive controls for such a diverse group while remaining thorough and providing superior quality.

ChemDoodle is integrated with the following iChemLabs Products:

- ChemDoodle Web Components
- ChemDoodle Mobile

About this Guide

This User Guide contains information for the ChemDoodle application for the Windows, Mac OS X and Linux operating systems. It assumes you are familiar with the basics of your operating system. If you are not, please refer to your system manual before using ChemDoodle.

Some tasks described in this guide require the use of third-party applications such as Microsoft Office Word or iWork Pages. If you are not familiar with these third-party applications, please consult the associated user guide provided with that product.

The chapters in this guide are organized by task. They are intended to help you familiarize yourself with the ChemDoodle application and to begin using it as quickly and efficiently as possible.

Most images are taken from the Mac OS X version of ChemDoodle and will be representative of all operating systems. If an operating system specific issue is discussed, any images are taken from the operating system under investigation.

Additional Information

Additional sources of ChemDoodle information include:

- ChemDoodle Support Pages. http://www.chemdoodle.com/support
- ChemDoodle Videos. http://www.chemdoodle.com/videos
- ChemDoodle Web Components. http://web.chemdoodle.com
- ChemDoodle Mobile. http://mobile.chemdoodle.com
- iChemLabs Customer Support. http://www.ichemlabs.com/contact-us
- iChemLabs Website. http://www.ichemlabs.com

Installation and System Requirements

Microsoft Windows Requirements

- Windows XP, Vista or 7+.
- Oracle Java 1.6 or more recent.
- A minimum of 1GB of memory.

Macintosh OS X Requirements

- Mac OS X 10.6 (Snow Leopard) or 10.7 (Lion) or 10.8 (Mountain Lion).
- Oracle Java 1.6 or more recent (installed by default on 10.6; for 10.7+, will be automatically installed when ChemDoodle is opened and you accept to install Java).
- A minimum of 1GB of memory.

Linux Requirements

- Any version of Linux, although we test with and *Ubuntu* (recommended), *Mint*, *Fedora*, *Debian* and *OpenSUSE* Linux.
- Any GUI, although we recommend and test with *GNOME*.
- Oracle Java 1.6 or more recent (OpenJDK, GNU Java, IcedTea or any non-official distributions are not supported).
- A minimum of 1GB of memory.

Installing Java

ChemDoodle requires the official Oracle (formerly Sun Microsystems) Java distribution to run. Java is free and can be easily installed from: http://www.java.com

Most contemporary Windows systems will have Java installed by default.

Mac OS X 10.6 will have Java installed by default. Mac OS X 10.7+ will prompt you to install Java when you first run a Java application. Accept that prompt to install Java.

ChemDoodle does NOT support **OpenJDK**, **IcedTea**, **GNU Java**, or any other non-Oracle version of Java. With unsupported Java distributions, ChemDoodle will run slowly, have broken functions and may not even run at all.

Installation

Installation, activation and uninstallation instructions are can be found on the ChemDoodle website.

Table 1: Websites for Installation Instructions

Operating System	Webpage
Windows	http://www.chemdoodle.com/windows-installation-instructions
Mac OS X	http://www.chemdoodle.com/osx-installation-instructions
Linux	http://www.chemdoodle.com/linux-installation-instructions

Installing for Multiple Users on a Single Computer

ChemDoodle will allow several users to use ChemDoodle on the same computer. All preferences and settings files are saved relative to the user's account, so that each user may save their own preferences. Note that even though ChemDoodle only needs to be installed once on the computer, each user

will still have to individually activate ChemDoodle for his/her user account, so he/she will need access to an activation code. Instructions for installing ChemDoodle for multiple users is operating system dependent and is described in the following subsections.

Windows

During the installation, keep the install folder in *C:\Program Files*. All users will be able to execute ChemDoodle from within this folder.

There will be periodic updates to ChemDoodle. For Windows Vista and later, ChemDoodle requires administrator privileges to update, so you will need to update ChemDoodle as administrator on the computer if none of the users have administrator privileges. This only needs to be done once for the computer, and all users will be using the update.

Mac OS X

During the installation, drag the *ChemDoodle* folder to the */Applications* folder as instructed. All users will be able to execute ChemDoodle from within this folder.

There will be periodic updates to ChemDoodle. Only superusers will be able to update ChemDoodle, so you will need to update ChemDoodle as superuser on the computer if none of the users are superusers. This only needs to be done once for the computer, and all users will be using the update.

Linux

Run the Linux *BIN* in a folder that all users have rights to execute binaries from. After the installation, verify that all users that will be using ChemDoodle have the necessary permissions to do so.

There will be periodic updates to ChemDoodle. You should restrict write privileges to the *ChemDoodle* installation folder if you do not want users to update ChemDoodle by themselves. This may be necessary, for instance, if you do not want one user to update the application while another user is finishing some work and does not yet want to learn the changes the update will bring. If you restrict write permissions, you will need to update ChemDoodle as root on the computer when all users are ready. This only needs to be done once for the computer, and all users will be using the update.

Folder Contents

There are two folders that the ChemDoodle application uses, the main *ChemDoodle* installation folder and the *ChemDoodleSettings* folder located in the operating system's standard *Documents* folder.

The contents of the main *ChemDoodle* installation folder are:

1. **ChemDoodle application** - ChemDoodle.exe on Windows, ChemDoodle.app on Mac OS X, and the ChemDoodle shell script on Linux
2. **config directory** - This folder contains various configuration files, such as *proxy.config*, for setting ChemDoodle to use your proxy. It also contains the site license configuration file for site licenses.
3. **docs directory** - This folder contains documentation such as this user guide.
4. **external directory** - This folder contains required packages that ChemDoodle needs to start up and run properly. Any licenses associated with these packages are also provided.

5. **resources directory** - This folder contains native application icon images and other resources such as the auto-updater and the ChemDoodle Web Components library.
6. **ChemDoodle.jar** - The executable java jar of ChemDoodle. Do not remove this file! This jar is not present in the Mac OS X distribution of ChemDoodle.
7. **ChemDoodle.vmoptions** - This file is only present in the Windows distribution of ChemDoodle. It contains parameters for the Java virtual machine.

WARNING: Do not remove or alter any of the contents of the ChemDoodle installation folder or unexpected behavior may occur. To move the application, you must move the entire ChemDoodle folder.

Standard Operating System Documents Folder

The standard operating system *Documents* folder varies depending on the operating system:

- **Windows XP** - *C:\Documents and Settings\[username]\My Documents*
- **Windows Vista/7** - *C:\Users\[username]\My Documents*
- **Mac OS X** - */Users/[username]/Documents*
- **Linux** - */Users/[username]/Documents*

Free Trials

Trials may be initiated by clicking the **Free Trial** button on the activation screen when ChemDoodle is opened. Trials will remain active for 14 days. After a trial expires, there is no option to try it again.

Trial Restrictions

- Documents show a watermark at the top and will render a background texture.
- The **Save...**, **Save as Image...** and **Convert...** functions are disabled.
- Only images and ChemDoodle data can be pasted from ChemDoodle.
- All copied and printed content will contain a watermark.
- Templates cannot be saved.
- Certain ChemDoodle Web Components functions are disabled (such as PDB file optimization).

Unrestricted Trials

If your trial has expired and you still require the use of ChemDoodle, or if you would like to try ChemDoodle without the trial restrictions, you may purchase an unrestricted 14 day trial on the ChemDoodle website.

Student Version Restrictions

The student version of ChemDoodle has several restrictions:

- No iChemLabs account is provided.
- Round-trip editing is not available.
- Images output from ChemDoodle will not contain chemical metadata.
- Formatted documents and publishing style sheets are not available.
- Import/Export of style sheets is disabled.
- Only ChemDoodle Documents can be saved.
- No conversion utility.

- The only chemical data format you can copy is the ChemDoodle format.

Activation

Activation is performed when one uses a purchased activation code to associate a license with the ChemDoodle application for a given user account.

Activation can be performed in two ways. The first is by using the activation code in the activation screen when ChemDoodle has not been activated or a trial started. The second way is to use the **Activate ChemDoodle** menu item in the **Purchase** menu while a trial is active.

The activation code may be manually typed into the activation form, but it is easier to just copy and paste the entire code from the receipt into the form. Once activated with a purchased license, all restrictions from the trial are removed.

Activation requires an active internet connection. Our server is sent the activation code which is validated and gives permission to create the license file. This method prevents piracy and allows us to minimize the cost of ChemDoodle. There are no exceptions to this activation procedure.

Connection Issues

Activation is an important part of the setup procedure, and there are a few issues, usually in corporate environments, that may occur.

Firewall Issues

If your firewall blocks internet connections from Java applications, then ChemDoodle will not be allowed to connect to the internet. An administrator should set up a special exception to allow ChemDoodle to connect to the internet, at least for activation.

Proxy Issues

If you use a proxy to access the internet, ChemDoodle will use the default system proxy information to connect to the internet. If that fails, then you will need to manually define the proxy settings in the *proxy.config* file that is located in the *config* folder in the ChemDoodle installation folder.

Usage Restrictions

There are no restrictions on how to use ChemDoodle as long as the user abides by the license he/she accepts when activating ChemDoodle.

There are no restrictions on your created chemical drawings generated from activated copies of ChemDoodle. You may use your created chemical drawings for whatever purpose you choose.

Using ChemDoodle to output the glassware graphics for the sole purpose of publishing, selling, or distributing them individually or as a set is forbidden.

Attributions

Attribution of graphics and output to ChemDoodle are welcome, but are not necessary in any form.

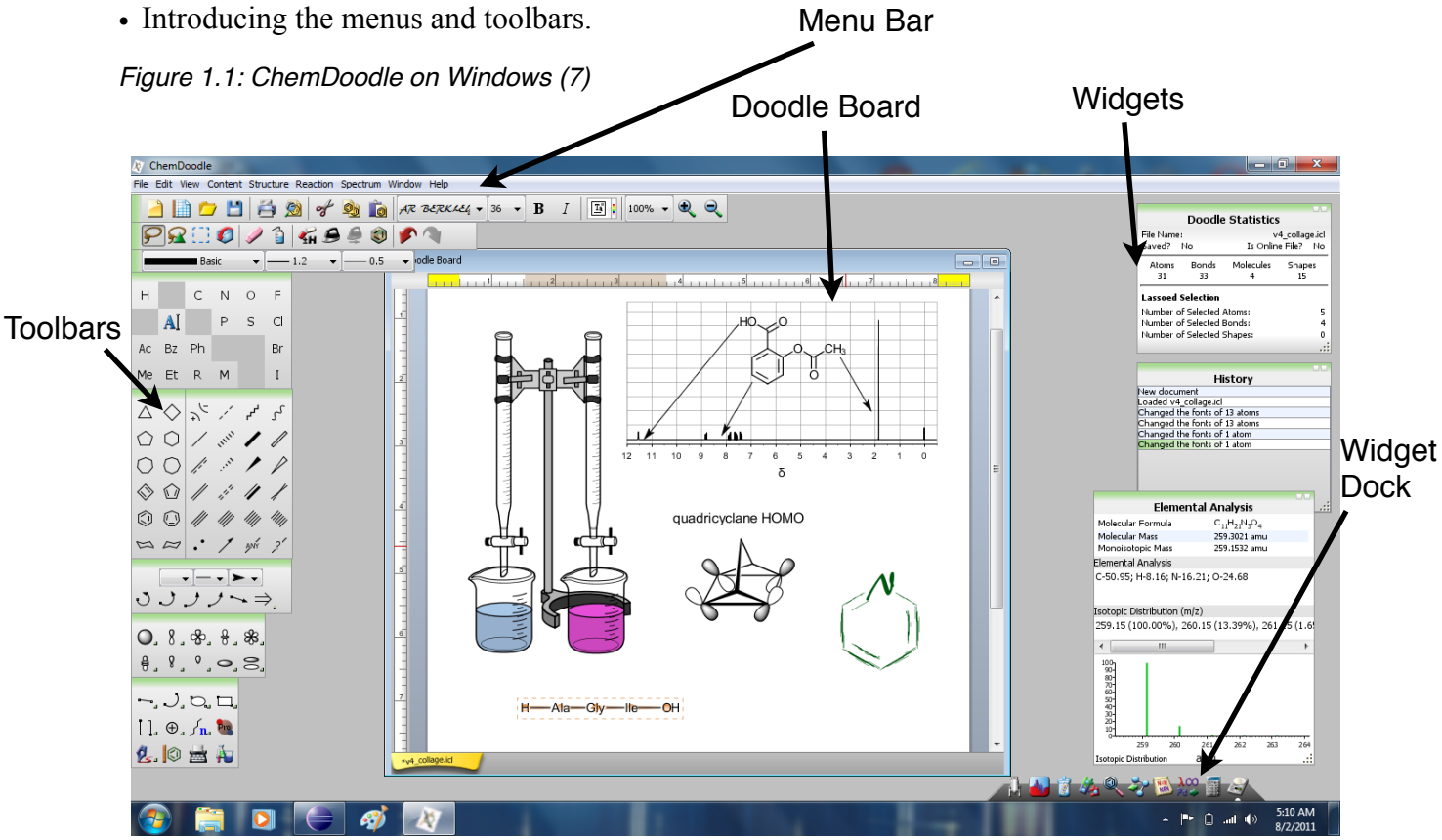
Chapter 1: Introducing ChemDoodle

Overview

This section introduces the new user to the ChemDoodle graphical user interface. It covers the following topics:

- Identifying the parts of the ChemDoodle interface.
- Creating, opening and saving documents.
- Introducing the menus and toolbars.

Figure 1.1: ChemDoodle on Windows (7)



The ChemDoodle Graphical User Interface

Although the Windows, Mac OS X and Linux versions of the ChemDoodle graphical user interface (GUI) differ slightly, the main elements of the GUI are consistent across platforms. The Windows version of ChemDoodle is shown in *Figure 1.1*. The Mac OS X version of ChemDoodle is shown in *Figure 1.2*. The Linux version of ChemDoodle is shown in *Figure 1.3*.

Figure 1.2: ChemDoodle on Mac OS X (10.6)

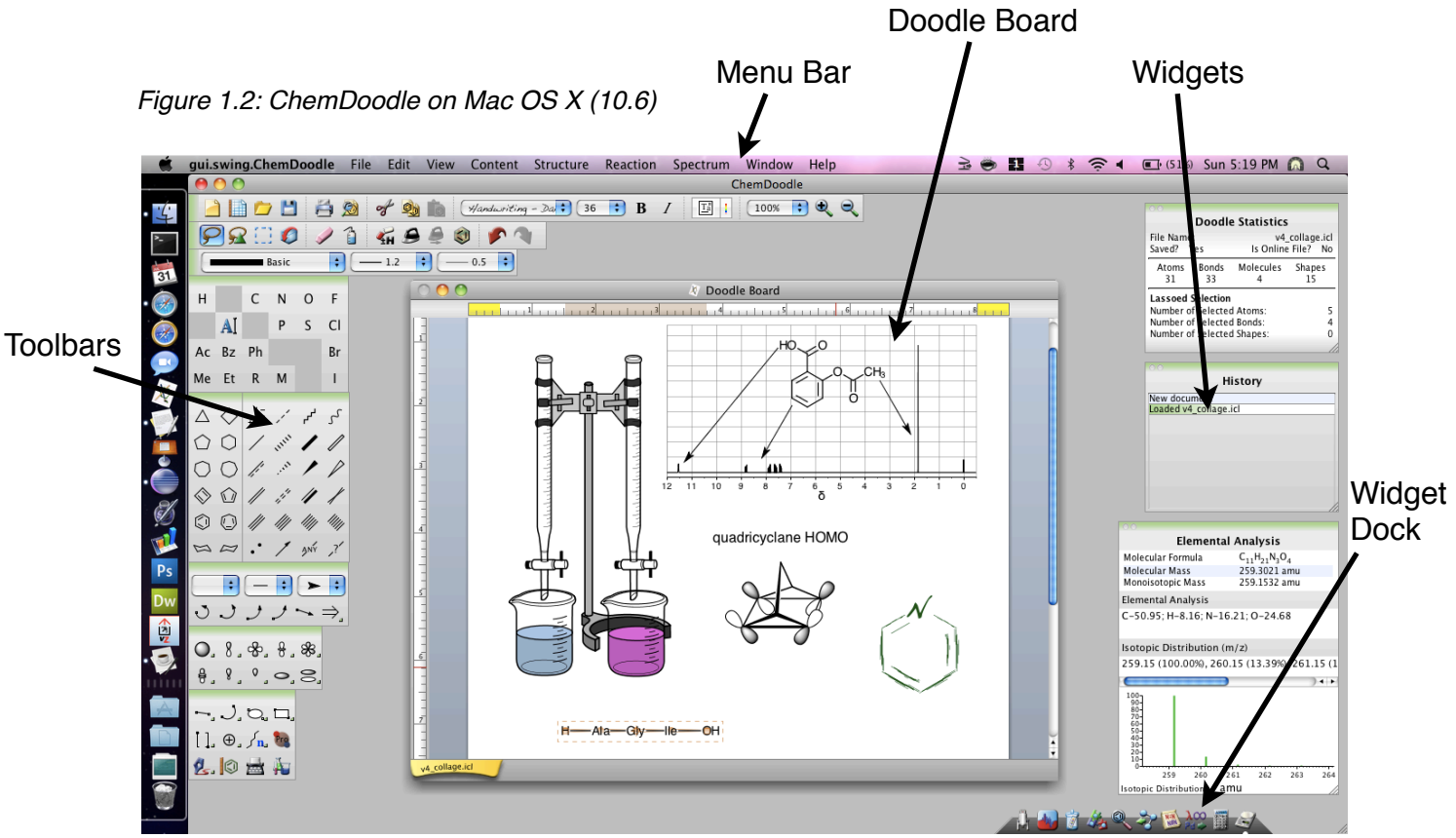
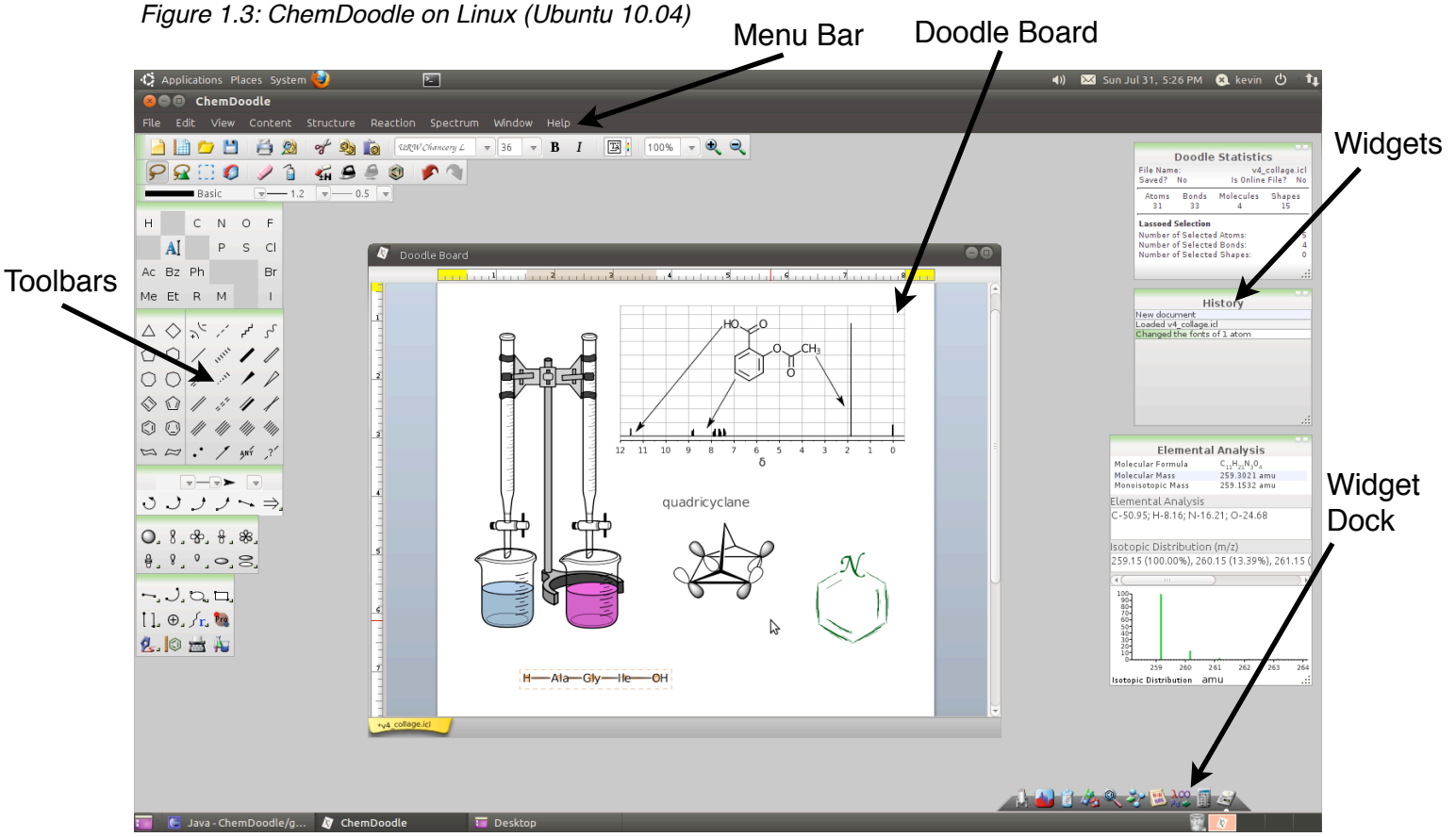


Figure 1.3: ChemDoodle on Linux (Ubuntu 10.04)



Using the Graphical User Interface

ChemDoodle's functions are accessed through interaction with several types of components:

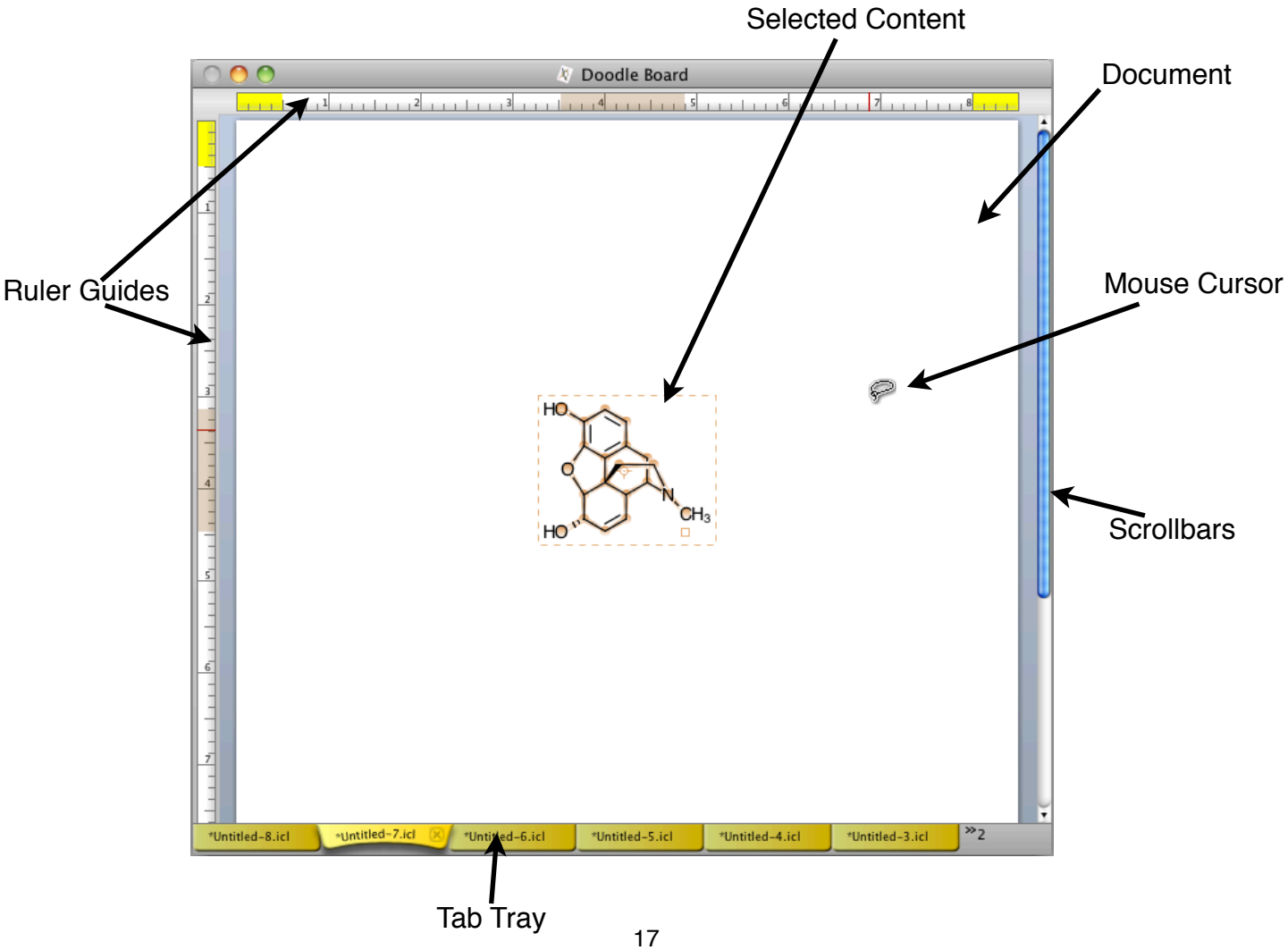
- **Doodle Board** - The main drawing window.
- **Menus** - Core application functions.
- **Toolbars** - Quickly access functions and modify how mouse gestures interact with the **Doodle Board**.
- **Widgets** - Mini applications within ChemDoodle that perform powerful and complementary tasks.

These components are identified in *Figures 1.1-1.3* and are discussed in the following sections. Widgets are explained in *Chapter 2*.

Doodle Board

The Doodle Board is the main drawing window and contains all of the documents you create and edit. You may use mouse gestures to interact with the Doodle Board and to draw your figures. *Figure 1.4* displays the main components of the Doodle Board.

Figure 1.4: The Doodle Board



Ruler Guides

There are two rulers aligned with the currently displayed document on the Doodle Board. The ruler to the left of the document allows for vertical measurements and the ruler to the top of the document allows for horizontal measurements.

When the document rendering scale is changed, the ruler scale will also change to match the new dimensions. When the scrollbars are used to focus on a different area of the document, the rulers will also scroll to match the new location.

The ruler displays full ticks at each inch, half-ticks at each half-inch, and quarter-ticks every eighth of an inch. Several colored ticks and areas may also be present on the rules for visual feedback. These feedback tips can be disabled in the **Preferences** window under the **General** tab.

- **Margin Areas** - Margins are highlighted in a yellow color.
- **Mouse Pointer Ticks** - Mouse pointer locations are ticked on the rules with a red color.
- **Selection Dimension Area** - Marks the bounds of the currently selected content. This is denoted by an amber area. This area corresponds to the internal coordinates of the content and not the visual bounds. For example, it will denote the bounding box given the atom coordinates, but will ignore the dimensions of the labels for those atoms.

Scrollbars

Scrollbars will appear to the right and bottom of the document if the height and width, respectively, of the document are too large to fit on the Doodle Board. You can click and drag the scroll bars to change which area of the document is displayed on the Doodle Board. You can also use the mouse scroll gesture to change the perspective. Horizontal mouse scrolling is only supported on Mac OS X.

Tab Tray

The Doodle Board stores all drawing content and organizes them into documents that can be saved as files or images. Each document has a corresponding tab, located at the bottom of the Doodle Board in the tab tray. When a tab is pressed, the corresponding document will be selected and viewed. This allows you to manage a large number of files at once, without having to manage a large number of windows.

The number of tabs present in the tab tray will change depending on how many documents are open. If only a single document is present, then only one tab is displayed and will be selected. Selected tabs are colored a light blue, as is shown in *Figure 1.5*.

Figure 1.5: A single tab.

When multiple documents are open, multiple tabs will be displayed in the tab tray. The tab corresponding to the currently selected document will be selected and displayed over other tabs as is shown in *Figure 1.6*.

Figure 1.6: Multiple tabs.

If there are more tabs than can fit in the tab tray, then only the most recently viewed tabs that fit in the tab tray will be displayed. A number and two right-oriented chevrons are displayed to the right of the last tab to notify you that some tabs are not displayed as is shown in *Figure 1.7*.

Figure 1.7: There is 1 non-displayed tab.

Click on the chevrons and number to open a popup menu that lists the undisplayed tabs as is shown in *Figure 1.8*. Click on a choice to select that document.

Figure 1.8: List non-displayed tabs.

There are also tab specific functions that can be accessed by right-clicking on any given tab:

- **Close** - Close the current tab. This option is only enabled if multiple tabs are present.
- **Close Others** - Close the other tabs, but leave the current one open. This option is only enabled if multiple tabs are present.
- **New Document** - Create a new document and tab.
- **Restore** - If the corresponding document was created by opening a file, then this function will be enabled, allowing you to undo all of your changes and reload the file.

The name of the file is displayed on the tab. If the name is too long, it may be cropped and appended with "...". You may also see a '*' and/or '^' displayed before a file name in a tab. The '*' is a reminder that the file has been changed since the last save, and the '^' marks it as an online file.

Documents

The document represents a virtual sheet of paper. Each document embodies one page of the structures, objects and figures that you create. The document is fully customizable and also contains a definition of the styles of the content within it. You can create new blank documents, or read one from a file that ChemDoodle recognizes.

> *Note: A visual specification is a definition about how some object is rendered. For example, a bond line width is a visual specification for a bond. In this document, such a concept may be referred to as a visual specification, a style or a document setting. They all mean the same thing.*

Creating a Document

You can create a new, blank document using the default ChemDoodle document settings, or use a Chemical Document Settings file to create a new formatted document.

To create a new blank document using the default style sheet, select the **New** menu item in the **File** menu.

To create a new blank document using a predefined style sheet, select **New Formatted Document...** in the **File** menu.

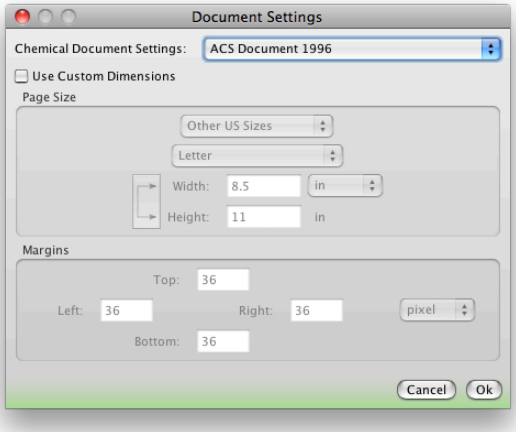
ChemDoodle provides built-in Chemical Document Settings files. For example, the *ACS Document 1996* style is configured to create documents that are set with the bond lengths, bond width, spacing, and fonts used in the 2-column format of all **American Chemical Society** journals. Currently, ChemDoodle provides the following style sheets:

- ACS Document 1996
- Adv. Synth. Catal Document
- J. Chin. Chem. Soc. Document
- J. Het. Chem. Document
- J. Mol. Mod. Document (1 Column)
- J. Mol. Mod. Document (2 Column)

- Phytomedicine Document
- RSC Document (1 Column)
- RSC Document (2 Column)
- Science of Synthesis Document
- SYNTHESIS, SYNLETT Document
- Verlag Helv. Chim. Acta Document
- Wiley Document

These style sheets are presented when you create a new formatted document as is shown in *Figure 1.9*.

Figure 1.9: Creating a New Formatted Document.



The style sheets are organized into 3 sections. The first contains just the default style sheet, the second contains all the built-in style sheets and the last contains custom style sheets. Select the style sheet that you prefer, and choose to set any custom dimensions, and then click the **Ok** button to create your new formatted document.

If you would like to modify the document dimensions of the formatted document, then select the **Use Custom Dimensions** checkbox and edit the **Page Size** and **Margins** fields.

Opening a Document

To open a document, select the **Open...** menu item from the **File** menu, locate the file you would like to open with the file chooser that appears and click the **Open** button.

ChemDoodle can read many file formats, and the default file type the file chooser searches for is a **ChemDoodle Document**. To allow other file types, click on the format drop down selection at the bottom of the file chooser and select the file type you would like to open, or select the **All Files** type.

> *NOTE: Selecting **All Files** will allow you to select any file, including files that ChemDoodle cannot read. If such a file is chosen, you will see a file read error displayed. Otherwise, ChemDoodle will try to determine the type of file chosen by analyzing the file extension and file content to open it accordingly.*

To open a recently opened document, enter the **Open Recent** submenu in the **File** menu and select the document you would like to open. Only the 10 most recently opened files are remembered.

File Chooser Previews

The file choosers that you use to open your files will closely resemble the standard file choosers that you use in all of your other applications. However, we have added some enhancements when using ChemDoodle. One addition is chemical file type previews.

On all operating systems, you will see a preview of chemical files that you select in file choosers. On Windows, Mac OS X and Linux, the file chooser will show a preview of the entire document on the right as shown in *Figures 1.10*, *1.11*, and *1.12*. On Windows and Linux, these previews are interactive, if you hover your mouse over the preview, that area will zoom in for a closer inspection. On

Mac OS X, a tray is added to the bottom of the file chooser to list the individual molecules present in the file as shown in *Figure 1.12*.

Figure 1.10: The file chooser on Windows showing the file preview.

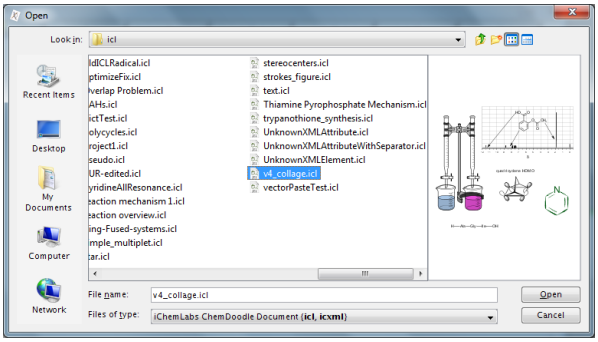


Figure 1.11: The file chooser on Linux showing the file preview.

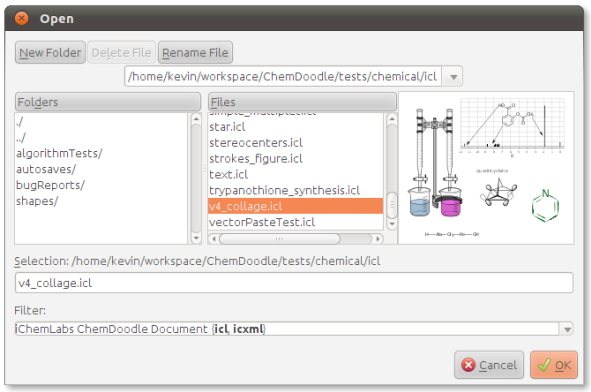
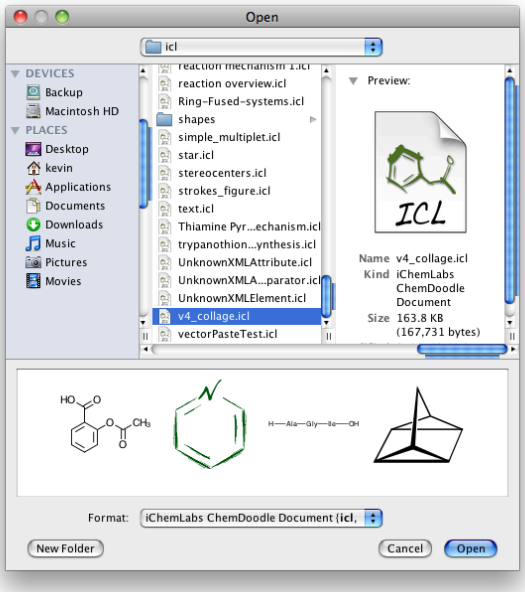


Figure 1.12: The file chooser on Mac OS X showing the file preview and preview tray.



You can disable file chooser previews in the **Preferences** window, under the **General** tab in the **Filechooser Settings** section.

Changing Document Size

To change the size of the current document, perform the following steps:

1. Choose the **Resize Document...** menu item in the **Edit** menu.
2. Use the form to select a preset document size or manually type in the desired document dimensions.
3. Click the **Ok** button to resize the document.

Discard Recent Changes to a Document

To retrieve the last saved version of a file without using **Undo** functions, select the **Restore** menu item in the **File** menu. All changes made to the file since it was last saved are discarded and the saved version of the file will appear.

Saving Documents

To save your document as a file, select the **Save** or **Save As...** menu items from the **File** menu. **Save** will automatically save the document to the file it is associated to, while **Save As...** will allow you to save that file to a new location or override other files. If there is no file associated with a document, the **Save** function will work identically to the **Save As...** function.

After selecting a save function, a file chooser will appear. Select the location you would like to have the document saved in and type in a name for the file if you do not like the default name. You do not need to type in an extension as ChemDoodle will do this for you.

After you are satisfied with a location and name, select the file type of the document to be saved. By default, a **ChemDoodle Document** is chosen, but you can choose from a large selection of file types that ChemDoodle can interpret.

> *NOTE: Only the **ChemDoodle Document** can store your document with 100% accuracy. Other file types are for other purposes and may not define the same objects and properties in ChemDoodle. Keep this in mind while saving files. If you forget, a small warning will popup when saving to a file type other than a **ChemDoodle Document**. These warnings can be disabled in the **Preferences** window under the **Saving** tab.*

After selecting the file type to be used, press the **Save** button to save your document as a file.

Autosaving

ChemDoodle will automatically save unsaved content for you at regular intervals. If your computer shuts off unexpectedly, the next time ChemDoodle opens, all autosaved content will be displayed.

You can turn off autosaving in the **Preferences** window under the **Saving** tab. You can also specify the autosave interval in the same section. The default autosave interval is 5 minutes.

Reversing Actions

ChemDoodle keeps track of the actions you perform. You can reverse actions one at a time by selecting the **Undo** menu item in the **Edit** menu then restore them with the **Redo** menu item in the **Edit** menu. Once you close your document, the undo queue is reset.

More advanced undo/redo functionality is associated with the **History** widget.

Mouse Cursors

The mouse pointer is context sensitive and will change when hovered over the document to display visual feedback about the current mouse gestures that can be performed. The different mouse cursors are described in *Table 3*.

Table 3: Mouse Cursors

Cursor	Means that...
	Clicking and dragging perform obvious functions.
	This is the lasso cursor. Clicking and dragging will generate an outline following the drag path. All content within the drag path will be selected.
	This pinpoints the exact location that your click will hit. This enhances accuracy when using the rectangular marquee or when placing shapes.

Cursor	Means that...
	This signifies that a single object may be selected.
	This means that content can be grabbed. Individual objects or selected content can be grabbed.
	This means that content has been grabbed and dragging gestures will perform appropriate actions.
	This cursor only appears when rotating structures in 3D. It means that content can be grabbed.
	This cursor only appears when rotating structures in 3D. It means that content has been grabbed and drag gestures will perform appropriate actions.
	This cursor signifies that resize actions can be performed by clicking and dragging. This cursor will also appear when translating the rotation anchor.
	This cursor signifies that rotation actions can be performed by clicking and dragging.

Selected Content

Content that is selected will be bordered by a dashed amber line. Selected content can be used in functions and sent to other components. A crawling ants effect is on by default to help the user keep track of selected content. The crawling ants effect can be disabled in the **Preferences** window under the **General** tab.

For instructions on selecting content and editing selected content, read *Chapter 5*.

The Workspace

The ChemDoodle workspace consists of the application window and all interface elements contained within. You may freely place toolbars, select widgets, change the document scale, select view options, etc., and the next time you open ChemDoodle, your choices will have been remembered. ChemDoodle also provides several functions for managing your workspace, so you have control over how the application behaves.

Resizing the Workspace

A minimum screen resolution of 1280 by 800 pixels is recommended to neatly fit all of the components in ChemDoodle on the screen. Slightly smaller resolutions are still acceptable when shrinking the document scale. For much smaller resolutions, the workspace will display scrollbars to access the entire ChemDoodle interface.

On devices that just fit the ChemDoodle window, ChemDoodle will expand to fit the entire screen. On larger resolution devices, ChemDoodle will open to take only as much room as necessary. At any time, you may un-expand the application or resize it to your preference. Upon resizing, the widgets will be replaced to the right of the workspace, and the **Doodle Board** will be centered.

The workspace will keep track of the size and location of ChemDoodle when it was last closed.

Resetting to the Default Workspace

To reset to the default workspace that was presented when ChemDoodle was first opened, select the **Default Workspace** menu item in the **Window** menu.

Reverting to the Last Saved Workspace

To revert to the last saved workspace, select the **Revert Workspace** menu item in the **Window** menu.

Saving the Current Workspace

To save the current workspace, which will override the revert workspace, perform the following steps:

1. Organize the workspace to your preference.
2. In the **Window** menu, select the **Save Workspace** menu item.

The current workspace is now saved and can be reverted to.

Note: ChemDoodle will automatically save your current workspace upon close, so make sure to revert the workspace to your saved workspace before you close, if necessary. Otherwise, ChemDoodle will open up to look exactly like it was when it was closed.

Menus

Menus are located on the top of the ChemDoodle application. On Mac OS X, the ChemDoodle menu bar is displayed in the screen menu bar, as would be expected of Mac OS X applications.

For menu item keyboard shortcuts, consult the *KeyboardShortcuts.pdf* document in the *docs* folder in the *ChemDoodle* installation folder.

There are 9 menus in the menu bar (10 on Mac OS X), not including the **Purchase** menu that is present during the free trial:

- **ChemDoodle** - This is a Mac OS X specific menu bar and contains access to several Mac OS X specific tasks as well as the **About**, **Preferences** and **Quit** menu items.
- **File** - This menu handles all input and output of data, as well as file specific functions such as **Annotations...**. You also have access to your iChemLabs account through this menu and the **Quit** menu item is located here on non-Mac OS X platforms.
- **Edit** - Standard global document functions are located here including **Cut**, **Copy** and **Paste**.
- **View** - Functions for changing how documents are shown are located here as well as access to the elemental and chemical data provided with ChemDoodle. The dynamic periodic table is also accessible through this menu.
- **Content** - Contains all non-chemical functions for editing content in the current document.
- **Structure** - Contains all functions related to editing and analyzing molecules.
- **Reaction** - Contains all functions related to editing and analyzing reactions.
- **Spectrum** - Contains all functions related to editing and analyzing spectra.
- **Window** - Manage your workspace and the entire ChemDoodle application window.
- **Purchase** - This menu is only present during the free trial and provides functions for purchasing and activating licenses for ChemDoodle.
- **Help** - This menu contains several functions to access this user guide, list references, contact customer service and other common help items.

ChemDoodle Menu (Mac OS X Only)

- **About ChemDoodle** - Display information about ChemDoodle, your activation code and your license expiration, if any.

- **Preferences...** - Open the **Preferences** window to edit ChemDoodle preferences.

- **Services** - Standard Mac OS X submenu that will likely be empty.

- **Hide ChemDoodle** - Hide the ChemDoodle application.
- **Hide Others** - Hide other applications.
- **Show All** - Show all hidden applications.

- **Quit ChemDoodle** - Quit the ChemDoodle application.

File Menu

- **New** - Add a new blank document to the **Doodle Board**.
- **New Formatted Document...** - Add a new blank formatted document to the **Doodle Board**.

- **Open** - Open a recognized chemical file that you locate with a file chooser.
- **Open Recent>** - The 10 most recently opened chemical files are listed here. Click a file to open it.
- **Insert Image...** - Add a recognized image file to the current document that you locate with a file chooser.

- **Close** - Close the current document. This function is only enabled if two or more documents are present.
- **Close Others** - Close all but the current document. This function is only enabled if two or more documents are present.
- **Restore** - Restores a file from its last save. This function will only be enabled for files that have been previously saved or were opened from a preexisting file.

- **Annotations...** - Associate annotations with the current document or view previously set annotations.
- **Save** - Saves the current file with the present save settings determined when opening the file or by previously saving it. This action will act exactly like the **Save As...** function if the document is not yet associated with a save location.
- **Save As...** - Save the current document as a file type of your choice in a new file (or override one) that you will locate with a file chooser.
- **Save As Image...** - Save the current document as an image that you will place with a file chooser. Several bitmap and vector image types are supported.
- **Save Selection As Image...** - Save the currently selected objects as an image that you will place with a file chooser. Several bitmap and vector image types are supported. This menu item is disabled if no objects are selected.
- **Convert...** - Displays a window to convert chemical files to different chemical file types that ChemDoodle interprets. Nothing is loaded to the **Doodle Board**, as output is written directly to a new file that is created.

- **Generate Web Component...** - Generate a **ChemDoodle Web Component**. An entire window will appear for you to define and edit the **ChemDoodle Web Component**, as well as preview and generate the *Javascript* for it. More information on this feature is covered in Appendix F.

- **Sync with Online Account...** - Login to your iChemLabs Account to access special online features in ChemDoodle.
- **Open Online File>** - Your online files will be listed in this submenu. Click on a file to open it on the **Doodle Board**.
- **Save As Online File..**. - Save your file online. This is useful for using ChemDoodle efficiently on several computers or for interacting with iChemLabs cloud services. This feature also allows you to transfer structures drawn on your desktop to ChemDoodle Mobile on your phone.
- **Refresh** - Revalidate the menus and re-sync your information with your online account. This should be done when you transfer a new file into your account from a source other than ChemDoodle desktop.

- **Logout** - Logout from your iChemLabs account.

- **Page Setup...** - Display the operating system specific window for selecting initial print settings.
- **Print Preview** - View the current document in its entirety on the screen, ignoring extraneous graphics such as errors and visual aids.
- **Print...** - Print the current document.

- **Exit** - Exits ChemDoodle. This menu item is in the **ChemDoodle** menu on Mac OS X, listed as **Quit ChemDoodle**.

Edit Menu

- **Undo** - Undo the last action.
- **Redo** - Redo the last undone action.

- **Cut** - Copy the selected objects to the system clipboard in addition to removing them from the document.
- **Copy** - Copy the selected objects to the system clipboard.
- **Copy As>** - Contains convenience functions for quickly placing specific data on the system clipboard as text and as a chemical to be transferred to a range of 3rd party applications that use that data type. This submenu is only enabled if content is selected.
    - **Daylight SMILES** - Place a *SMILES* string for the currently selected content on the system clipboard as text and as a chemical.
    - **IUPAC InChI** - Place an *InChI* string for the currently selected content on the system clipboard as text and as a chemical.
    - **ChemDoodle JSON** - Place *ChemDoodle JSON* for the currently selected content on the system clipboard as text.
    - **MDL MOLFile** - Place a complete *molfile* for the currently selected content on the system clipboard as text and as a chemical.
    - **Tripos SLN** - Place a *SLN* string for the currently selected content on the system clipboard as text and as a chemical.
- **Paste** - Paste the system clipboard data of highest priority into the document.
- **Paste and Match Style** - Paste the system clipboard data of highest priority into the document and match the style to the current style sheet.
- **Paste Text as Chemical>** - Pastes the current text on the clipboard, interpreted as chemical data, as any of the options provided in the submenu.
    - **Beilstein ROSDAL** - Paste text as ROSDAL.
    - **ChemDoodle JSON** - Paste text as ChemDoodle JSON.
    - **Daylight SMILES** - Paste text as SMILES.
    - **IUPAC InChI** - Paste text as InChI.
    - **Tripos SLN** - Paste text as SLN.
    - **XYZ-Like Data** - Paste text as a chemical, interpreted from a text blob where XYZ-like data is parseable.

- **Guess Chemical Format** - Paste text as chemical, where the format is guessed from the content.

- **Paste Special...** - Lists all data that ChemDoodle can interpret from the system clipboard. You may then choose the data of choice to be pasted into the document. This function is useful, for instance, when you would like to paste *SMILES* string text instead of a structure into the document. A structure has higher priority than text.

- **Clear** - Remove all content from the current document.

- **Resize Document...** - Resize the current document. You may also change the page margins in the **Preferences** window under the **Visuals** tab under the **Page** tab.
- **Conform Document...** - Conform all objects in the current document to a selected style sheet. This function will also change all fonts and scale all objects if you choose to do so.

- **Purge Clipboard** - This function clears the system clipboard.
- **Purge History** - This function clears the undo/redo history, which will reset the **History** widget. This may be convenient if the action list gets so long that it becomes unmanageable and causes memory issues, or if you would like to prevent yourself from undoing past a certain action.

- **Preferences...** - Open the **Preferences** window to edit ChemDoodle preferences. This menu item is in the **ChemDoodle** menu on Mac OS X.

View Menu

- **Hide Warnings** - Hide all the warnings in the document.

- **Drawing Aids>** - Display various guides to help when drawing figures.
  - **Atoms>** - Display guides associated to atoms.
    - **Show Circular Guidelines** - Display circular guides around atoms with radii equal to the current bond length document setting.
    - **Show Orthogonal Guidelines** - Display vertical and horizontal guidelines that intersect through the atom for aiding in alignment tasks.
  - **Bonds>** - Display guides associated to bonds.
    - **Show Parallel Guidelines** - Display a line that goes through the bond to extrapolate where they point to.
  - **Rings>** - Display guides associated to rings.
    - **Color in Rings** - Color in Euler facet rings with a color code that depends on the size of the ring.
  - **Molecules>** - Display guides associated to molecules.
    - **Show Molecule Bounds** - Draw rectangular bounding guides around molecules to show their visual bounds.
    - **Show Orthogonal Guidelines** - Display vertical and horizontal guidelines that intersect through the center of the molecule for aiding in alignment tasks.

- **Background>** - Display guides associated to the page.
  - **Show Crosshair** - Displays a crosshair.
  - **Show Grid Guidelines**> - Displays grids.
    - **Every Quarter-Inch** - Displays a grid with quarter-inch spacing.
    - **Every Half-Inch** - Displays a grid with half-inch spacing.
    - **Every Inch** - Displays a grid with inch spacing.
  - **Show Margin Guidelines** - Displays a rectangular region that specifies the printable area of the page.
- **Unique IDs>** - Associates ID attributes to objects.
  - **On Atoms>** - Associate IDs to atoms.
    - **Incremental** - Associate incremental IDs to atoms. The atoms are numbered in chronological order from when they were created.
    - **Morgan Indices** - Associate Morgan indices to atoms.
  - **On Bonds** - Associate incremental IDs to bonds. The bonds are numbered in chronological order from when they were created.

- **Elemental Data** - View the entire elemental database packaged in ChemDoodle that is used for all calculations and cheminformatics functions. The data is displayed in a dynamic table.
- **Ionization Energies** - View ionization energies of the elements in a dynamic table. This data is part of ChemDoodle's elemental database.
- **Isotopes** - View isotope data for the elements in a dynamic table. This data is part of ChemDoodle's elemental database.

- **Interactive Periodic Table** - View an interactive periodic table that can be customized and printed. You may also use its dynamic features to create nice demonstrations.

- **Actual Size** - Negate any zoom effects.
- **Current Selection** - Center the current selection on the **Doodle Board**. This function is useful if the document perspective is zoomed in and it is difficult to locate selected content.
- **Zoom Out** - Zoom out and decrease the document scale, you may also use the drop down selection provided in the **Files + Formatting** toolbar.
- **Zoom In** - Zoom in and increase the document scale, you may also use the drop down selection provided in the **Files + Formatting** toolbar.

Content Menu

- **Select>** - Contains various tools for selecting content.
  - **All** - Select all content in the current document.

  - **Inverse** - Select all content in the current document that isn't currently selected while deselecting all content in the current document that is currently selected.

- **Next Molecule** - Select the next molecule in the document. This function will traverse chronologically through the molecules in the current document based on the time they were drawn. If a molecule isn't currently selected, it will first select the last molecule drawn.
- **Next Shape** - Select the next shape in the document. This function will traverse chronologically through the shapes in the current document based on the time they were drawn. If a shape isn't currently selected, it will first select the last shape drawn.

- **SMARTS...** - A textfield will appear. Type in the desired *SMARTS* pattern here and then click the **Accept** button. Any content in the current document that matches the *SMARTS* pattern will be selected.

- **Deselect** - Deselect all content that is currently selected. This function is only enabled if content is currently selected.
- **Reselect** - Reselect the last content that was selected. This function is only enabled if no content is currently selected. This function may not work as expected when content is removed. For instance, if you selected content and then deleted it, then pressing reselect will have no action because the content to be reselected no longer exists.

- **Center>** - Contains various functions for centering content.
  - **All on Page** - Center all content on the page.

  - **Selection on Page** - Center only the currently selected content on the page.
  - **Selection Horizontally** - Horizontally center only the currently selected content.
  - **Selection Vertically** - Vertically center only the currently selected content.
- **Flip>** - Contains functions for flipping selected content.
  - **Horizontally** - Flip the currently selected content horizontally over its midpoint.
  - **Vertically** - Flip the currently selected content vertically over its midpoint.
- **Rotate>** - Contains various functions for rotating selected content.
  - **90° CW** - Rotate selected content clockwise by 90 degrees.
  - **90° CCW** - Rotate selected content counterclockwise by 90 degrees.
  - **180° -** Rotate selected content by 180 degrees.
  - **Arbitrary...** - Rotate selected content by an arbitrary angle that you input.
- **Scale...** - Scale the currently selected objects. You will be presented with a window to set various options to define how the content will be scaled. You can even choose to scale all molecules individually, to set them all to a common bond length for instance.

- **Align Bond>** - Contains functions for aligning a single selected bond, rotating the molecule it is contained in. This function is enabled when only a single bond is selected.
  - **Up** - Align bond up.
  - **Right** - Align bond right.

- **Down** - Align bond down.
- **Left** - Align bond left.

- **Flip Bond Orientation** - Flip the orientation of the bond. Non-symmetrical bonds will face the other direction.

- **Align>** - Contains functions for aligning selected content.
  - **Left Edges** - Align all selected content by the left edges of their visual bounds.
  - **Horizontal Centers** - Align all selected content by the horizontal centers of their visual bounds.
  - **Right Edges** - Align all selected content by the right edges of their visual bounds.

  - **Top Edges** - Align all selected content by the top edges of their visual bounds.
  - **Vertical Centers** - Align all selected content by the vertical centers of their visual bounds.
  - **Bottom Edges**-Align all selected content by the bottom edges of their visual bounds.
- **Distribute>** - Contains functions for distributing selected content.
  - **Horizontally on Page** - Distribute selected content horizontally on the page such that they are evenly distributed based on their visual bounds and fit within the page margins.
  - **Vertically on Page** - Distribute selected content vertically on the page such that they are evenly distributed based on their visual bounds and fit within the page margins.
  - **Horizontally by Buffer Space...** - Distribute selected content horizontally on the page such that they are evenly distributed based on their visual bounds by a value that you input.
  - **Vertically by Buffer Space...** - Distribute selected content vertically on the page such that they are evenly distributed based on their visual bounds by a value that you input.
- **Grid All on Page...** - Grid all content on the page. A window will appear to ask for row and column information.
- **Stack All on Page** - Stack all content on the page. Stacking will place all content within the page margins based on their visual bounds. Stacking proceeds by placing content from left to right, and then top to bottom, on the page using a small buffer space.

- **Group** - Group the currently selected content into a single shape. Single items in grouped content can not be edited and transformations will affect the entire group as a whole. Groups can also be grouped into larger groups.
- **Ungroup** - Ungroup grouped content. Ungrouping is not recursive, so if the group being ungrouped contains a group, then that inner group will remain grouped.

- **Join** - If two atoms are selected, then they will be joined into a single atom, and their bonds will all point to the new joined atom. If those atoms were part of two discrete molecules, then one molecule is translated to the other. If two bonds are selected, then they will be joined together, and all bonds connected to the joined bonds will connect to the new joined bond. Two bonds within

the same molecule cannot be joined. One molecule will be translated and rotated to the other to aesthetically display the new joined molecule. This function is disabled in all other cases.

- **Flatten** - This function will change all z-coordinates of selected atoms to be 0, thereby flattening 3D structures.

- **Add Frame>** - Contains various functions for surrounding selected content with shapes based on their visual bounds.
  - **Square Brackets** - Surround selected content with square brackets based on the content's visual bounds.
  - **Parenthesis** - Surround selected content with parenthesis based on the content's visual bounds.
  - **Curly Brackets** - Surround selected content with curly brackets based on the content's visual bounds.
  - **Chevrons** - Surround selected content with chevrons based on the content's visual bounds.
  - **Rectangle** - Surround selected content with a rectangle based on the content's visual bounds.
- **Measure>** - Contains various functions for measuring selected content.
  - **Diagonal** - Place one ruler object diagonally over selected content based on its visual bounds to measure its diagonal. You can change the units of the ruler object.
  - **Width and Height** - Place two ruler objects, one vertically to the left and one horizontally below selected content based on its visual bounds to measure its width and height. You can change the units of the ruler object.

- **Conform to Document Settings** - Conform all currently selected objects to the current chemical document settings, including scaling and changing fonts.

Structure Menu

- **Add/Remove Hydrogens>** - Contains functions for adding Hydrogens to structures. Settings for defining how Hydrogens will be added to structures can be set in the **Preferences** window under the **Visuals** tab under the **Atoms** tab.
  - **All** - Add Hydrogens to all structures in the current document.
  - **From Selection** - Add Hydrogens only to the currently selected structures.
- **Add Attribute...** - Add an attribute to the selected object. This will only be enabled if a single atom or bond is selected.
- **Place Formal Charges** - Will place formal charges on atoms based on their valency.

- **Calculate Covalent Bonds** - This function will deduce covalent bonds in structures based on atomic 3D distances and the covalent radii present in ChemDoodle's elemental database. This function is dependent on the **Ångström/Bond Length** document setting present in the **Preferences** window under the **Visuals** tab. Only single bond orders will be placed. This function is very useful for working with files that may not contain explicit topology, such as *PDB* or *XYZ* files.
- **Remove Selected Bonds** - This function will remove all selected bonds, leaving the constituent atoms.

- **Saturate** - This function will change the bond orders of all selected bonds to the single bond order.
- **Kekulize** - This function will convert a delocalized substructure (defined with resonance bonds) or a single bond skeleton to a Kekulé structure with the most delocalized area.
- **Delocalize** - Converts a Kekulé structure to the delocalized equivalent.
- **Graph Reduction>** - Contains several functions for reducing the underlying graph data structures that represent the selected structures. This is ideal for extracting information about small molecule building blocks for drug discovery purposes.
    - **Reduce 0° (Lone)** - This function will remove all 0 degree nodes, so all lone atoms will be removed.
    - **Reduce 1° (Terminals)** - This function will remove all 1 degree nodes, so all terminal atoms will be removed.
    - **Repeatedly Reduce 1°** - This function will repeatedly remove all 1 degree nodes until none remain, so all isolated chains will be removed.
    - **Reduce 1° + 0°** - This function will remove all 0 and 1 degree nodes, so all lone and terminal atoms will be removed.
    - **Reduce 2° (Chains)** - This function will remove all 2 degree nodes, so all inner chain atoms will be removed.
    - **Reduce 2° + 1° + 0°** - This function will remove all 0, 1 and 2 degree nodes, so all lone, terminal and chain (including non-isolated chains) atoms will be removed.
- **Expand Labels** - Will expand all complex atom labels to their all-atom equivalents.
- **Rings>** - Contains several functions for defining ring sets in selected structures. If a highly overlapping figure results, just stack the content for a cleaner layout.
    - **Explode Smallest Set of Smallest Rings** - Explode out the smallest set of smallest rings (SSSR) for selected structures. The SSSR is the standard for defining ring sets in flat 2D structures.
    - **Explode Euler Facet Rings** - Explode out the Euler facet rings for selected structures. The Euler facet ring set is better than the SSSR at defining essential rings in 2D depictions of 3D structures.
    - **Explode Hanser (All) Rings** - Explode every last graph cycle in selected structures.
- **Stereochemistry>** - Contains several functions for deducing the stereochemistry of selected structures.
    - **Assign R/S (CIP)** - Finds and assigns CIP stereochemistry to chiral centers.
    - **Assign E/Z (CIP)** - Finds and assigns CIP stereochemistry to stereochemical double bonds.
    - **Assign cis/trans** - Finds and assigns cis/trans stereochemistry to appropriate double bonds.
- **Chemical Suppliers>** - Contains functions to search for chemical suppliers for drawn structures.

- **Substructure Match** - Find chemical suppliers for the selected structure by substructure search.
- **Exact Match** - Find chemical suppliers for the selected structure by exact match.

- **Clean>** - Contains various functions for optimizing and beautifying selected structures.
  - **2D Optimization** - The CCG depiction algorithm is performed on your selected structures to clean them in 2D.
  - **Distance Geometry Embedding** - Distance geometry is used on the bond distance matrix of the selected structures to embed them in 3D. This is great for highly connected structures like buckyballs and will produce suitable 3D coordinates. It will not work very well on less connected structures like chains.
- **Descriptors>** - Contains various functions that will display the named descriptor for the first of the selected molecules. Details about these algorithms are described in *Chapter 6*.
  - ***Last Chosen*** - This menu item is a placeholder that will remember the last chosen descriptor for easy repeat access.
  - **Constitutional>** - Contains any constitutional descriptors; descriptors that are defined by the chemical makeup of the molecule.
    - **Atom Count** - Calculates the atom count.
    - **Bond Count** - Calculates the bond count.
    - **Degree of Unsaturation** - Calculates the degree of unsaturation.
    - **Element Counts** - Calculates the element counts.
    - **Euler Facet Ring Count** - Counts the total number of Euler facet rings present in a molecule.
    - **Exhaustive Ring Count** - Counts every last graph cycle in a molecule.
    - **Frèrejacque Number** - Calculates the Frèrejacque number. This is also the SSSR number.
    - **Hydrogen Bond Acceptor Count** - Calculates the Hydrogen bond acceptor count.
    - **Hydrogen Bond Donor Count** - Calculates the Hydrogen bond donor count.
    - **Rotatable Bond Count** - Counts the number of rotatable bonds.
    - **Total Electron Count** - Counts the total number of electrons present in the molecule.

    - **Lightest Isotopic Mass** - Calculates the molecular mass based on the lightest isotope for each element, regardless of abundance.
    - **McGowans Characteristic Volume** - Calculates McGowan's characteristic volume.
    - **Molecular Mass** - Calculates the molecular mass based on ChemDoodle's elemental database.

- **Molecular Mass** - Calculates the molecular mass based on ChemDoodle's elemental database.
- **Volume as a Sum of Atomic and Bond Contributions** - Calculates the ABC volume.

- **Empirical Formula** - Generates the empirical formula of the first selected structure.
- **Molecular Formula** - Generates the molecular formula of the first selected structure.

- **Topological>** - Contains any topological descriptors; descriptors that are defined by the bond connectivity of the molecule.
  - **Centric Index** - Calculates the Centric index.
  - **Diameter** - Calculates the longest topological path in a molecule.
  - **Hosoya Index** - Calculates the Hosoya index.
  - **Molecular Topological Index** - Calculates the Molecular Topological index.
  - **Platt Index** - Calculates the Platt index.
  - **Ring Complexity** - Calculates the Ring Complexity.
  - **Szeged Index** - Calculates the Szeged index.
  - **Wiener Index** - Calculates the Wiener index.
  - **Zagreb Indexes** - Calculates various Zegreb indexes.

  - **Balaban Index** - Calculates the Balaban index.
  - **Bertz Complexity Index** - Calculates the Bertz Complexity index.
  - **Branching Index** - Calculates the Branching index.
  - **Chi Molecular Connectivity Indexes>** - Calculates various Chi Molecular Connectivity Indices.
  - **Fraction Molecular Framework** - Calculates the Fraction Molecular Framework ratio.
  - **Harary Index** - Calculates the Harary index.
  - **Kappa Shape Indices>** - Calculates various Kappa Shape Indices.
  - **Superpendentic Index** - Calculates the Superpendentic index.

  - **Adjacency Matrix** - Generates the bond connectivity matrix.
  - **Bond Distance Matrix** - Generates the bond distance matrix.
  - **Bond Electron Matrix** - Generates the bond electron matrix.
  - **Detour Matrix** - Generates the detour matrix.
  - **Incidence Matrix** - Generates the incidence matrix.
  - **Laplacian Matrix** - Generates the Laplacian matrix.

- **Physicochemical>** - Contains any physicochemical descriptors; descriptors

that are defined by physics or chemistry of the molecule.

- **Average Molecular Polarizability>** - Calculates the average molecular polarizability given several algorithms.
- **Critical Pressure** - Calculates the critical pressure of a molecule.
- **Critical Temperature** - Calculates the critical temperature of a molecule.
- **Critical Volume** - Calculates the critical volume of a molecule.
- **Enthalpy of Formation (ideal gas at 298K)** - Calculates the enthalpy of formation of a molecule at the stated conditions.
- **Enthalpy of Fusion** - Calculates the enthalpy of fusion of a molecule.
- **Enthalpy of Vaporization (at Tb)** - Calculates the enthalpy of vaporization of a molecule at the stated conditions.
- **Gibbs Energy of Formation (ideal gas, unit fugacity, at 298K)** - Calculates the Gibbs energy of formations of a molecule at the stated conditions.
- **Heat Capacity (ideal gas, at 298K)** - Calculates the heat capacity of a molecule at the stated conditions.
- **Lipophilicity, logP>** - Calculates logP given several algorithms.
- **Liquid Viscocity (at 298K)** - Calculates the liquid viscocity of a molecule at the stated conditions.
- **Molar Refractivity>** - Calculates the molar refractivity of a molecule given several algorithms.
- **Normal Boiling Point** - Calculates the normal boiling point of a molecule.
- **Normal Freezing Point** - Calculates the normal freezing point of a molecule.
- **Topological Polar Surface Area** - Calculates topological polar surface area (TPSA).

- **ADME Filters>** - Contains descriptors that assess bioactivity.
  - **Bioavailability Score** - Calculates the Bioavailability score.
  - **Egan Violations Count** - Calculates the number of violations to Egan's rules.
  - **Lipinski's Rule of 5 Violations Count** - Calculates the number of violations to Lipinski's rule of 5.
  - **Veber Violations Count** - Calculates the number of violations to Veber's rules.

- **Generate Line Notation>** - Contains functions for generating line notations of selected structures.
  - **SMILES** - Generates simplified molecular input line entry specification (*SMILES*).
  - **SLN** - Generates Sybyl Line Notation (*SLN*).
  - **InChI** - Generates the international chemical identifier (*InChI*).

- **ROSDAL** - Generates the representation of organic structure descriptions arranged linearly (*ROSDAL*).

- **Parse IUPAC Name...** - A text field will appear. Type or paste in a correct IUPAC name and the structure will be generated and inserted into the current document.

- **Abbreviations>** - Contains functions for maintaining ChemDoodle's abbreviations database.
  - **Add New...** - Pops up a window to add a new abbreviation to ChemDoodle's abbreviations database.
  - **Manage Recognized...** - Pops up a window to add, edit and delete abbreviations from ChemDoodle's abbreviations database.
- **Manage My Templates...** - Contains functions for maintaining ChemDoodle's templates database.

Reaction Menu

- **Clean** - Clean the selected reaction. The reaction must first be defined using the **Build Implied Reaction** or **Edit Reaction...** functions. This function will align and distribute the reaction as well as beautify the reaction arrow. Settings to control how reactions are cleaned can be set in the **Preferences** window, under the **Visuals** tab, under the **Reaction** tab.

- **Build Implied Reaction** - When an arrow and structures are selected, this function will become enabled. All selected structures with midpoints to the left of the arrow midpoint become reactants while all selected structures with midpoints to the right of the arrow midpoint become products.
- **Edit Reaction...** - Will open up a window showing all the structures in the current document. Click and drag structures from the document tray to the reactant and product trays to explicitly define the reaction. This function is enabled when an arrow is selected.
- **Dissolve Reactions** - Will dissociate any selected reaction data structures.

Spectrum Menu

- **View XY Data** - View the XY plot data of the first selected spectrum. You can copy and paste this data into other programs, like Excel.

- **Edit Perspective...** - Will open up a window showing several tools for editing the spectrum view and axis. Once closed, the spectrum in the document will update.
- **Expand Perspective** - Will expand the spectrum perspective to view the entire domain and range of the plot. This function is enabled when a spectrum is selected.

- **Generate>** - Contains various functions for generating and simulating spectra.
  - **^{1}H NMR** - Generate a proton nuclear magnetic resonance spectrum of the first selected structure.
  - **^{13}C NMR** - Generate a carbon-13 nuclear magnetic resonance spectrum of the first selected structure.

  - **Mass Parent Peak** - Generate a mass parent peak from the mass spectrum of the first selected structure. This will

show the magnitude of the parent ion and the isotopic distribution.

Window Menu

- **Minimize** - Iconify the main ChemDoodle window to the dock or system tray. ChemDoodle's menu bar will remain focused on Mac OS X.
- **Zoom** - Expand the ChemDoodle window to fill the entire screen without overlapping any docks or system trays.

- **Select Tab Right** - This function is enabled if there are one or more tabs present in the tab tray. This function will select the tab to the right of the currently selected tab. If the currently selected tab it the right-most tab, then the first tab is selected.
- **Select Tab Left** - This function is enabled if there are one or more tabs present in the tab tray. This function will select the tab to the left of the currently selected tab. If the currently selected tab it the left-most tab, then the last tab is selected.

- **Save Document Settings...** - Set the currently defined document settings as the default document settings.

- **Default Workspace** - Return the configuration of windows within the main ChemDoodle window to the default layout.
- **Revert Workspace** - Revert the ChemDoodle workspace to the last saved workspace.
- **Save Workspace** - Save the current configuration of the windows within the main ChemDoodle window. This also saves file chooser paths and other workspace settings. This function is automatically performed when ChemDoodle is closed.

Purchase Menu

This menu is only present during the free trial, and is removed when ChemDoodle is activated with a purchased activation code.

- **Activate ChemDoodle** - Displays the activation form to input a purchased activation code and generate the license for the ChemDoodle application.

- **Buy an Activation Code** - Opens the default internet browser to the purchase page of the ChemDoodle website.

Help Menu

- **About ChemDoodle** - Display information about ChemDoodle, your activation code and your license expiration, if any. This menu item is in the **ChemDoodle** menu on Mac OS X.

- **ChemDoodle User Guide** - View this user guide in the program most appropriate for opening *PDF* files.
- **ChemDoodle Keyboard Shortcuts** - View a cheat sheet for all keyboard shortcuts and actions available in ChemDoodle in the program most appropriate for opening *PDF* files.
- **References** - View an organized list of references for the data and algorithms used in ChemDoodle. You can use this list to assess ChemDoodle's quality.

- **View User License** - View the user license that you accepted when you activated ChemDoodle.
- **Deactivate ChemDoodle** - ChemDoodle can only be used on the number of computers determined in your license. To switch from one computer to another, use this function first. This function is also

useful if you need to reinstall your operating system.

- **Contact Customer Service** - Open the iChemLabs customer support form and pre-populate fields. This is the preferred way to contact iChemLabs customer service.
- **iChemLabs Newsfeed** - View the iChemLabs newsfeed *RSS*.

- **Check for Updates** - Check for updates to ChemDoodle. If any are found, you will see the changes listed and you will be requested to update ChemDoodle. If allowed, ChemDoodle will automatically update itself. There is no need to redownload or reinstall ChemDoodle for updates.

Toolbars

Toolbars are located at the top-left of the ChemDoodle window. They contain buttons for changing how mouse gestures affect documents, such as placing bonds or placing a rectangle. There are also buttons for quickly accessing menu items.

Toolbars can be moved at any time. They will automatically lock to the borders of the main ChemDoodle window and to their original position. To save the current placement of toolbars so they will remain in that position when you next open ChemDoodle, select the **Save Workspace** menu item in the **Window** menu. The placement of toolbars will also be saved when the ChemDoodle application is closed.

There are 8 toolbars:

- **Files + Formatting** - Contains buttons for saving files, transferring content and formatting fonts and scale.
- **Content** - Contains functions for manipulating content including the selection tools.
- **Strokes** - Contains 3 drop down selections for defining bond stroke brush styles.
- **Labels** - Contains preset labels that can be used on atoms as well as the **Atom Label** tool which will allow you to type whatever content you would like in atom labels.
- **Rings** - Contains buttons for drawing common ring types.
- **Bonds** - Contains buttons for accessing all bond types in ChemDoodle.
- **Arrows** - Contains 3 drop down selections for defining arrows and buttons for drawing the defined arrow with several preset arc angles.
- **Orbitals** - Contains various orbital graphics for standalone figures or for attaching to structures.
- **Shapes** - Contains any remaining buttons, including shapes, carbon chains, brackets, pens, glassware clipart, text, etc.

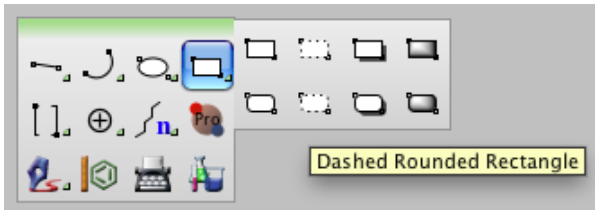
Additionally, there are also text formatting toolbars that will appear when convenient, such as when editing text areas.

Group Buttons

In some cases, similar buttons are grouped into a single unified group button. These group buttons are decorated with a small highlighted triangle at the bottom-right of the button. Clicking on the button will select it and perform the displayed function as one would expect.

To change to a different function of the group button, click down and hold the button for one second or click down and drag slightly to expand the group button as is shown in Figure *1.13*. Once expanded, just drag the mouse pointer over the function you would like to use and release the mouse. The function the mouse was over when it was released will become selected and will now display as the main function of the group button.

Figure 1.13: An expanded group button.



Files + Formatting Toolbar

Figure 1.14: Files+Formatting Toolbar

➡Create a new blank document

➡Create a new blank formatted document

➡Open a file

➡Save a file

➡Print document

➡Print preview

➡Cut

➡Copy

➡Paste

➡Font family (font functions affect selected content only)

➡Font size

➡Bold font

➡Italicize font

➡Quick Colors button

➡Color button and color selection button

➡Document scale

➡Zoom In

➡Zoom Out

Content Toolbar

Figure 1.15: Content Toolbar

➡Lasso selection tool

➡Rectangular Marquee selection tool

➡Lasso only Shapes selection tool

➡Rotate in 3D tool

➡Eraser tool

➡Clear tool

➡Add/Remove Hydrogens

➡Clean Structure

➡Clean Reaction

➡Conform to Document Settings

➡Fragmentation Tools

➡Undo

➡Redo

Strokes Toolbar

Figure 1.16: Strokes Toolbar

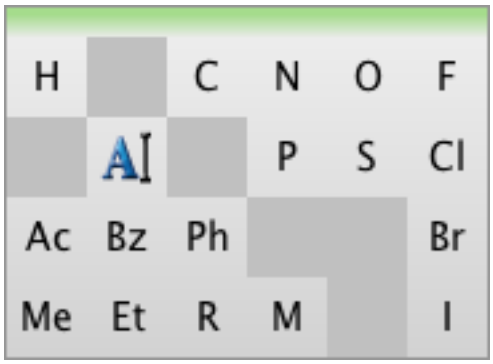
➡Stroke Style

➡Stroke Width

➡Texture Magnitude

Labels Toolbar

Figure 1.17: Labels Toolbar

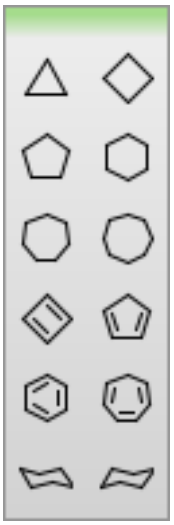


The labels toolbar contains the element labels: H, C, N, O, F, P, S, Cl, Br and I. It also contains the superatom labels: Ac, Bz, Ph, Me, Et, R and M. Clicking on any of these labels will change the cursor to that label and then clicking on an atom will change that atom's label to the selected label.

The middle of the toolbar contains the **Set Atom Label** tool . The atom label tool, when selected, will allow you to click on any atom and open a text field. Type in anything you want into the text field and then click on the page or press the *return* key to close the text field, setting the selected atom's label to the contents of the text field.

Rings Toolbar

Figure 1.18: Rings Toolbar



Clicking on any ring will change the drawing mode to place rings.

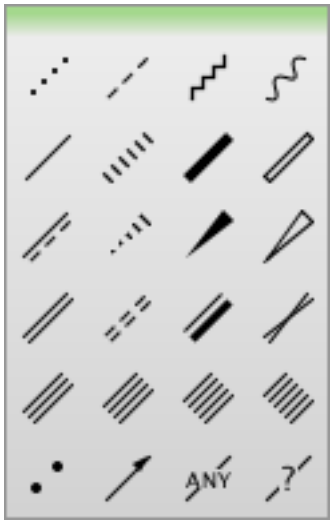
Rings include, from top-left to bottom-right:

- cyclopropane ring
- cyclobutane ring
- cyclopentane ring
- cyclohexane ring
- cycloheptane ring

- cyclooctane ring
- cyclobutadiene ring
- cyclopentadiene ring
- benzene ring
- cycloheptatriene ring
- cyclohexane chair conformer 1
- cyclohexane chair conformer 2

Bonds Toolbar

Figure 1.19: Bonds Toolbar



Just click any bond type and the drawing mode will change to place bond orders of that type. Clicking on a bond will change that bond's current bond type to the selected bond type.

The single bond order will add to other bond orders by default. So clicking on a single bond will change it to a double bond, clicking on a double bond will change it to a triple bond, etc. Clicking on a sextuple bond will change it to a single bond. Clicking on decorated bond orders (protruding, ambiguous double, etc.) will convert it to a non-decorated (single, double, etc.) bond before incrementing it. To stop single bond orders from adding to bonds, you can set the single bond behavior to instead override other bond orders in the **Preferences** window under the **General** tab.

Bond types include, from top-left to bottom-right:

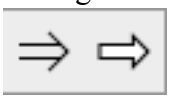
- Zero Order/Hydrogen/Ionic bond
- Half bond
- Zigzag bond
- Wavy bond
- Single bond
- Bold Dashed bond
- Bold Single bond
- Bold Hollow bond
- Resonance bond
- Recessed bond
- Protruding bond
- Double bond
- Double Dashed bond
- Bold and Thin Double bond
- Ambiguous Double bond
- Triple bond
- Quadruple bond
- Quintuple bond
- Sextuple bond
- Two Electron bond
- Covalent bond (coordinate covalent by default, can be changed to a polar covalent bond)
- Any Order bond

- Unknown Order bond

Arrows Toolbar

Figure 1.20: Arrows Toolbar

The top row of contains three drop down selections. The first defines the style of the start arrow, the second defines the style of the connector between arrows and the third defines the style of the end arrow. The first five buttons beneath the drop down selections allow you to place the arrow in the document and will preset a given angle. The preset angles include (from left to right): 270°, 180°, 120°, 90° and 0°. At any time, you can change the arc angle of a placed arc to any arbitrary angle of your choice.

The last button is the special arrow presets button. This group button contains presets for common non-standard arrow types, such as retrosynthetic arrows. The arc angles of these arrows cannot be changed. 

Orbitals Toolbar

Figure 1.21: Orbitals Toolbar

The orbitals toolbar contains two rows of orbital types that can be placed into figures and attached to structures. From top-left to bottom-right are Atomic s, Atomic $p_{x|y|z}$, Atomic $d_{xz|yz|xy|x^2-y^2}$, Atomic d_{z^2}, Atomic $f_{xz^2|xy^2|x(x^2-3y^2)|y(3x^2-y^2)}$, Atomic f_{z^3}, Hybrid sp^3, Hybrid sp lobe, Bonding σ and Bonding π.

Each button is a group button containing different shading an fill options for that orbital shape.

Shapes Toolbar

Figure 1.22: Shapes Toolbar

The shapes toolbar contains many group buttons and other functions for changing the current drawing mode to place both chemical and non-chemical objects.

The tools include, from top-left to bottom-right:

- **Lines** - Straight, dotted, wavy and zigzag.

- **Arcs** - 90°, 120°, 180° and 270°.

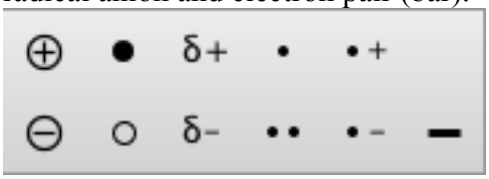
- **Ovals** - Plain, dotted, shadowed and

shaded.

- **Rectangles** - Plain, dotted, shadowed, shaded, plain rounded, dotted rounded, shadowed rounded and shaded rounded.

- **Brackets** - Square (pair), parenthesis (pair), curly (pair), chevrons (pair), dynamic brackets, square, parenthesis, curly, chevron.

- **Chemical Attributes** - increment charge, add radical, positive dipole, single electron, radical cation, decrement charge, remove radical, negative dipole, electron pair, radical anion and electron pair (bar).



- **Carbon Chains** - 120° Carbon chains, Fisher Projection chains and Random Carbon chains.

- **Sequence Tool** -  Draw an amino acid sequence.
- **Polylines** - Pen, pen-poly tool and polyline.

- **Rulers** -  Place a measurement ruler.
- **Text Areas** -  Place a text area with a background and border that can be resized to any dimension and is associated with text formatting tools.
- **Glassware Templates** -  Opens the laboratory glassware templates window to build diagrams with glassware clipart.

Interface Options

In addition to being a very powerful application for your chemical data, ChemDoodle is also very customizable so you can fit its behavior to your preference. ChemDoodle provides many options for changing the way it looks, how it works, and the visual effects that you will see.

To access the interface options, select the **Preferences...** menu item in the **Edit** menu (in the **ChemDoodle** menu on Mac OS X). The first tab, **General**, will contain the interface options.

Drawing Controls

Drawing Mode
There are two drawing modes, Quick and Control. Quick mode will do a complete multistep-action in a mousedown-drag-mouseup procedure, while Control mode will complete a multistep-action in a click-move-click procedure. The default is Quick mode.

Optimize Zone Size
The Optimize Zone is a special component in ChemDoodle to help you place bonds in the optimal position around atoms. It is the blue circle that appears when placing bonds and other molecule fragments. To use the Optimize Zone, just place the mouse pointer in the blue circle. The bond or fragment being placed will automatically be oriented in the most optimal position. You can change the size of the optimize zone to be Small, Medium or Large. It is Medium by default.

Hover Distance
The hover distance controls how close the mouse pointer must be to an object for it to be considered hovered. The default is 10 pixels, but you can make this shorter or longer depending on your preference.

Snap to Grid
By default, coordinates for all objects can be placed anywhere. However, you can set a 5 pixel or 10 pixel grid for objects to snap to.

Single Bond Behavior
By default, **Single** bonds will increment bond orders. So using the **Single** bond tool, if you click on a **Single** bond it will become a **Double** bond and so forth. However, you can change this behavior to instead override bond orders so any bonds clicked on with the **Single** bond tool become **Single** bonds.

Label Behavior
Label tools can either edit the atom clicked on or add a new bond connected to the atom clicked on with the new atom having that label. By default, atom label tools will modify the selected atom.

Auto-connect Rings and Templates
This option is enabled by default and will have the atoms placed by ring and template tools automatically merge with any overlapping atoms present in the document.

Fix Bond Lengths
This options is enabled by default and fixes the bond lengths of the drawing tools. You can quickly reverse this setting when drawing by holding down the *shift* key.

Fix Bond Angles
This options is enabled by default and fixes the bond angles of the drawing tools. You can quickly reverse this setting when drawing by holding down the *alt* key.

Require Starting Atom
Many chemical sketchers have the bond as the smallest building block. ChemDoodle uses atoms as the smallest building blocks, and all drawing functions require a starting atom. You can disable this requirement and

allow new bonds to be placed with a single mouse click.

Rotate Atom Text with Structures
By default, text will not rotate when you rotate structures. This way text is always horizontally readable. You can enable this setting to have atom text rotate when you rotate structures.

Bonds are Focusable
If you are working with only atoms or you don't want to touch bonds, enabling this setting will make editing easier. When enabled, bonds cannot be hovered or selected.

3D Rotation Mode
When using the structure perspective tool, mouse movements will correspond to X and Y axis movements during 3D rotation. You can change this to correspond to a quaternion rotation if you are more familiar with that behavior.

Appearance

Recently Opened Files
Recently opened files can be displayed at the bottom of the **File** menu, or in a submenu in the **File** menu. By default they are displayed in a submenu, but you may wish to switch this option for quicker access if you have a tall screen.

Interface Font
If you prefer a different font from the standard sans-serif font that ChemDoodle uses, you can change it in the **Preferences** window under the **General** tab in the **Appearance** section. This is also helpful if you need to switch to a different font that supports characters for another language.

Interface Color
If you prefer a color other than the default light green color, you can choose to change this in the **Preferences** window under the **General** tab in the **Appearance** section. Light, pale color choices are easiest on the eyes and are least distracting.

Decorations

Show Unfixed Drawing Measurements
When enabled, statistics are rendered to show you lengths and angles if they are not fixed.

Show Transform Measurements
When enabled, statistics are rendered to show you how your lasso functions are altering your figures.

View Crawling Ants Effect When Lassoing
When enabled, the lasso outline will exhibit a crawling ants effect so you can easily see it.

View Shimmer Effect on Button Hover
When enabled, buttons will display a shimmer effect when you hover the mouse cursor over them. This makes it easy to detect which button you are pressing.

View Mouse Position on Rules
When enabled, the mouse position will be ticked on the document's rulers in red.

View Selection Bounds on Rulers
When enabled, the lasso selection will be highlighted on the document's rulers in amber.

Filechooser Settings

Unified Filechooser Memory
By selecting this option, all filechoosers, regardless of function will remember the last location of any of the file choosers. Otherwise, they will each retain their own memory.

Include Previews in Filechooser
You may wish to disable this to hide file chooser previews.

Chapter 2: Widgets

Overview

Widgets could be individual applications on their own, but with ChemDoodle, they provide added functionality and benefit from ChemDoodle's useful capabilities.

This section introduces the new user to widgets within ChemDoodle. It covers the following topics:

- Identifying the widgets.
- Using the widgets.
- Thorough guides for the widgets.

Widget Windows

Each widget has its own unique interface contained within a widget window. A widget window is a simple, movable and resizable window that contains the widget interface and other buttons for maximizing and minimizing the widget as is shown in *Figure 2.1* and *Figure 2.2*. Widget window decorations will be slightly different between Windows/Linux and Mac OS X.

The top bar contains two buttons, one for minimizing the widget to the ChemDoodle desktop tray and one for maximizing the widget to fit the entire ChemDoodle application window. You can also use the drag anchors to resize widgets.

To move widgets, just click and drag the top bar. Widgets will automatically lock to the borders of the ChemDoodle application and to their origins.

The entire widget interface is presented in the rest of the widget window below the title, which is displayed below the top bar.

Figure 2.1: Widget Window on Windows/Linux

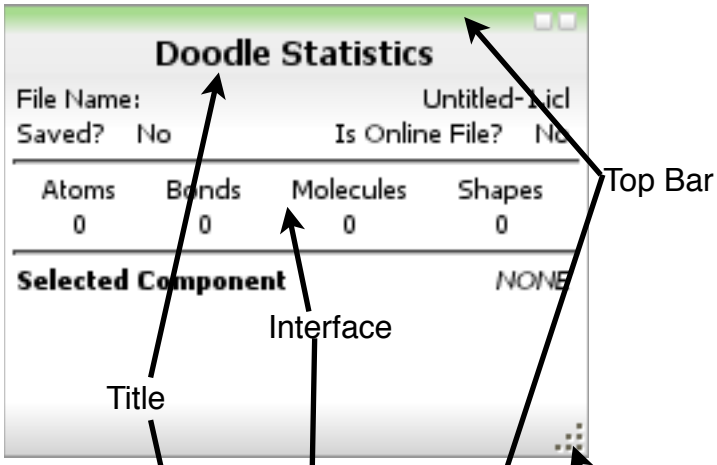
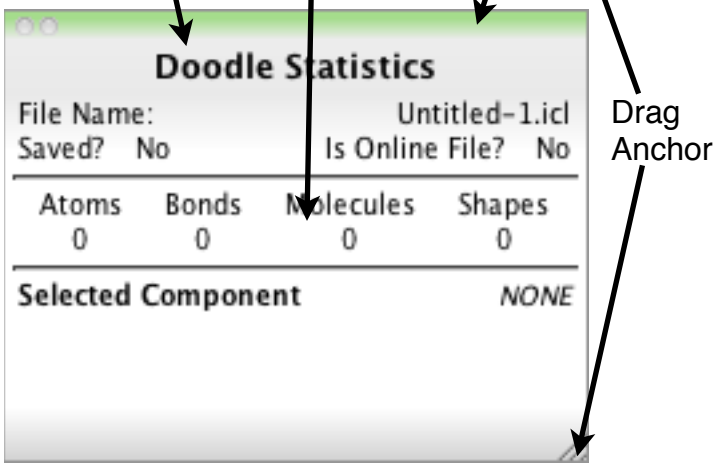


Figure 2.2: Widget Window on Mac OS X



Widget Expansion

Some widgets are initially in a collapsed state. Each collapsed widget will have some gesture to expand it. For example, the **MolGrabber** widget is initially collapsed. Just type a search term in the text field and press the *return* key to expand it as showing in *Figures 2.3-2.4*. Every collapsable widget will also have a collapse button to collapse it.

Figure 2.3: A collapsed widget

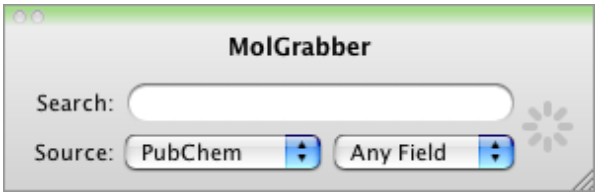
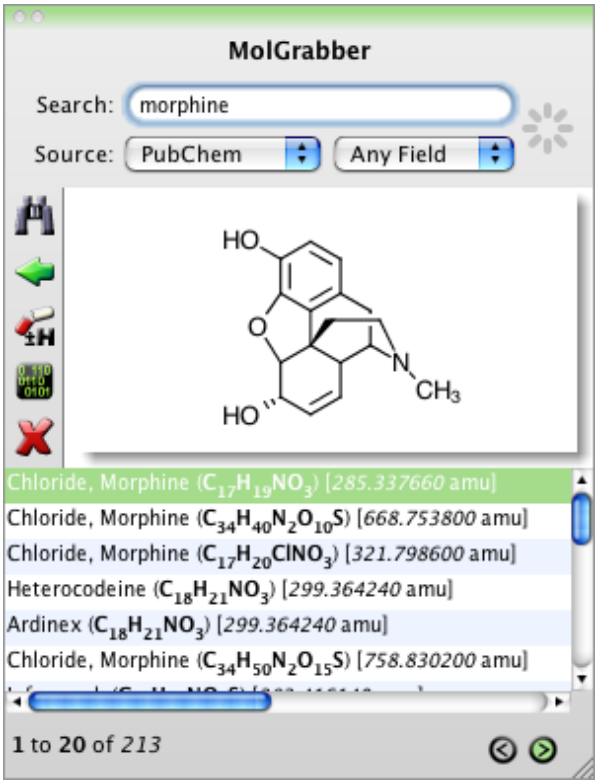


Figure 2.4: An expanded widget



Widget List

There are currently 12 widgets provided in ChemDoodle:

- **Elemental Analysis** - Calculates molecular masses, elemental analysis and isotopic distributions for structures.
- **History** - Provides full access to the undo/redo queue.
- **Line Notation Pad** - Generates and parses line notations and will also correct your input.
- **MolGrabber** - Search databases for chemical structures.
- **Multiplet Tool** - Simulate multiplets.
- **NMR SignalSeek** - Simulate nuclear magnetic resonance and associate peaks to nuclei as well as provide more thorough information about the spectrum and simulation.
- **Properties** - Calculates molecular descriptors.
- **Search** - Search your computer and attached storage devices for chemical structures.
- **Statistics** - Displays document and drawing statistics.
- **Symbols** - Quick access to chemically relevant symbols and the full unicode range.
- **Templates** - Organizes chemical structure templates for your use.
- **TLC Canvas** - Draw thin layer chromatography plates.

Widget Dock

The **Statistics** and **History** widgets are shown at all times. Only one other widget is shown in addition to these two at any given time. You can switch the widget that is shown by clicking on the widget icon of the widget you would like to be shown in the widget dock. The widget dock is located at the bottom-right of the ChemDoodle window and appears as shown in *Figure 2.5*.

Figure 2.5: The widget dock

If you hover over any of the icons, that icon will be enlarged, and the title of the widget will appear to the left of the widget dock as shown in *Figure 2.6*.

Figure 2.6: Hovering an icon in the widget dock

Just click on the hovered widget icon to select and show the corresponding widget.

You can also move the widget dock along the bottom of the application desktop, by pressing the mouse down and dragging on the **(< >)** symbol displayed at the bottom right of the dock.

Widget Icons

In addition to selecting widgets, these icons may also perform additional functions. For instance, if you drag a structure onto the Line Notation Pad widget icon, that structure will be loaded into the widget. Information on these additional functions are provided in the next sections.

Table 4: Widget Buttons

Button	Widget
	Elemental Analysis
	Line Notation Pad
	MolGrabber
	Multiplet Tool
	NMR SignalSeek
	Properties
	Search
	Symbols
	Templates
	TLC Canvas

Elemental Analysis Widget

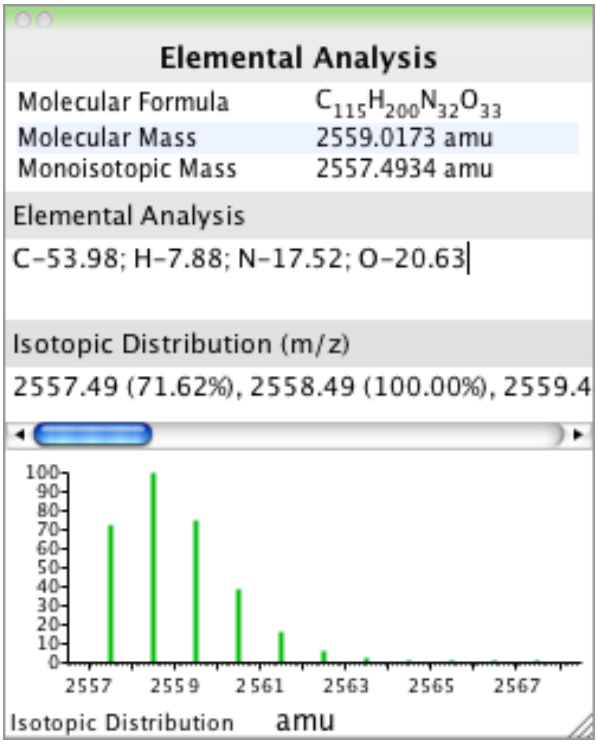
Purpose

The **Elemental Analysis** widget calculates several data that are useful to chemists. It calculates formulas and masses, performs elemental analysis, and simulates isotopic distributions.

Interface

The interface consists of 4 sections. From top to bottom, the first section displays the molecular formula, molecular mass and monoisotopic mass. The second section shows the elemental analysis, with each element shown with its percent composition. The third section lists the isotopic distribution, with mass values and intensities. The fourth section shows an interactive spectrum of the isotopic distribution.

Figure 2.7: Elemental Analysis Widget



History Widget

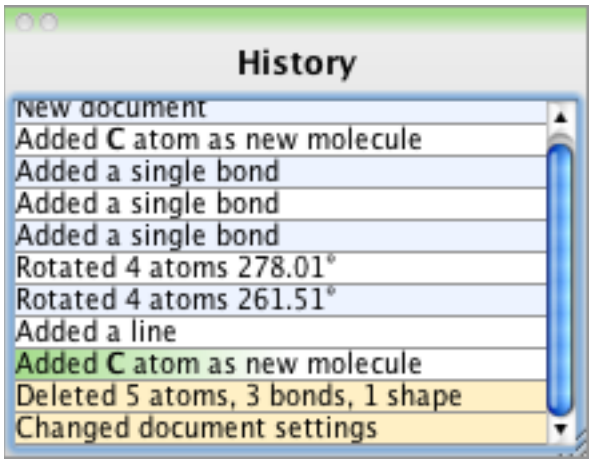
Purpose

The **History** widget is an advanced undo/redo tool and provides access to the complete log of all actions performed since the document was created or opened. Click on a given action to jump back and forth to the document state when that action was performed.

Interface

The interface consists of a single list in a scrolling pane as shown in *Figure 2.8*. The current state of the document is signified with a green highlight over the left side of the latest action. Any actions performed earlier are undecorated and listed above the current state, while any actions that have been undone are highlighted in an amber color and are listed below the current state. By clicking on any actions above the current state, the document will revert back to that action, undoing all actions between the current state and the action clicked. By clicking on any actions below the current state, the document will redo all actions between the current state and the action clicked. Therefore, the History widget allows you to easily revert and restore any actions performed during the edit history of the document.

Figure 2.8: History Widget

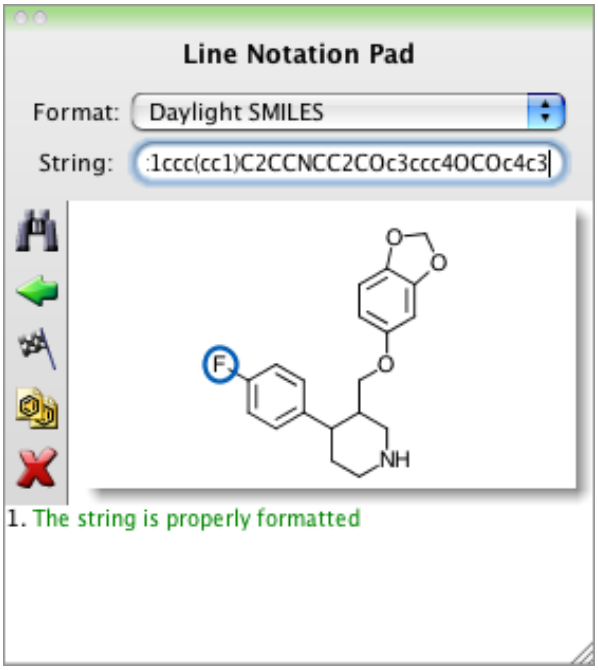


Line Notation Pad Widget

Purpose

The Line Notation Pad widget can interpret and generate *SMILES*, *SLN*, *InChI* and *ROSDAL* chemical line notation formats as well as convert between them with ease. The interface for the Line Notation Pad widget is shown in *Figure 2.9*.

Figure 2.9: Line Notation Pad Widget



Interface

The interface, from top to bottom, consists of a **Format** drop down selection for choosing the format, a **String** text field for inputting and outputting the line notation, a vertical row of buttons for performing various functions, the main structure panel and the input analysis list. Initially, the interface is collapsed. Drag a structure onto the Line Notation Pad widget button or type in a line notation in the **String** text field and press the *return* key to expand it.

Using the **Format** drop down selection, you can choose any of the line notations available to set the current line notation format. If content is present in the text field, then that content will be converted into the new format.

The **String** text field will display the generated line notation when a structure is dropped on the main structure panel or the Line Notation Pad widget button. You may also explicitly type your line notation in this component and then press the *return* key or the **View in 2D** button to interpret it and display the corresponding structure in the main structure panel.

The buttons perform functions as described in *Table 5*.

Table 5: Line Notation Pad Widget Buttons

Button	Function
	The **View in 2D** button will interpret the current string in the **String** text field using the format in the **Format** drop down selection and display the structure in the main structure panel as well as provide feedback in the input analysis list.
	The **Add to the Doodle Board** button will place the current structure in the main structure panel onto the current document. Alternatively, you can click on the main structure panel and drag onto the document to place it.

Button	Function
	The **Choose Start Point** button will allow you to click on an atom in the main structure panel to denote it as the start point for the generation of the line notation. Note that if the line notation format is canonical or if such an option is set, then setting the starting point will have no effect.
	The **Copy to System Clipboard as Text** will copy the current text in the **String** text field onto the system clipboard as plain text. For MIME type specific clipboard contents, set the appropriate options in the **Advanced** tab of the **Preferences** window, then copy from the **Doodle Board**.
	The **Clear** button will clear the current contents and collapse the widget.

Beside the buttons in the main structure panel which will display the structure associated with the line notation in the **String** text field. You can generate a line notation for a structure on the **Doodle Board** by selecting the structure and then by clicking and dragging that structure onto the main structure panel of this widget. Structures from the main drawing panel can also be dragged onto the **Doodle Board**.

The last component of the interface is a scrollable list. Any errors or warnings perceived when interpreting the line notation will be listed here. Use these suggestions to help correct malformed strings.

MolGrabber Widget

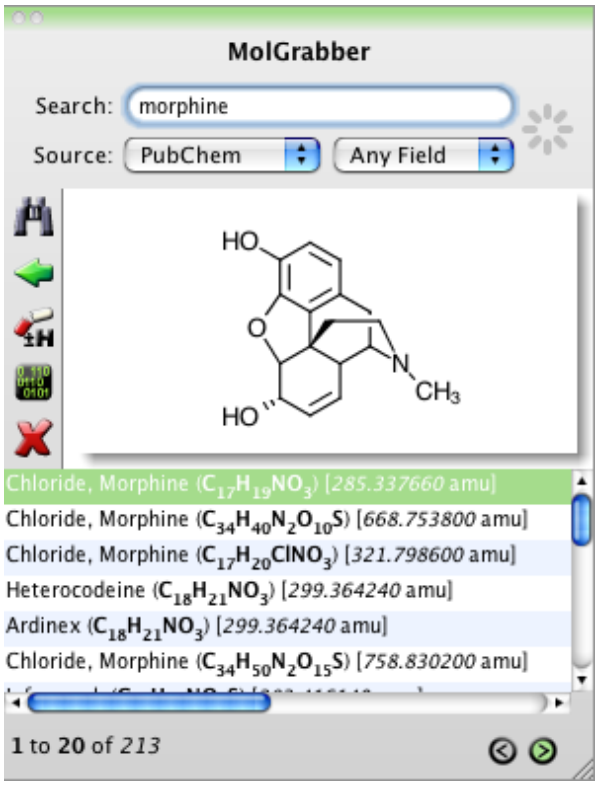
Purpose

MolGrabber is a web application for obtaining pre-drawn molecular structures and properties from online databases. The interface is shown in *Figure 2.10*. Currently, MolGrabber interfaces with the following databases:

- **ChemExper** - http://www.chemexper.com/
- **ChemSpider** - http://www.chemspider.com/
- **PubChem** - http://pubchem.ncbi.nlm.nih.gov/

NOTE: Because MolGrabber connects to online databases, it requires an active internet connection for use.

Figure 2.10: MolGrabber Widget



Interface

The interface, from top to bottom, consists of a **Search** text field for inputting a search

term, a **Source** drop down selection for choosing the database to search through followed by a second drop down selection to restrict the search, a progress spinner to the right of those three components to notify you that a search is currently being performed, a main structure panel with a button column to the left of it for performing various functions, a scrollable list to hold all search results and, at the bottom, statistics about the search result with traversal buttons for navigating through large numbers of results.

Initially, the interface is collapsed. Type a search term in the **Search** text field and press the *return* key to expand it. This can be any search term that the associated database can handle. After pressing the *return* key, the progress spinner will activate to notify you that it is performing the search. After the search completes, the progress spinner will deactivate, the results will populate the result list and the first result will appear in the main structure panel.

The **Source** drop down selection can be used to select which database to search. The second drop down selection will restrict your search to a specific data field type supported by the database. Just choose a specific field and the search will only match results in that field for the input search term.

The buttons perform functions as described in *Table 6*.

Table 6: MolGrabber Widget Buttons

Button	Function
	The **Search** button will begin the search query using the search term input into the **Search** text field and restrict it to matching the field selected in the **Source** drop down selections.
	The **Add to the Doodle Board** button will place the current structure in the main structure panel onto the current document. Alternatively, you can click on the main structure panel and drag onto the document to place it.
	The **Show/Hide Hydrogens** button will add and remove Hydrogens from the structure in the main structure panel based on the coordinates for Hydrogens provided by the database. Some databases may not provide Hydrogen coordinates and therefore this function will have no effect.
	The **Show Associated Data** button will display all associated database data for the structure displayed in the main structure panel.
	The **Clear** button will clear the current contents and collapse the widget.

To the right of the buttons is the main structure panel that will display the structure for the selected result. After obtaining the structures you would like to include in your figures, all you have to do is drag and drop

the structure from the main structure panel onto the **Doodle Board**.

Below the buttons is the search result list. This list will display a maximum of 20 results and follows the following format for each entry:

Name (**Molecular Formula**) [*Molecular Mass amu*]

Click on any of the results to display them in the main structure panel.

Below the search results is a label to inform you of which search results are presented in the current result set along with traversal buttons to navigate through large numbers of results. Just press the left and right arrows to view the previous 20 and next 20 results respectively. If there are no previous or no next results, then the corresponding arrow will be disabled.

NOTE: ChemSpider does not currently support pagination of results, so be careful with generic queries as they may return many, many results and may take a long time to complete.

Directing to the Online Database

After a molecule has been loaded, clicking on the **Show Associated Data** button will list associated data from that database. The top item will be the specific database id as a hyperlink. The link will open up your default browser to the selected database's page for the current result.

Database Notes

ChemDoodle only provides an interface to the databases supported in the MolGrabber widget. You should inform yourself about the copyrights, disclaimers and warranty information provided by these databases before using them.

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PubChem User Requirements

http://eutils.ncbi.nlm.nih.gov/entrez/query/static/eutils_help.html

Do not overload NCBI's systems. Users intending to send numerous queries and/or retrieve large numbers of records from Entrez should comply with the following:

- Run retrieval scripts on weekends or between 9 pm and 5 am Eastern Time weekdays for any series of more than 100 requests.
- Make no more than one request every 3 seconds.
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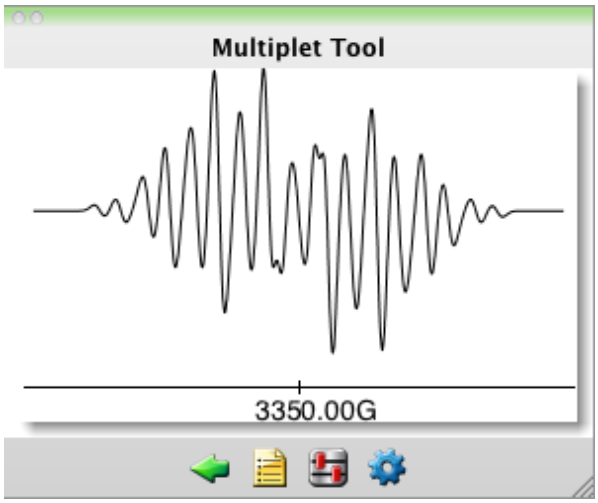
Multiplet Tool Widget

Purpose

The Multiplet Tool widget is a comprehensive tool for generating multiplet trees, simulating signals and producing their figures. It is perfectly suited for simulating nuclear magnetic resonance (NMR) or electron paramagnetic resonance (EPR, a.k.a. ESR) signals. The interface is shown in *Figure 2.11*.

Figure 2.11: Multiplet Tool Widget



Interface

The interface, from top to bottom, consists of the main multiplet panel and a row of buttons for performing various functions.

Use the buttons to set up the simulation and layout of the multiplet. The buttons perform functions as described in *Table 9*.

Table 9: Multiplet Tool Widget Buttons

Button	Function
	The **Add to the Doodle Board** button will place the current multiplet from the main multiplet panel into the current document.

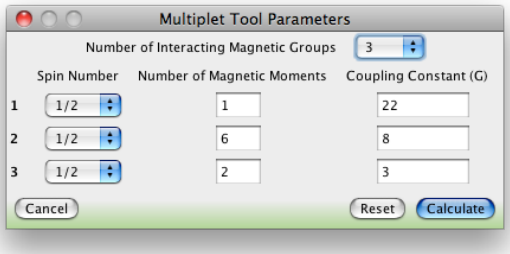
Button	Function
	The **Input Parameters** button pops up a window for you to define parameters for the simulation including the number of neighboring nuclei, their spin and coupling magnitude.
	The **Real-Time Sliders** button provides a window with sliders for each parameter. Changing the sliders will affect the simulation in real time.
	The **Settings** button will display a window to define how the simulation is performed and how the multiplet figure is laid out and displayed.

Once you have completed your simulation, just drag and drop the multiplet from the main multiplet panel onto the **Doodle Board**.

Simulating Multiplets

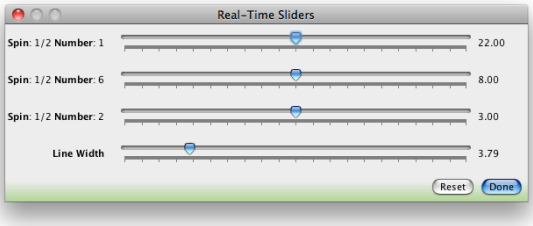
To simulate multiplets, define the parameters in the **Input Parameters** window that appears after clicking the **Input Parameters** button and then click the **Calculate** button as shown in *Figure 2.12*. Press the reset button in this window to reset all parameters.

Figure 2.12: Multiplet Input Parameters



To tweak the input parameters to analyze their affect on the simulation, just use the Real-Time Sliders button and change the values slowly in the window that appears as shown in *Figure 2.13*. When you are satisfied with the simulation, press the **Done** button. The **Reset** button will reset the parameters to their initial values before the window was opened.

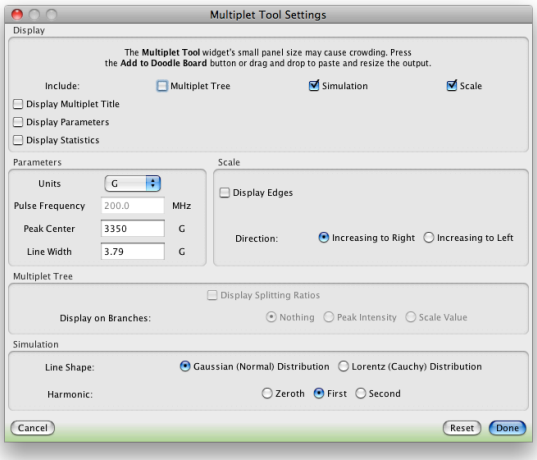
Figure 2.13: Real-Time Sliders



Setting up the Multiplet Figure

To define how the simulation is performed and how the multiplet figure is displayed, click on the **Settings** button to show the **Multiplet Settings** window as shown in *Figure 2.14*.

Figure 2.14: Multiplet Settings



Editing Multiplets from the Doodle Board

To edit a multiplet from the **Doodle Board**, just select it and then drag and drop it onto

the **Multiplet Tool** widget button or onto the main multiplet panel. A copy will be made and can be edited using the **Multiplet Tool** widget. Just add this new edited multiplet to the **Doodle Board** and delete the old one.

Memory and Runtime Issues

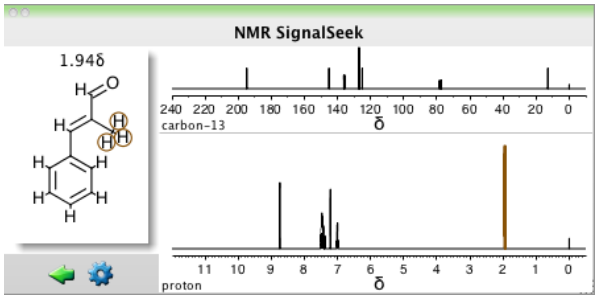
A nucleus of any spin may be used, including hypothetical spins, however more complex simulations require more memory and processor power leading to longer runtimes. Some extremely complex simulations may cause memory issues.

NMR SignalSeek Widget

Purpose

The NMR SignalSeek widget simulates ^{1}H and ^{13}C nuclear magnetic resonance and also associates peaks with nuclei. Full information about each simulation is provided for in-depth analysis. The interface is shown in *Figure 2.15*.

Figure 2.15: NMR SignalSeek Widget



Interface

The interface, from left to right, consists of the main structure panel and a row of buttons for performing various functions, followed by a set of panels for displaying the simulated NMR spectra with ^{13}C displayed on top and ^{1}H displayed on the bottom.

The main structure panel displays the structure being analyzed and is interactive. The spectra are also interactive and display the simulation results. Use the buttons to set up the simulation and copy content to the **Doodle Board**. The buttons perform functions as described in *Table 10*.

Table 10: NMR SignalSeek Widget Buttons

Button	Function
	The **Add to the Doodle Board** button will place both the simulated ^{1}H and ^{13}C spectra onto the current document.

Button	Function
	The **Settings** button will display a window to define how the simulation is performed.

Simulating NMR

To simulate NMR spectra for a structure, drag and drop that structure from the **Doodle Board** onto the NMR SignalSeek widget button or the main structure panel. The ^{1}H and ^{13}C NMR spectra are instantly generated and displayed.

All variables for the simulation can be customized. To define the variables, click on the **Settings** button to display a window containing the parameters, as show in *Figure 2.16*. When you are finished, click the **Simulate** button to recalculate the spectra. Adjust these parameters to match an experimental spectrum for correlated figures on the **Doodle Board**. Settings include:

- **TMS** - Display or hide the reference peak.
- **Roof Effects** - Simulate roof effects.
- **Line Shape** - Lorentzian or Gaussian.
- **Pulse Frequency** - The spectrum resolution. The value is appropriate for ^{1}H NMR. ^{13}C NMR will be simulated to a resolution of a quarter of this value to remain consistent with experimental spectrometers.
- **Line Width** - Control the line width.
- **Dilution** - Affect the solvent/solute intensity ratio.
- **Temperature** - Change the simulation temperature.
- **Solvent** - Choose a solvent. Splitting is fully calculated with the appropriate spin of the nuclei (Deuterium has a spin of 1 and you will see this splitting correctly in the solvent peaks).

Figure 2.16: NMR Simulation Settings

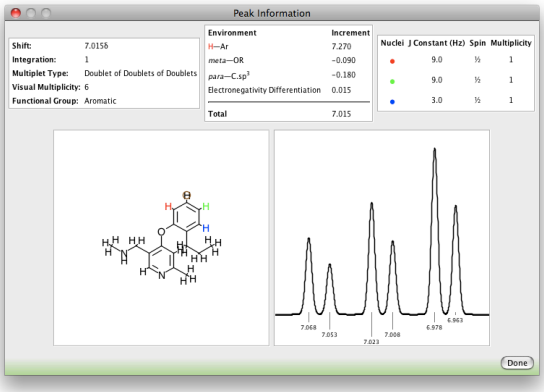
Analyzing the Results

The spectra are completely interactive. You can easily change the view of the spectrum by clicking and dragging to zoom in on the x-axis. Double clicking on the spectrum will revert it to the full view. Scrolling will change the scale of the y-axis.

Peaks and nuclei are hoverable. Hovering over a peak will highlight the corresponding nuclei and vice versa. The chemical shift of the nuclei is displayed above the structure in the main structure panel.

Clicking on a highlighted peak or nuclei set will display further data from the simulation, including the shift prediction, splitting nuclei and j-constant predictions as shown in *Figure 2.17*. Use this to gain further information about multiplets.

Figure 2.17: In-depth Simulation Information



Lastly, the widget is initially small to conserve space. But with all widgets, you can resize or maximize them if you would like more interaction space.

How NMR is Simulated

The simulations in the NMR SignalSeek widget are based on empirical algorithms, with a database of incremental constants compiled from publications and some unpublished work. These references are listed by clicking the **References** menu item in the **Help** menu. Further information on the algorithms used to simulate NMR is provided in *Appendix E*.

Properties Widget

Purpose

The **Properties** widget calculates and displays descriptors for molecules. There are two unique interfaces displayed by the **Properties** widget depending on the situation. If and only if a single molecule is being drawn, a table will be displayed. Otherwise, a drop-down tree will be presented to show data for each of the selected molecules. The **Properties** widget will automatically update to reflect any changes if allowed to. The interface displayed when a single molecule is being edited is shown in *Figure 2.18*, and the interface displayed when molecules are selected is shown in *Figure 2.19*.

Figure 2.18: Properties Widget Interface with a Single Molecule is being Drawn

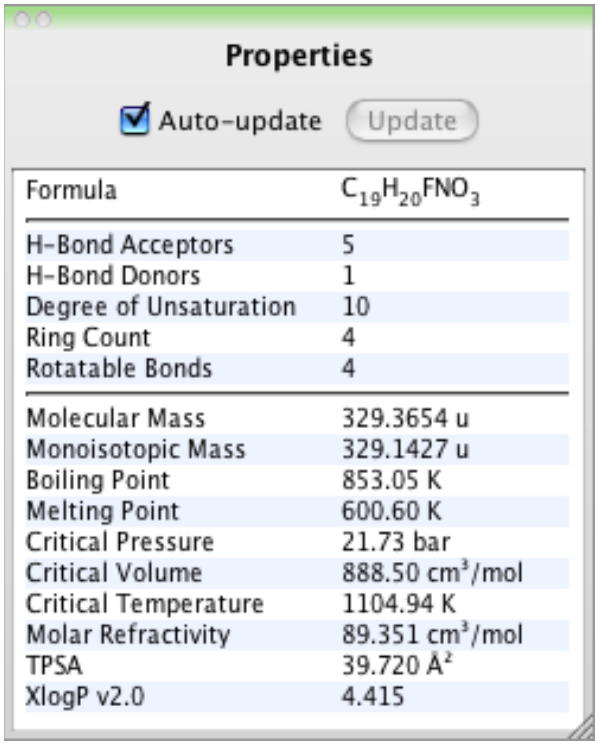
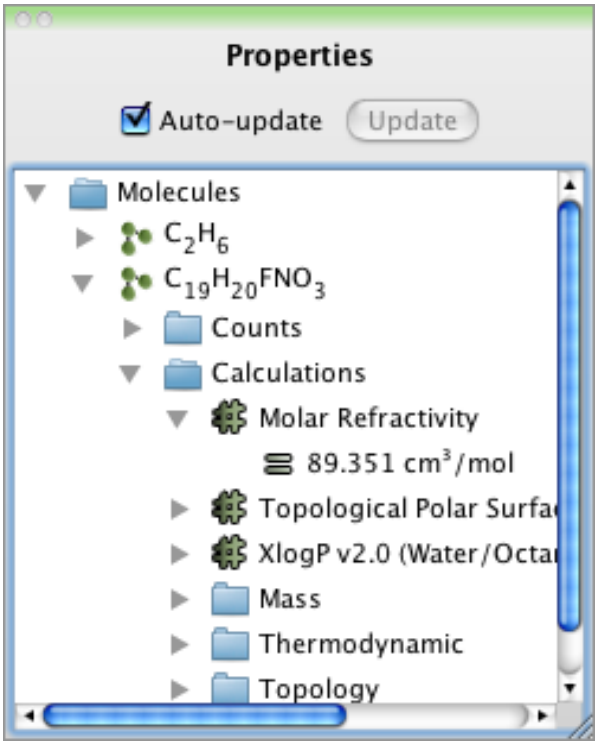


Figure 2.19: Properties Widget Interface when Molecules are Selected



Interface

The interface consists of a checkbox and button at the top that control when the widget updates and the data component at the bottom which displays a table or drop-down tree depending on the situation.

The table is non-interactive and only displays the most important information. For the rest of the descriptors, select the molecule to display the organized tree. To use the tree, just click the arrow to the left of each item, or double click on the item to expand it.

When the **Auto-update** checkbox is selected, the Properties widget will refresh automatically when any content is changed. Deselect the checkbox to improve drawing performance when handling large molecules. When the **Auto-update** checkbox is deselected, the **Update** button will be enabled to manually control when the widget refreshes.

Currently, the **Properties** widget calculates the following properties for each molecule:

- Molecular Formula
  - Counts
    - Atoms
    - Bonds
    - Rings
      - Frèrejacque Number
      - All Rings
    - Hydrogen Bond Acceptors
    - Hydrogen Bond Donors
    - Degree of Unsaturation
    - Lipinski's Rule of 5 Violations
    - Wiener Index
  - Calculations
    - Molar Refractivity
    - Topological Polar Surface Area
    - XlogP v2.0
    - Mass
      - Molecular
      - Monoisotopic
      - Elemental Composition

To copy content from the **Properties** widget, just right-click on any item and choose the **Copy** menu item.

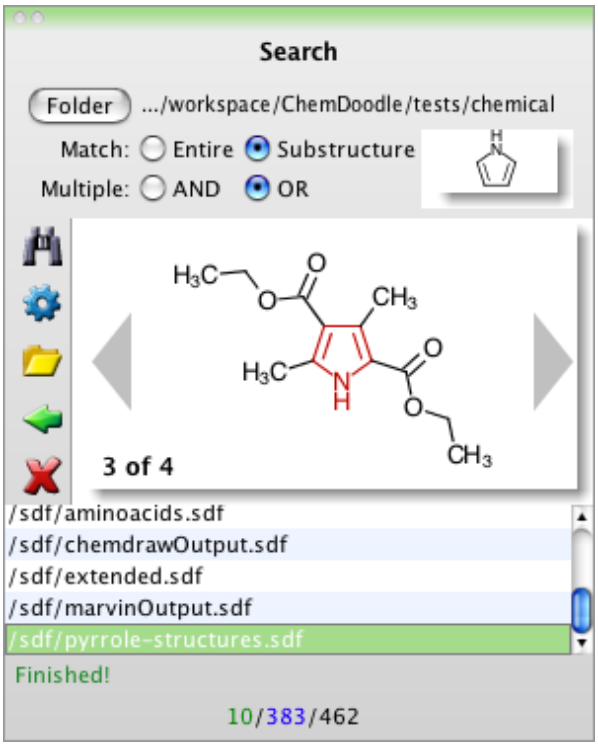
It may take a lot of clicks to access information through the **Properties** widget. For quicker access to all molecular descriptors, use the **Descriptors** submenu of the **Structure** menu.

Search Widget

Purpose

The **Search** widget allows you to search your hard drive and any attached storage devices for chemical structures. The **Search** widget recognizes all formats that ChemDoodle understands, so you will be able to find the old files you thought you lost a long time ago and edit them in ChemDoodle. The interface is shown in *Figure 2.20*.

Figure 2.20: Search Widget



Interface

The interface, from top to bottom, consists of a **Folder** button to select the root directory of the search, **Match** and **Multiple** options to define how the search is performed, a small drop panel to drop the structures to be searched for and to notify you that a search is currently being performed, a column of buttons for various functions with a main structure panel to the right of them, a list of search results and then labels to notify you of search progress.

The top section will allow you to select a root folder for the search. Just click on the **Folder** button and use the file chooser that appears to select a folder. Try to be as exclusive as possible when choosing a root folder, as searching your entire hard drive can take a very long time and may cause memory issues. The **Match** and **Multiple** options will affect how the search is performed. Setting **Match** to **Entire** will guarantee that all results are exact matches of the query structures, while selecting **Substructure** will match any structures where the query structures are matched exactly or contained within larger structures. Setting **Multiple** to **AND** will ensure that all query structures are matched in a file for that file to be considered a result, while selecting **OR** will allow any matched query structure to qualify the file as a result.

Initially, the interface is collapsed. Drag and drop a structure or group of structures from the Doodle Board onto the small drop panel or onto the **Search** widget button to expand it and set the query structure content.

The buttons perform functions as described in *Table 7*.

Table 7: Search Widget Buttons

Button	Function
	The **Search** button will begin the search query using the query structure(s) dropped on Search widget button and the search options set.
	The **Settings** button will allow you to control search parameters and improve performance.

Button	Function
	The **Open** button will open the currently selected result on the **Doodle Board**.
	The **Add to the Doodle Board** button will place the current structure in the main structure panel onto the current document. Alternatively, you can click on the main structure panel and drag onto the document to place it.
	The **Clear** button will clear the current contents and collapse the widget.

While the search is being performed, a pulsing stop sign will become visible on top of the small drop panel to notify you of search progress. Clicking on the stop sign will terminate the search. At the bottom of the interface are two labels. The first label names the file currently being searched, and will display Finished! when completed. The second label displays statistics about the files searched since the search was initialized in the following format:

Files Matched/Chemical Files Searched/Total Files Searched

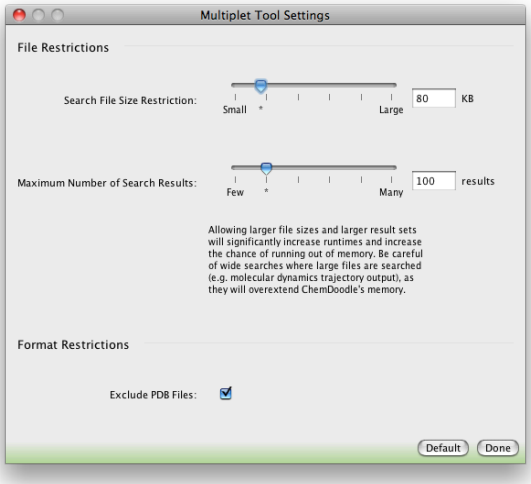
Be careful with the search! Searching large numbers of files may cause ChemDoodle to run out of memory, causing slow response in ChemDoodle. Choose the root search folder and the search settings described in the next section with care.

Once the search is completed, all matched files will be listed in the results list. Click on any result to view all the structures in that file, one at a time, in the main structure panel. All hits are highlighted in red. If a file contains multiple structures, clicking the grey arrows that appear to the left and right of the structure will allow you to browse through them. The total number of structures in the file is noted at the bottom left of the main structure panel. Once you have found the structure you were looking for, just drag and drop the structure from the main structure panel onto the **Doodle Board**. You can also use the **Open** button to open the entire file on the **Doodle Board**.

Search Settings

Search parameters can be defined by clicking on the **Settings** button. A window with the options will appear as shown in *Figure 2.21*.

Figure 2.21: Search Settings for the Search Widget



There are currently 3 options:

1. **Search File Size Restriction** - This value determins the maximum file size that the **Search** widget will include in its search, avoiding memory issues.
2. **Maximum Number of Search Results** - This value will control the maximum number of search results. The search will continue until all the files in the selected root search folder are visited or when this maximum result value is reached. Keeping

it low and providing smaller root search folders will avoid runtime and memory issues.

3. **Exclude PDB Files** - Many times, *PDB* files are very large and contain *molecular dynamics* trajectories or *Monte Carlo* distributions. To avoid all of these files, which will cause runtime and memory issues, keep this option selected. If you need to search through *PDB* files, turn this option off.

Statistics Widget

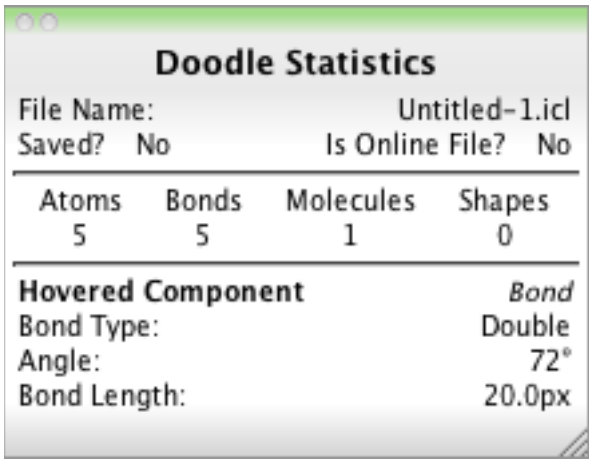
Purpose

The **Statistics** widget will display information about the current document and hovered or selected items. Use it to help with drawing and placement tasks.

Interface

The interface is separated into three sections as shown in *Figure 2.22*. The top section displays information about the document, the middle section displays information about the content, and the final section displays specific information about hovered or selected objects.

Figure 2.22: Statistics Widget



Symbols Widget

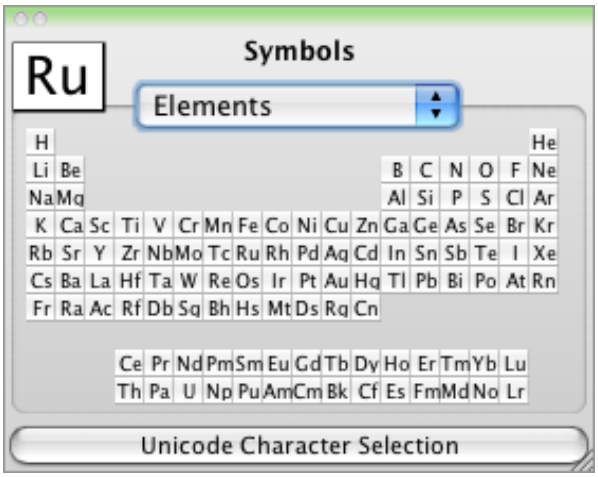
Purpose

The **Symbols** widget is a complement to the **Labels** toolbar. This widget contains an abbreviation library, a periodic table of elements, arrows, greek letters and many other symbols. A few selected tabs are shown in *Figures 2.24-2.26*.

Interface

The content in the **Symbols** widget is small and may be difficult to read. As can be seen in *Figure 2.23*, hovering over any symbol will show a larger preview at the top left hand corner of the widget. Hovering for a few seconds will also display a tooltip description.

Figure 2.23: Symbol Preview



When abbreviations or elements are chosen, you may modify atoms as described in the labels section. Other symbols, such as arrows may not be used directly as atom labels. However, you can open up an atom label text field, and then input the symbol. If you are modifying any text component, clicked symbols will be inserted into the component's content.

Figure 2.24: Abbreviations Tab

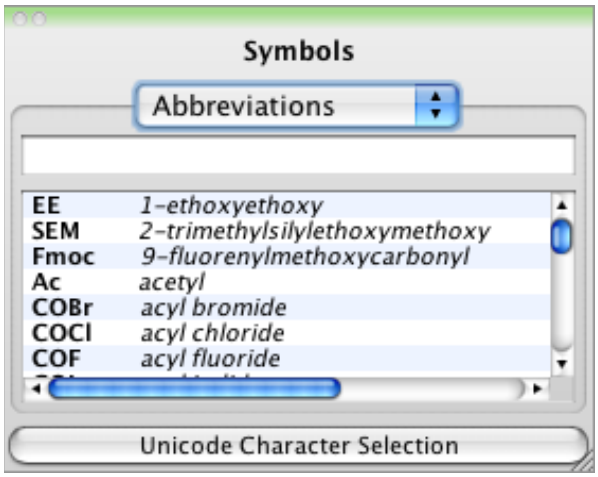


Figure 2.25: Arrows Tab

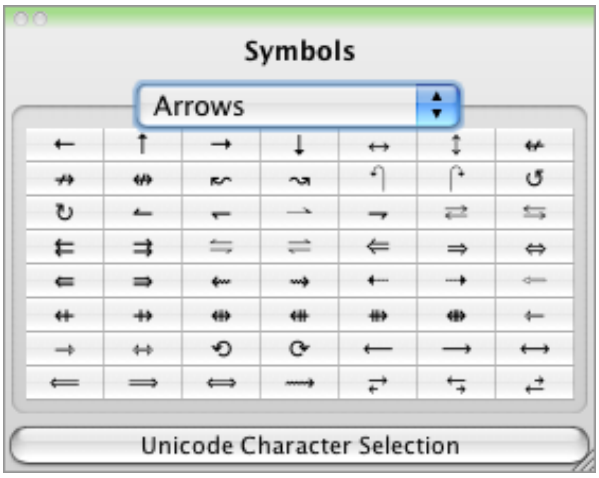
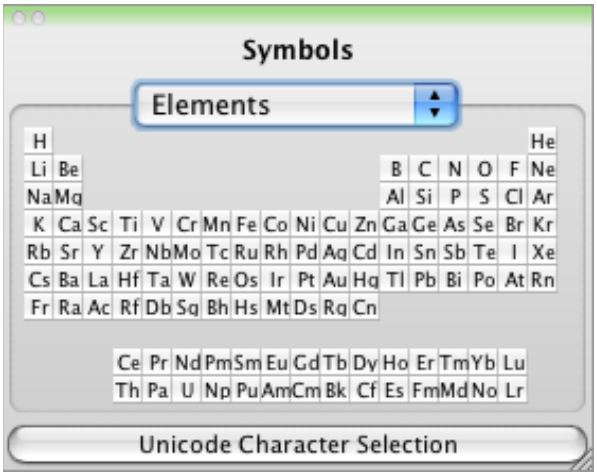
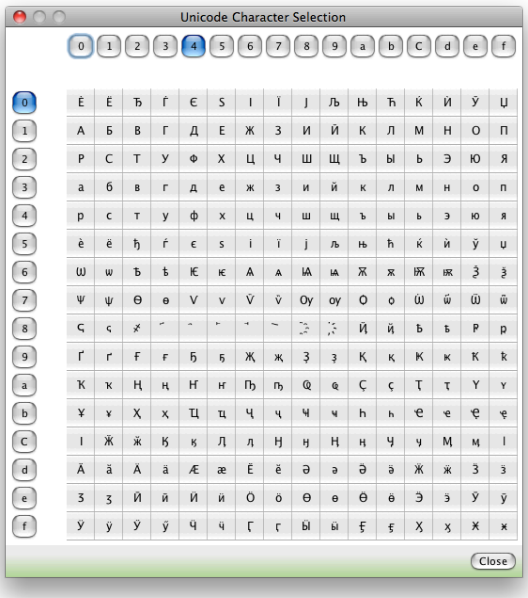


Figure 2.26: Elements Tab



If you set an atom's label to one that is not recognized or parsed by ChemDoodle, an unrecognized warning will appear. You may dismiss this warning or edit the current list of abbreviations to allow unrecognized tokens by selecting the **Add New...** menu item in the **Structure** menu in the **Abbreviations** submenu.

Figure 2.27: The Unicode Character Selector



All possible symbols available are accessible in the Symbols widget, even if they are not displayed immediately in the tab sets. Just click the **Unicode Character Selection** button at the bottom of the widget to view the unicode character selector shown in *Figure 2.27*. Using hex, you can traverse the entire Unicode range and easily insert any desired symbols into text components. Note that not all fonts will have character glyphs assigned to each hex value. In these cases, a blank space or empty rectangle will appear in your text component and in the unsupported symbol button.

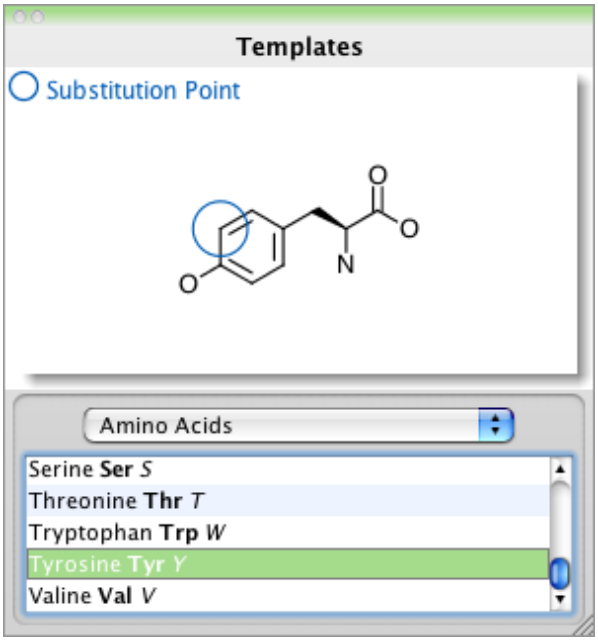
NOTE: Some programs use the Symbol font to display symbols. This is an archaic solution and the standard is to now use unicode characters, which ChemDoodle fully supports. ChemDoodle will try to recognize and correct such cases when reading in files from other programs.

Templates Widget

Purpose

The **Templates** widget organizes your templates and allows you to easily use them. The interface is shown in *Figure 2.28*.

Figure 2.28: Templates Widget



Interface

The interface, from top to bottom, consists of a main structure panel, a drop down selection for selecting a template group and a scrollable list for selecting a template.

The main structure panel displays the selected template. An atom can be set to be the substitution point by clicking on it. The substitution point is the atom that will be overlapped with the atom the template is connected to.

The template group drop down selection will allow you to select a group of templates to browse. After selecting a template group, the template list will populate with templates from that group. Just click on a template to display it in the main structure panel for use.

Using Templates

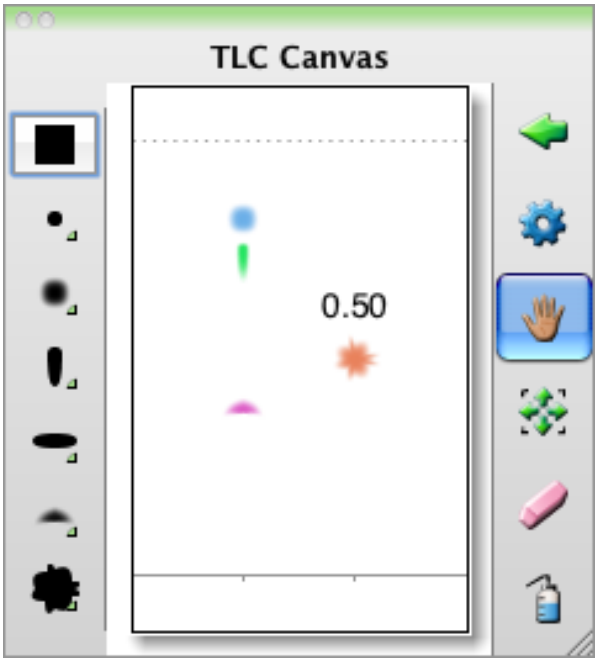
Drawing with templates and creating templates is discussed in detail in *Chapter 3*.

TLC Canvas Widget

Purpose

The **TLC Canvas** widget provides a tool for creating graphics of thin layer chromatography (TLC) plates. The interface is shown in *Figure 2.29*.

Figure 2.29: TLC Canvas Widget



Interface

The interface, from left to right, consists of a column of buttons for spot types, the main TLC panel for drawing the TLC plate and a column of buttons for performing various functions.

The top button in the spot type column sets the color of spots. Beneath the color button are 6 different shapes of spots:

- **Compact Spot** - a small dot
- **Expanded Spot** - a circle
- **Trailing Spot** - a small dot with a trail
- **Widened Spot** - an oval aligned horizontally
- **Crescent Spot** - a crescent shape with bowl facing downwards
- **Custom Spot** - a splatter shape that can be changed

Click on any of the spot types to set the drawing mode to place the spot.

Each spot button is a group button. Expand the group button for more spot styles. For each spot there are three spot styles:

- **Solid Style** - Solid throughout
- **Empty Style** - Just a line border
- **Diffuse Style** - Gradient from the center to the edges

The main TLC panel contains the TLC plate being drawn. You can edit it using the controls to the right. When finished editing the TLC plate, use the **Add to Doodle Board** button to place it on the **Doodle Board**.

The right-most button column contains function buttons to control how to edit the TLC plate. The buttons perform functions as described in *Table 8*.

Table 8: TLC Plate Widget Buttons

Button	Function
	The **Add to the Doodle Board** button will place the current TLC plate in the main TLC panel onto the current document.
	The **TLC Settings** button will popup a window to edit the visual specifications of the TLC plate.

Button	Function
	The **Move** button allows you to translate spots along their lanes and allows you to move the origin and solvent front.
	The **Resize Spots** button will display the anchor points for all spots and allow you to click and drag them to alter spot shapes.
	The **Delete** button will all you to remove spots by clicking on them and allow you to delete lanes by clicking on the lane tick at the origin.
	The **Clear** button removes all spots, leaves a single lane, and resets the origin and solvent front.

Drawing TLC Plates

There are 13 buttons associated with the TLC Canvas. The controls on the left are the simplest. The top button is the color of the spots, just click it to choose a different color. The rest of the buttons in that column correspond to spot shapes. These are the compact, expanded, trailing, widened, crescent and custom spots, in that order. Just click on a spot button, then hover over the TLC plate for a preview and R_f calculation. Once you are satisfied with a location, click to place the spot. You can create new lanes by placing spots in between the existing lanes.

These spot buttons are group buttons and more spot styles will appear when hovered. All of the spots can be initialized with a solid, hollow or gradient style. The gradient styled spots most closely represent actual spots.

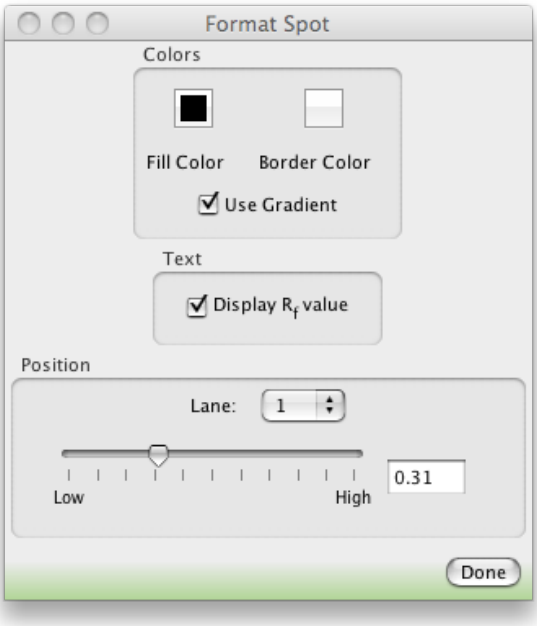
Using the **Move** button, you hover over spots to highlight them, and then click and drag to move them along their lanes. R_f values are displayed while you move spots. You may also click and drag the origin and solvent front to move them, preserving R_f values.

When spots are hovered, you can right click on them to open a popup menu with the following functions:

- **Duplicate Spot** - Will produce a duplicate spot of the hovered spot, underneath the hovered spot in the same lane.
- **Remove Spot** - Will delete the spot.
- **Format Spot** - Opens the **Format Spot** window.

The Format Spot window will provide several options for precisely defining its color, style, display settings and position as shown in *Figure 2.30*.

Figure 2.30: Format Spot Window



To resize and reshape spots on the TLC plate, use the **Resize Spots** button. Just hover over

the control points that appear, and then click and drag to move them. All spots except the custom spot are defined by 4 control points. You may move all four to create different shapes. The custom spot is unique and is defined by 8 control points. You may use custom spots to create much more complicated shapes.

To remove spots and lanes, use the **Delete** button. Hover over spots to highlight them, then click to remove them. You may delete a lane by clicking its lane tick at the origin. Deleting a lane will also delete its contained spots. To clear and reset the entire TLC plate, click the **Clear** button.

Editing TLC Plates from the Doodle Board

To edit a TLC plate from the **Doodle Board**, just select it and then drag and drop it onto the **TLC Canvas** widget button or onto the main TLC panel. A copy will be made and can be edited using the **TLC Canvas** widget. Just add this new edited TLC plate to the **Doodle Board** and delete the old one.

Chapter 3: Basic Structures

Overview

You can draw any structure imaginable with ChemDoodle. However, with all of the drawing tools available, drawing basic structures may seem overwhelming to the new user.

This section introduces the new user to the basic structure drawing tools within ChemDoodle. It covers the following topics:

- Recognizing the structure drawing tools.
- Drawing atoms.
- Setting atom labels.
- Drawing bonds.
- Changing bond orders.
- Drawing chains.
- Drawing rings.
- Drawing templates.
- Adding attributes to structures, such as charges, radicals and symbols.
- Setting mass number values to isotopes.
- Placing orbitals on structures.

KeyBoard Shortcuts

There are many keyboard shortcuts to help you draw structures quickly and efficiently. The full list of keyboard shortcuts is given in the *KeyboardShortcuts.pdf* file located in the *docs* folder in the main *ChemDoodle* installation folder.

Atoms

Atoms are the basic building blocks in chemistry and are the basic building blocks in ChemDoodle. Before any other chemical objects can be drawn, an atom must be present as the starting point.

Placing Carbon Atoms

When you first use ChemDoodle, you will notice a gray dot following your mouse pointer on the **Doodle Board** as shown in *Figure 3.1*.

Figure 3.1: Trailing Carbon Atom

To set a carbon atom at the current location of the mouse pointer, just click the mouse. This will set the carbon atom and structures can be grown from it.

At any time while drawing chemical structures, if there is no hovered atom to grow from, a carbon atom will trail your mouse to be placed and grow a new structure.

> *NOTE: More advanced users may find it inconvenient to always require a starting atom to draw structures. You can turn off this restriction in the **Preferences** window under the **General** tab, by check the **Require Starting Atom** checkbox. Clicks with the bond tools will then immediately place those bonds and ring, templates and chains will not require a starting atom.*

Placing Other Elements

To place atoms with element symbols other than carbon, use the **Labels** toolbar or the **Elements** panel in the **Symbols** widget. Just click on the desired element symbol, and the mouse cursor will change to be that symbol with a small arrow at the bottom-left. Once

you have located where to place the atom using the bottom-left arrow of the new mouse cursor, just click to place it.

If you click while an atom is hovered, then that atom's label will change to the currently selected element symbol.

Placing Atoms with Non-elemental Labels

To place atoms with any text you desire, click on the **Set Atom Label** tool  located in the **Labels** toolbar. Then click on the **Doodle Board** in the desired location to place the new atom and to open up an atom label text field. Type in the desired atom label text into the text field and then click elsewhere on the **Doodle Board** or press the *return* key to close the text field and set the atom.

If you click while an atom is hovered, then a text field will appear for that atom's label for you to edit.

Hovering Atoms

With most tools in ChemDoodle, atoms can be hovered. Exceptions include the shape tools, such as when drawing rectangles. Hovering an atom is very simple, just get your mouse close enough to an atom so that it is surrounded by an amber circle as shown in *Figure 3.2*.

Figure 3.2: A Hovered Atom

The atom is then defined as being hovered and further actions pertaining to it can be performed.

By default, most carbon atoms have their labels hidden to create skeleton figures. To modify when carbon labels are displayed, please refer to the **Carbon Labels** section in **Chapter 6**.

Selecting Atoms

To select atoms, first hover them and then press the mouse down. The amber circle will turn into a blue circle as shown in *Figure 3.3*.

Figure 3.3: A Selected Atom

The blue circle is actually a special component called the **Optimize Zone**, which will be discussed in the **Bonds** section.

To deselect atoms, just release the mouse.

Changing Atom Labels to other Elements

To change an atom's label to another element symbol, use the **Labels** toolbar or the **Elements** panel in the **Symbols** widget. Just click on the desired element symbol, and the mouse cursor will change to be that symbol with a small arrow at the bottom-left. Once you have hovered the atom with the label to be changed, just click to set the new label.

Additionally, when an atom is hovered, you can press any of the letter keys on the keyboard to cycle through the element symbols that begin with that letter.

Changing Atom Labels to Non-elemental Text

To change an atom's label to any text you desire, click on the **Set Atom Label** tool  located in the **Labels** toolbar. Then hover the atom with the label to be changed and click to open up its atom label text field. Type in the desired atom label text into the text field and then click elsewhere on the **Doodle Board** or press the *return* key to close the text field and set the new label.

Additionally, you can hover the atom in any mode and then press the *space* key to open the atom's label text field.

Repeating the last Typed Atom Label for other Atoms

When writing a complex atom label, you may want to repeatedly use that label for other atoms. After typing the label, just hover the other atoms with labels to be changed and press the *enter* key. The hovered atom's label will be set to the last typed label.

You can also define the label text to be used by the *enter* key by opening up a previously typed atom label text box and then closing it.

Moving an Atom

To move an atom, first select one of the selection tools discussed in *Chapter 5*. Make sure that no content is currently selected by emptying the lasso. Perform the following steps:

1. Hover the atom to be moved.
2. Press the mouse down to select the atom.
3. Drag the mouse to move the atom.
4. Release the mouse to finish the move action.

If the atom is a terminal atom in a molecule, then the above instructions will move the atom and bond with fixed angles and lengths as described in the **Bonds** section.

If the atom is part of a molecule and not a terminal atom, the the above instructions will move that entire molecule. Just hold down the *shift* key while performing the above instructions to move the atom by itself.

Deleting an Atom

To delete an atom, hover it and then press the *delete* or *backspace* key. All attached bonds will also be removed, leaving the adjacent atoms.

Chemical Labels

The last section described how to use the atom label tool to assign any arbitrary text to an atom. This text is chemically interpreted; a label of *CH3* will be interpreted as one carbon atom with three hydrogen atoms attached to it. Much more advanced labels can be written and parsed. More information on chemical interpretation, and expanding these labels, is described in *Chapter 6*.

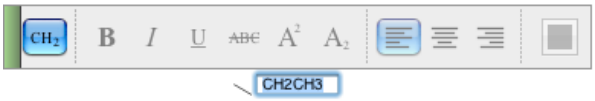
In addition to chemical interpretation, the label will automatically be formatted for display; the *CH3* label will display as CH_3. Stacking will also be applied, so as bond overlap with labels is kept to a minimum. ChemDoodle's intuition may not always be what you intended though, and you may want to format more advanced labels, such as for rendering isopropyl groups (*i*Pr and ^{i}Pr) or adding indexes to carbon chain groups (R^{10}). In these cases, you can override ChemDoodle's chemical interpretation and apply your own formatting.

Atom Label Tool

When opening an atom label field, a format toolbar will appear above it containing several controls. The only enabled button will

be the **Interpret Chemically** button, which is selected by default as shown in *Figure 3.4*.

Figure 3.4: Only one button is enabled by default.

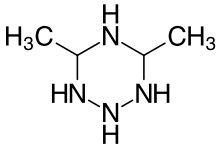


Without further editing, closing this label will assign an ethyl group to the atom and the text will be automatically formatted as CH_2CH_3.

Atom Label Token Stacking

When labels are chemically interpreted, they will be split up into tokens that describe each discrete unit. For instance, *NH* will be split into *(N)(H)* and *CCH2COOH* will be split into *(C)(CH2)(COOH)*. More about this is covered in *Chapter 6*. ChemDoodle will automatically stack tokens in atom labels such that they overlap with surrounding bonds as little as possible as shown in *Figure 3.5*.

Figure 3.5: Atom label tokens are stacked to overlap with bonds as little as possible.



By default, if not on a terminal atom, and stacking will help reduce clutter, the second token and all subsequent tokens will be stacked to the next line. There are two visual specifications for more precise control over this behavior:

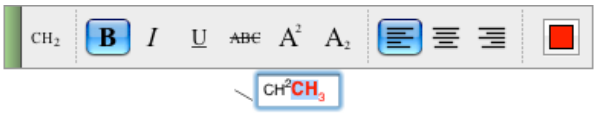
- **Stack Lone/Terminal** - In the **Preferences** window, in the **Visuals** tab in the **Atoms** section under the **Labels** subsection, you can set this checkbox to determine if lone and terminal labels will also stack labels.
- **Token Stacking** - In the **Preferences** window, in the **Visuals** tab in the **Atoms** section under the **Labels** subsection, you can set multi-choice option to declare whether token stacking occurs for all individual tokens, for only the second token or never for any token.

In addition to the token behavior settings, you also have full control of the spacing between tokens. All of these settings are present in the **Preferences** window, in the **Visuals** tab in the **Atoms** section under the **Labels** subsection.

Formatting Atom Labels

If a different format is desired, just deselect the **Interpret Chemically** button and the formatting options will be enabled as shown in *Figure 3.6*.

Figure 3.6: Applying a custom format to an atom label.



Use the controls in the toolbar that appears above the atom label field to explicitly format the atom label. *Table 11* lists how to change the following attributes.

Table 11: How to change these formatting attributes

Attribute	Control
Bold	Select the text to be bold and press the **Bold** button.
Italics	Select the text to be italicized and press the **Italic** button.
Underline	Select the text to be underlined and press the **Underline** button.

Attribute	Control
Strikethrough	Select the text to display the strikethrough and press the **Strikethrough** button.
Superscript	Select the text to be superscript and press the **Superscript** button.
Subscript	Select the text to be subscript and press the **Subscript** button.
Alignment	The entire label will be aligned to the selection of the **Align Left**, **Align Center** or **Align Right** buttons.
Color	Select the text to be colored and press the **Choose Color** button. Then select the color.
Font Family	Select the text to change the font family of and then use the font chooser in the **Format** toolbar to select the font family.
Font Size	Select the text to change the font size of and then use the size chooser in the **Format** toolbar to select the font size.

Note: When disabling chemical interpretation, the label will lose all chemical significance, and will not be expandable or suitable for any chemical algorithms.

Atom Label Orientation

By default, atom label tokens will orient themselves in the direction of least overlap with the rest of the structure. Some times, it may be necessary to force the label to flush in a specific direction. To do so, perform the following steps:

1. Hover the atom with label to orient.
2. Right-click on the atom and expand the **Label Flush** submenu.
3. Choose the direction to orient the label. Choose **Auto** if you want ChemDoodle to automatically determine the best orientation.

Bonds

Bonds are the second most important building blocks in chemistry. Bonds in ChemDoodle are graphical connectors between atoms. There are many options for bond types and for defining how they look.

Placing a Single Bond

To place a single bond, click the **Single Bond** tool  in the **Bonds** toolbar which should be selected by default when ChemDoodle is opened.

Then hover over an atom and press the mouse down. A preview of the new bond and atom will be drawn as shown in *Figure 3.7*.

Figure 3.7: New Bond Placement Preview

Drag the mouse and use the techniques discussed in the following subsections to

place the bond in the preferred orientation. Then release the mouse to set the bond.

Placing Bonds other than Single Bonds

To place bond types other than **Single** bonds, just click on the desired bond type in the **Bonds** toolbar. Then follow the instructions for placing a **Single** bond.

Optimize Zone

The Optimize Zone is a special component in ChemDoodle to help you place bonds in the optimal position around atoms. It is the blue circle that appears when placing bonds and other molecule fragments. To use the Optimize Zone, just place the mouse pointer in the blue circle. The bond or fragment being placed will automatically be oriented in the most optimal position.

The Optimize Zone size can be changed in the **Preferences** window under the **General** tab.

Placing Bonds with Fixed Lengths and Angles

By default, fixed widths and fixed angles are enforced when drawing structures. To place a bond within these restraints, hover over an atom and press the mouse down with a bond tool. You will see the **Optimize Zone** appear. Drag the mouse pointer out of the **Optimize Zone**. The new bond placement will now orient towards the mouse pointer.

The default fixed length is defined by the **Bond Length** visual specification in the Preferences window under the **Visuals** tab under the **Bonds** tab. Angles are fixed every 30° starting at 0°.

You can set whether fixed lengths and/or fixed angles are on by default in the **Preferences** window under the **General** tab.

Placing Bonds at Non-fixed Lengths

When placing bonds outside of the **Optimize Zone**, fixed lengths will be enforced. To break from fixed lengths, hold down the *shift* key while placing the bond.

You may turn off fixed lengths in the **Preferences** window under the **General** tab. In this case, the *shift* key will then enforce fixed lengths.

Placing Bonds at Non-fixed Angles

When placing bonds outside of the **Optimize Zone**, fixed angles will be enforced. To break from fixed angles, hold down the *alt* key while placing the bond.

You may turn off fixed angles in the **Preferences** window under the **General** tab. In this case, the *alt* key will then enforce fixed angles.

Placing Bonds at Non-fixed Lengths and Non-fixed Angles

When placing bonds outside of the **Optimize Zone**, fixed angles and fixed lengths will be enforced. To break from fixed lengths and fixed angles at the same time, hold down both the *shift* and *alt* key while placing the bond.

You may turn off fixed lengths and fixed angles in the **Preferences** window under the **General** tab. In this case, holding the *shift* and *alt* keys will then enforce fixed lengths and angles.

Connecting two Atoms with a New Bond

If two atoms are already present in the document and you want to connect them with a bond, just initiate drawing a new bond from one atom and without releasing the mouse, drag over the second atom until it is highlighted with a red circle. Then release the mouse and the new bond will be formed.

Hovering Bonds

With some tools in ChemDoodle, bonds can be hovered. Hovering a bond is very simple, just get your mouse close enough to the center of the bond so that it is encapsulated by a pair of amber semicircles as shown in *Figure 3.8*.

Figure 3.8: A Hovered Bond

The bond is then defined as being hovered and further actions pertaining to it can be performed.

Selecting Bonds

Bonds can only be selected when using the selection tools discussed in *Chapter 5*. To select bonds, first hover them and then press the mouse down. The amber semicircles will turn a blue color as shown in *Figure 3.9*.

Figure 3.9: A Selected Bond

Changing a Bond Type

To change a bond type, first select the bond type you would like to change the bond to in the **Bonds** toolbar. Then hover the bond with the type that you would like to change and click the mouse. The new bond type will override the old type.

Changing Selected Bonds to Single Bonds

To change the bond types of a large number of bonds to all be **Single** bonds, perform the following steps:

1. Select the bonds to be changed to **Single** bonds using a selection tool as discussed in *Chapter 5*.
2. Press the **Saturate** menu item in the **Structure** menu.

Incrementing a Bond Order

When using the **Single Bond** tool, clicking on hovered bonds will not override other bond types. Instead the **Single Bond** tool will increment the bond order. For example, clicking on a **Double** bond will change it to a **Triple** bond and clicking on the **Triple** bond will change it to a **Quadruple** bond. Clicking on a **Sextuple** bond will change the order back to a **Single** bond.

This functionality can be disabled so that the **Single Bond** tool overrides bond types in the **Preferences** window under the **General** tab.

Deleting a Bond

To delete an bond, hover it and then press the *delete* or *backspace* key. The constituent atoms will remain.

Deleting Bonds Around Atoms

To delete bonds, but retain the atoms contained in the bonds, perform the following steps:

1. Select the bonds to be removed using a selection tool as discussed in *Chapter 5*.
2. Press the **Remove Selected Bonds** menu item in the **Structure** menu.

All selected bonds will be removed, but atoms will remain present.

Changing the Z-Order of Bonds

When bonds overlap, one bond will be rendered in front of the other. For structures with 3D coordinates, the bond with the most positive z-coordinates will be rendered on top. Without z-coordinates, the last bond drawn will be rendered on top.

To change the z-order of bonds when z-coordinates are present, perform the following steps:

1. Select the structure with the z-orders to be changed.
2. Select the **Rotate in 3D** tool in the **Content** toolbar.
3. Click and drag the mouse to rotate the structure in 3D so the desired bond is placed on top.
4. Release the mouse to stop the rotation and set the new coordinates.

To change the z-order of bonds when z-coordinates are not present, perform the following steps:

1. Delete the bond that is to be rendered on top.
2. Redraw the bond.

Chains

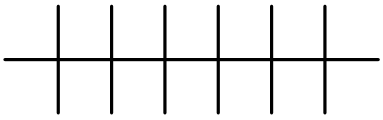
Chains are a group of carbon atoms, linked linearly by bonds. Three types of chains are provided in ChemDoodle:

- **Carbon Chain -**  A consistent linear carbon chain, with all chain angles alternating at ±120° as shown in *Figure 3.10*.

Figure 3.10: A Carbon Chain

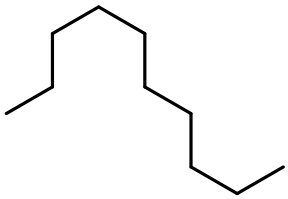
- **Fisher Projection Chain -**  A straight carbon chain, with all chain angles at 180°. All non-terminal chain atoms also have two additional carbon atoms depicted perpendicular to the chain orientation as shown in *Figure 3.11*.

Figure 3.11: A Fisher Projection Chain



- **Random Chain -**  A carbon chain where all chain angles are at 120°, but the chain itself can deviate in any direction as shown in *Figure 3.12*.

Figure 3.12: A Random Chain



Placing Chains at Fixed Angles

To place chains at fixed angles, perform the following steps:

1. Select a chain tool in the **Shapes** toolbar using the **Chain Tool** group button.
2. Choose a starting atom to sprout the chain from by hovering it. If you do not want to start the chain from any existing atoms, create an atom in a new place by clicking on the **Doodle Board** where no atoms are hovered.
3. Press the mouse down on the hovered atom.

4. Drag the mouse to the desired length of the chain. When using the **Random** chain, drag the mouse in the outline of the chain you would like to draw and the chain will grow following that path.

5. Release the mouse to set the chain.

By default, the chains will be oriented at fixed angles every 15° starting at 0°. All bond lengths are defined by the **Bond Length** visual specification in the **Preferences** window under the **Visuals** tab under the **Bonds** tab.

When dragging the mouse to define the chain, a number will be displayed below the mouse cursor to keep track of the number of bonds being added.

Placing Chains at Non-fixed Angles

To place chains at non-fixed angles, hold down the *alt* key while dragging the mouse when defining the chain to break from the fixed chain orientation angles.

Forcing the Placement of Chains Vertically and Horizontally

To place chains oriented vertically or horizontally, hold down the *shift* key while dragging the mouse when defining the chain. The chain preview will then automatically orient vertically or horizontally depending on angle from the starting atom to the current mouse cursor position.

Inverting Carbon Chains

Carbon chains can be inverted by holding down the *slash* key (/) while placing. The preview will update to reflect this.

Rings

Rings are a chain of carbon atoms where the last atom in the chain connects to the first. There may be bond types other than **Single** bonds in rings. Currently the following rings can be drawn quickly from the **Rings** toolbar, with more ring choices in the **Templates** widget:

- Cyclopropane ring
- Cyclobutane ring
- Cyclopentane ring
- Cyclohexane ring
- Cycloheptane ring
- Cyclooctane ring
- Cyclobutadiene ring
- Cyclopentadiene ring
- Benzene ring
- Cycloheptatriene ring
- Cyclohexane chair conformer 1
- Cyclohexane chair conformer 2

Placing a Ring

To place a ring, click the preferred ring tool in in the **Rings** toolbar.

Then hover over an atom and press the mouse down. A preview of the new ring will be drawn as shown in *Figure 3.13*.

Figure 3.13: New Ring Placement Preview

Drag the mouse and use the techniques discussed in the following subsections to place the ring in the preferred orientation. Then release the mouse to set the ring.

Optimize Zone
The Optimize Zone can be used to optimize ring placement as described in the **Bonds** section.

Placing Rings with Fixed Lengths and Angles
By default, fixed widths and fixed angles are enforced when drawing structures. To place a ring within these restraints, hover over an atom and press the mouse down with a bond tool. You will see the **Optimize Zone** appear. Drag the mouse pointer out of the **Optimize Zone**. The new ring placement will now orient towards the mouse pointer.

The default fixed length is defined by the **Bond Length** visual specification in the **Preferences** window under the **Visuals** tab under the **Bonds** tab. Angles are fixed every 30° starting at 0°.

You can set whether fixed lengths and/or fixed angles are on by default in the **Preferences** window under the **General** tab.

Placing Rings at Non-fixed Lengths
When placing rings outside of the **Optimize Zone**, fixed lengths will be enforced. To break from fixed lengths, hold down the *shift* key while placing the bond.

You may turn off fixed lengths in the **Preferences** window under the **General** tab. In this case, the *shift* key will then enforce fixed lengths.

Placing Rings at Non-fixed Angles
When placing rings outside of the **Optimize Zone**, fixed angles will be enforced. To break from fixed angles, hold down the *alt* key while placing the bond.

You may turn off fixed angles in the **Preferences** window under the **General** tab. In this case, the *alt* key will then enforce fixed angles.

Placing Rings at Non-fixed Lengths and Non-fixed Angles
When placing rings outside of the **Optimize Zone**, fixed angles and fixed lengths will be enforced. To break from fixed lengths and fixed angles at the same time, hold down both the *shift* and *alt* key while placing the bond.

You may turn off fixed lengths and fixed angles in the **Preferences** window under the **General** tab. In this case, holding the *shift* and *alt* keys will then enforce fixed lengths and angles.

Adding Rings to Bonds
When adding rings to atoms, you may not always find it easy to achieve an aesthetic fuse angle. To solve this, add the ring to a bond instead of an atom. The ring will automatically align to the bond it is being added to.

To add rings to bonds, perform the following steps:

1. Select a ring tool from the **Rings** toolbar.
2. Hover the bond a ring will be added to.
3. Click and drag the mouse pointer to the side of the bond the ring should be added to.
4. Release the mouse to set the ring.

When the mouse pointer is close to the bond the ring is sprouting from, ChemDoodle will automatically select the optimal side of the bond to add to.

Templates

ChemDoodle contains a very advanced structure templates system. Several sets of predefined templates are already packaged

with ChemDoodle and can be accessed through the **Templates** widget. Currently, the following template sets are provided:

- Amino Acids
- Cycloalkanes
- Functional Groups
- Hexoses
- Nucleotides
- Polycyclic Aromatic Hydrocarbons
- Polycycles
- Ring Conformers
- Stereocenters and Geometries

Selecting a Template for Use

The **Templates** widget organizes your templates and allows you to easily use them. Just follow these three steps to select a template for use:

Activate the **Templates** widget by clicking on the **Templates** widget button.

1. Choose a template group from the drop down selection.
2. Click on a template choice to choose a template from the list.
3. Define a substitution atom by clicking on the preferred atom in the main structure panel. The substitution point will overlap with the atom used as the growth position.

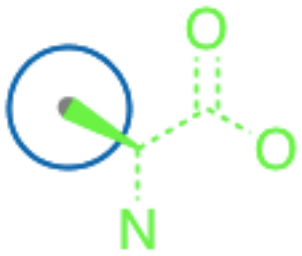
Placing templates is discussed in the following subsections.

Placing a Template

To place a template, set up a template and choose a substitution atom in the **Templates** widget.

Then hover over the atom in the document that you are attaching the template to and press the mouse down. A preview of the template will be depicted as in *Figure 3.14*.

Figure 3.14: New Template Placement Preview



Drag the mouse and use the techniques discussed in the following subsections to place the template in the preferred orientation. Then release the mouse to set the template.

Optimize Zone

The Optimize Zone can be used to optimize template placement as described in the **Bonds** section.

Placing Templates with Fixed Lengths and Angles

By default, fixed widths and fixed angles are enforced when drawing structures. To place a template within these restraints, hover over an atom and press the mouse down with a bond tool. You will see the **Optimize Zone** appear. Drag the mouse pointer out of the Optimize Zone. The new bond placement will now orient towards the mouse pointed.

The default fixed length is defined by the **Bond Length** visual specification in the Preferences window under the **Visuals** tab under the **Bonds** tab. Angles are fixed every 30° starting at 0°.

You can set whether fixed lengths and/or fixed angles are on by default in the **Preferences** window under the **General** tab.

Placing Templates at Non-fixed Lengths

When placing templates outside of the **Optimize Zone**, fixed lengths will be enforced. To break from fixed lengths, hold down the *shift* key while placing the template.

You may turn off fixed lengths in the **Preferences** window under the **General** tab. In this case, the *shift* key will then enforce fixed lengths.

Placing Templates at Non-fixed Angles

When placing templates outside of the **Optimize Zone**, fixed angles will be enforced. To break from fixed angles, hold down the *alt* key while placing the template.

You may turn off fixed angles in the **Preferences** window under the **General** tab. In this case, the *alt* key will then enforce fixed angles.

Placing Templates at Non-fixed Lengths and Non-fixed Angles

When placing templates outside of the **Optimize Zone**, fixed angles and fixed lengths will be enforced. To break from fixed lengths and fixed angles at the same time, hold down both the *shift* and *alt* key while placing the template.

You may turn off fixed lengths and fixed angles in the **Preferences** window under the **General** tab. In this case, holding the *shift* and *alt* keys will then enforce fixed lengths and angles.

Saving a New Template

To save a template into the **Templates** widget library, perform the following steps:

1. Draw the desired template on the **Doodle Board**.
2. Select the template with the selection tools discussed in *Chapter 5*. Only a single structure can be used in any template.
3. Right-click after selecting the structure.
4. Press the **Add Fragment as Template...** menu item to pop up the **Add Template** window.
5. Type in a name for the template in the **Template Name** text field.
6. Choose a template group to add the template to using the drop down selection. You can create a new template group using the **Add Group** button.
7. Click the **Done** button to add the template.

All of your templates are stored in the *templates* folder in the *ChemDoodleSettings* folder located in your operating system's standard *Document* folder. You may distribute your template groups to other ChemDoodle users or place third party template groups in this folder to use them in ChemDoodle. If ChemDoodle is open when manually placing template groups in the *templates* folder, make sure to first close and then restart ChemDoodle for changes to take effect.

Managing your Templates

To manage your templates, click on the **Manage My Templates...** menu item in the **Structure** menu.

Attributes

Attributes are special objects in ChemDoodle that are associated with other chemical objects. These include charges, radicals, symbols and ids on atoms and ids on bonds. They are both spatially and semantically linked to the chemical object that they describe. Any number of attributes can be added to a single chemical object.

In addition to the standard attributes provided in ChemDoodle, you can add your own text based attributes as shown for the attribute with display text of “attribute” for the nitrogen atom as shown in *Figure 3.15*.

Figure 3.15: An Attribute on an Atom

Adding Attributes

To add a custom attribute, perform the following steps:

1. Hover the atom to add the attribute to.
2. Right-click on the hovered atom.
3. Press the **Add Attribute...** menu item.
4. Type in the text to be displayed in the **Display** text field.
5. Type in an identifying name for the attribute in the **Name** text field. This value is used for the internal semantics and is not rendered.
6. Press the **Add** button to set the attribute.

Hovering Attributes

You can hover attributes by using any of the selection tools. First, make sure the current selection is empty and then move the mouse cursor close to the center of the attribute so that it is closer to the attribute than any other chemical objects. The attribute will then be defined as hovered and an amber circle will be rendered on top of it as shown in *Figure 3.16*.

Figure 3.16: A Hovered Attribute

To help identify which object the attribute describes, a transparent amber circle is drawn over that object (the nitrogen atom in *Figure 3.16*).

Selecting Attributes

Attributes can only be selected when using the selection tools discussed in *Chapter 5*. To select attributes, first hover them and then press the mouse down. The amber circle will turn a blue color as shown in *Figure 3.17*.

Figure 3.17: A Selected Attribute

Editing Attributes

The display text and names of custom attributes can be edited at any time by performing the following steps:

1. Hover the attribute to be edited.

2. Right-click on the hovered attribute.
3. Press the **Format Attribute...** menu item.
4. In the visual specifications window that appears, change the **Name** and **Display** text to the new values.
5. Click the **Done** button to set the new text values.

Moving Attributes

To move attributes, perform the following steps:

1. Hover the attribute to be moved.
2. Press the mouse down to select the hovered attribute.
3. Drag the attribute to the new preferred location.
4. Release the mouse to set the new position.

Attributes can only be moved a certain distance from the object that they describe. This distance is specified by the **Allow Distance** visual specification in the **Preferences** window under the **Visuals** tab under the **Attributes** tab. Change this to suit your needs.

Removing Attributes

To remove an attribute, use the **Eraser** tool and to click on the hovered symbol or hover the symbol with the selection tools and press the *delete* or *backspace* key.

Charges

Charges are attributes can be associated with any atoms as shown in *Figure 3.18*. Both positive and negative values can be used.

Figure 3.18: A Charge Attribute

O^{2-}

Adding Charges

To add charge to an atom, perform the following steps:

1. Select the **Increase Charge** ⊕ or **Decrease Charge** ⊖ tools in the **Attributes** group button in the **Shapes** toolbar.
2. Hover the atom to add charge to.
3. Press the mouse down to add the charge.
4. If you prefer to have the charge placed elsewhere, then before releasing the mouse, drag the pointer to the desired location.
5. Release the mouse to set the charge.

Incrementing and Decrementing Charges

To change the charge of an atom, perform the following steps:

1. Select the **Increase Charge** ⊕ or **Decrease Charge** ⊖ tools in the **Attributes** group button in the **Shapes** toolbar.
2. Hover the atom to with the charge to be changed.
3. Click the mouse down to increment or decrement the charge.

The + and - keys on the keyboard can also be used to increment and decrement charge values.

Removing Charges

Removing charges can be done is several ways:

- Decrement or increment the charge value to 0 using the **Increase Charge** and **Decrease Charge** tools.
- Select the **Eraser** tool and click on a hovered charge to remove it.
- Hover the charge using the selection tools and press the *delete* or *backspace* key.

Radicals

Radical types can be associated with any atoms as shown in *Figure 3.19*. Currently only Monovalent and Divalent Singlet types are supported.

Figure 3.19: A Radical Attribute

Adding Radicals

To add a radical electron to an atom, perform the following steps:

1. Select the **Increase Number of Radical Electrons**  tool in the **Attributes** group button in the **Shapes** toolbar.
2. Hover the atom to add the radical to.
3. Press the mouse down to add the radical.
4. If you prefer to have the radical placed elsewhere, then before releasing the mouse, drag the pointer to the desired location.
5. Release the mouse to set the radical.

Incrementing and Decrementing the Number of Radical Electrons

To change the charge of an atom, perform the following steps:

1. Select the **Increase Number of Radical Electrons**  or **Decrease Number of Radical Electrons**  tools in the **Attributes** group button in the **Shapes** toolbar.
2. Hover the atom with the radical to be changed.
3. Click the mouse down to increment or decrement the the number of radical electrons.

Removing Radicals

Removing radicals can be done is several ways:

- Decrement the radical value to 0 using the **Decrease Number of Radical Electrons** tools.
- Select the **Eraser** tool and click on a hovered radical to remove it.
- Hover the radical using the selection tools and press the *delete* or *backspace* key.

Symbols

Symbols are standard types of atom decorations that can be associated with any atoms such as the **Radical Cation** symbol shown in *Figure 3.20*.

Figure 3.20: A Symbol Attribute

Currently, included symbols are:

1. Single Electron
2. Electron Pair *aka.* Non-bonding Pair, Lone Pair
3. Radical Cation
4. Radical Anion
5. Electron Pair (Bar)

6. Positive Dipole
7. Negative Dipole

Adding Symbols

To add a symbol to an atom, perform the following steps:

1. Select the desired symbol tool in the **Attributes** group button in the **Shapes** toolbar.
2. Hover the atom the symbol will added to.
3. Press the mouse down to add the symbol.
4. If you prefer to have the symbol placed elsewhere, then before releasing the mouse, drag the pointer to the desired location.
5. Release the mouse to set the symbol.

Removing Symbols

To remove a symbol, use the **Eraser** tool and to click on the hovered symbol or hover the symbol with the selection tools and press the *delete* or *backspace* key.

Isotopes

Mass numbers can be associated with atoms with element symbols as their label to designate isotopes. All mass numbers are displayed in superscript format to the left of element symbols as shown in *Figure 3.21*.

Figure 3.21: A Carbon-13 Isotope

^{13}C

If you later change an atom's label and there is a mass number associated with that atom, then the mass number will be removed.

Setting Published Isotope Mass Numbers

To set a published mass number to an element atom, perform the following steps:

1. Hover the atom with the mass number to be set.
2. Right-click on the hovered atom.
3. Expand the **Mass Number** submenu.
4. Press any of the listed values to set the mass number of the isotope.

Setting Arbitrary Isotope Mass Numbers

To set an arbitrary mass number to an element atom, perform the following steps:

1. Hover the atom with the mass number to be set.
2. Right-click on the hovered atom.
3. Expand the **Mass Number** submenu.
4. Press the **Other...** menu item.
5. Type in an integer value into the text field that appears.
6. Click the **Accept** button to set the mass number.

Removing Mass Numbers

To remove a mass number from an atom:

1. Hover the atom with the mass number to be removed.
2. Right-click on the hovered atom.
3. Expand the **Mass Number** submenu.
4. Press the **Remove Mass Number** menu item to remove the mass number.

Orbitals

2D graphics for various orbital shapes can be placed directly into the document or attached onto structures. Use them to show more detailed chemical figures. Each orbital shape has several different shading and fill styles.

The following orbital types are provided:

- Atomic s Orbitals
- Atomic $p_{x|y|z}$ Orbitals
- Atomic $d_{xz|yz|xy|x^2-y^2}$ Orbitals
- Atomic d_{z^2} Orbitals
- Atomic $f_{xz^2|xy^2|x(x^2-3y^2)|y(3x^2-y^2)}$ Orbitals
- Atomic f_{z^3} Orbitals
- Hybrid sp^3 Orbitals
- Hybrid sp Lobes
- Bonding σ Orbitals
- Bonding π Orbitals

Orbitals are defined by two anchor points as shown in *Figure 3.22*. The first anchor point defines the center of the orbital while the second anchor point defines the extent of the orbital.

Figure 3.22: Orbital and Anchors

Placing Orbitals at Fixed Lengths and Angles

To place an orbital, perform the following steps:

1. Select an orbital tool by expanding any of the **Orbital** group button in the **Orbitals** toolbar.
2. Press the mouse down on the **Doodle Board** to set the center of the orbital.
3. Drag the mouse to preview the placement of the extent of the orbital. A dotted green outline of the orbital will be shown.
4. Release the mouse to set the orbital.

You can also click the mouse to set the start center then move the mouse and click again to set the extent.

In step 2, you may want to attach the orbital to an atom or bond center. ChemDoodle will automatically lock onto atoms and bonds when placing orbitals if the mouse pointer gets close enough to them. Once the atom or bond has been highlighted, continue through step two to place the orbital and set the center to be the atom or bond center.

Placing Orbitals at Non-fixed lengths or Angles

To place lines at non-fixed lengths or angles, hold down the *alt* key while dragging the mouse when defining the orbital to break from the fixed lengths and angle orientations.

Forcing Orbitals to be Drawn Vertically and Horizontally

To place orbitals oriented vertically or horizontally, hold down the *shift* key while dragging the mouse when defining the orbital. The orbital preview will then automatically orient vertically or horizontally depending on the angle from the start point to the current mouse cursor position.

Moving Orbitals

To move orbitals, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the orbital so an open hand mouse cursor appears and the rectangle anchor points are drawn as shown in *Figure 3.19*.
2. Press the mouse down and drag to move the orbital.
3. Release the mouse to finish the move action.

Resizing Orbitals

To resize orbitals, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the orbital so an open hand mouse cursor appears and the orbital anchor points are drawn as shown in *Figure 3.19*.
2. Move the mouse pointer over one of the two end anchor points so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to resize the orbital.
5. Release the mouse to finish the resize action.

Removing Orbitals

Orbitals can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the orbital so an open hand mouse cursor appears and the rectangle anchor points are drawn as shown in *Figure 3.19*. Then press the *backspace* or *delete* key.
- Use the eraser tool to hover the mouse pointer over the orbital so the orbital anchor points are drawn. Then click with the mouse.

Chapter 4: Shapes

Overview

In addition to chemical structures, ChemDoodle provides tools for drawing shapes for advanced figures.

This section introduces the new user to shapes within ChemDoodle. It covers the following topics:

- The different types of shapes.
- How to draw shapes.
- Adding arrows to figures.
- Adding text to figures.
- How to move shapes.
- How to resize shapes.
- How to remove shapes.
- What the anchor decorations mean.

Anchors

Anchors are points that define a given shape. By moving them, you modify how the shape appears. There are two types of anchors, control anchors and corner/edge anchors.

Control Anchors

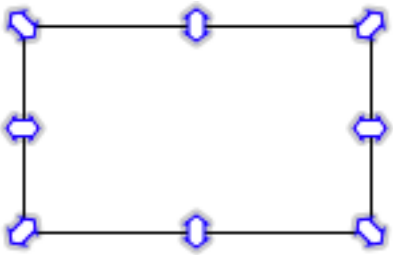
Control anchors represent points that can be moved anywhere and have no relationship to other anchors, such as in lines, custom shapes or orbitals. They appear as compass shapes as shown in *Figure 4.1*.

Figure 4.1: Control anchors

Corner/Edge Anchors

Corner edge anchors define corners and edges of shapes. Moving these anchors will change the shape in relationship to the other anchors. For instance, if you move a left-right pointing anchor, you will not affect the vertical positioning of the other anchors. These anchors are present for box shaped objects, like rectangles and ovals. They appear as double sided arrows as shown in *Figure 4.2*.

Figure 4.2: Corner/Edge Anchors



Lines

Lines are the most basic shape and are defined by two anchors placed at their endpoints as shown in *Figure 4.3*. There is also a third anchor at the midpoint for controlling the arc angle. This anchor point is discussed in the next section (Arcs).

Figure 4.3: Line Shape and Anchors

Drawing Lines at Fixed Angles

To draw a line at fixed angles, perform the following steps:

1. Select a line tool by expanding the **Lines** group button in the **Shapes** toolbar.
2. Press the mouse down on the **Doodle Board** to set the start point of the line.
3. Drag the mouse to preview the placement of the end of the line.
4. Release the mouse to set the line.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

By default, lines will be oriented at fixed angles every 15° starting at 0°.

Drawing Lines at Non-fixed Angles

To place lines at non-fixed angles, hold down the *alt* key while dragging the mouse when defining the line to break from the fixed orientation angles.

Forcing the Lines to be Drawn Vertically and Horizontally

To place lines oriented vertically or horizontally, hold down the *shift* key while dragging the mouse when defining the line. The line preview will then automatically orient vertically or horizontally depending on the angle from the start point to the current mouse cursor position.

Moving Lines

To move lines, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the line so an open hand mouse cursor appears and the anchor points are drawn as shown in *Figure 4.3*.
2. Press the mouse down and drag to move the line.
3. Release the mouse to finish the move action.

Resizing Lines

To resize lines, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the line so an open hand mouse cursor appears and the line anchor points are drawn as shown in *Figure 4.3*.
2. Move the mouse pointer over one of the two end anchor points so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to resize the line.
5. Release the mouse to finish the resize action.

Removing Lines

Lines can be removed in a number of ways. You can do the following:

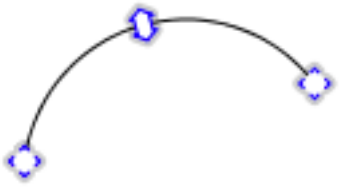
- Use a selection tool to hover the mouse pointer over the line so an open hand mouse cursor appears and the line anchor points are drawn as shown in *Figure 4.3*. Then press the *backspace* or *delete* key.
- Use the eraser tool to hover the mouse pointer over the line so the line anchor points are drawn. Then click with the mouse.

Arcs

Arcs are segments of a circle and are defined by two anchors placed at their endpoints as shown in *Figure 4.4*. There is also a third anchor at the middle for controlling the arc

angle. Only 90°, 120°, 180° and 270° arcs are directly provided in the **Arcs** group button, but an arc of any angle can be drawn. The only difference between the line shape and the arc shape is the angle, and either shape can be converted into the other by changing this value.

Figure 4.4: Arc Shape and Anchors



Drawing Arcs at Fixed Angles

To draw an arc at fixed angles, perform the following steps:

1. Select an arc tool by expanding the **Arcs** group button in the **Shapes** toolbar.
2. Press the mouse down on the **Doodle Board** to set the start point of the arc.
3. Drag the mouse to preview the placement of the end of the arc.
4. Release the mouse to set the arc.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

By default, arcs will be oriented at fixed angles every 15° starting at 0°.

Drawing Arcs at Non-fixed Angles

To place arcs at non-fixed angles, hold down the *alt* key while dragging the mouse when defining the arc to break from the fixed orientation angles.

Forcing the Arcs to be Drawn Vertically and Horizontally

To place arcs oriented vertically or horizontally, hold down the *shift* key while dragging the mouse when defining the arc. The arc preview will then automatically orient vertically or horizontally depending on the angle from the start point to the current mouse cursor position.

Moving Arcs

To move arcs, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the arc so an open hand mouse cursor appears and the arc anchor points are drawn as shown in *Figure 4.4*.
2. Press the mouse down and drag to move the arc.
3. Release the mouse to finish the move action.

Resizing Arcs

To resize arcs, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the arc so an open hand mouse cursor appears and the arc anchor points are drawn as shown in *Figure 4.4*.
2. Move the mouse pointer over one of the two end anchor points so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to resize the arc.
5. Release the mouse to finish the resize action.

Changing Arc Angles

Arc angles can be changed using the midpoint anchor. Choose a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the arc so an open hand mouse cursor appears and the arc anchor points are drawn as shown in *Figure 4.4*.
2. Move the mouse pointer over the middle anchor point so that it is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to change the arc angle.
5. Release the mouse to set the new arc angle.

While changing the angle of arcs, the arc angle will be displayed below the mouse cursor.

Flipping an Arc's Orientation

To flip an arc's orientation, so that the curve faces the opposite direction. use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the arc so an open hand mouse cursor appears and the line anchor points are drawn as shown in *Figure 4.4*.
2. Right-click on the hovered arc.
3. Select the **Flip Arc** menu item to flip the arc's orientation.

You can also click and drag the midpoint to the other side of the arc to perform this task.

Removing Arcs

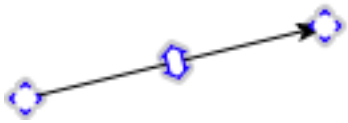
Arcs can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the arc so an open hand mouse cursor appears and the arc anchor points are drawn as shown in *Figure 4.4*. Then press the *backspace* or *delete* key.
- Use the eraser tool to hover the mouse pointer over the arc so the arc anchor points are drawn. Then click with the mouse.

Arrows

Arrows are essential in chemical graphics for many reasons, the most important being for reaction and mechanism diagrams. Arrows are so important that they have their own unique toolbar. Essentially, arrow shapes are just lines and arcs with arrowheads as shown in *Figure 4.5*.

Figure 4.5: Arrow Shape and Anchors



ChemDoodle also provides advanced features for building and defining reactions. Reactions are covered in *Chapter 7*.

Drawing Arrows at Fixed Angles

To draw an arrow at fixed angles, perform the following steps:

1. Select the desired **arrowheads** and connector styles in the Arrows toolbar.
2. Click on one of the arc angle buttons in the **Arrows** toolbar to enter the arrow placement mode.

3. Press the mouse down on the **Doodle Board** to set the start point of the arrow.
4. Drag the mouse to preview the placement of the end of the arrow.
5. Release the mouse to set the arrow.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

By default, arrows will be oriented at fixed angles every 15° starting at 0°.

Drawing Arrows at Non-fixed Angles

To place arrows at non-fixed angles, hold down the *alt* key while dragging the mouse when defining the arrow to break from the fixed orientation angles.

Forcing the Arcs to be Drawn Vertically and Horizontally

To place arrows oriented vertically or horizontally, hold down the *shift* key while dragging the mouse when defining the arrow. The arrow preview will then automatically orient vertically or horizontally depending on the angle from the start point to the current mouse cursor position.

Moving Arrows

To move arrows, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the arrow so an open hand mouse cursor appears and the arrow anchor points are drawn as shown in *Figure 4.5*.
2. Press the mouse down and drag to move the arrow.
3. Release the mouse to finish the move action.

Resizing Arrows

To resize arrows, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the arrow so an open hand mouse cursor appears and the arrow anchor points are drawn as shown in *Figure 4.5*.
2. Move the mouse pointer over one of the two end anchor points so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to resize the arrow.
5. Release the mouse to finish the resize action.

Changing Arrow Arc Angles

Arrow arc angles can be changed using the midpoint anchor. Choose a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the arrow so an open hand mouse cursor appears and the arrow anchor points are drawn as shown in *Figure 4.5*.
2. Move the mouse pointer over the middle anchor point so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to change the arrow arc angle.

5. Release the mouse to set the new arrow arc angle.

While changing the angle of arrow arcs, the arrow arc angle will be displayed below the mouse cursor.

NOTE: A few special arrow types, such as the retrosynthetic type, are straight, and you will not be able to change the arc angles for these types.

Removing Arrows

Arrows can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the arrow so an open hand mouse cursor appears and the arrow anchor points are drawn as shown in *Figure 4.5*. Then press the *backspace* or *delete* key.
- Use the eraser tool to hover the mouse pointer over the arrow so the arrow anchor points are drawn. Then click with the mouse.

Editing Arrowheads

Arrowheads can be added/removed from the ends of the line shape. This can be done before they are drawn, with the **Arrow** toolbar, or afterwards by using the **Format Arrow** window.

There are several settings that control how arrowheads are drawn:

- **Indented** - When selected, the back end of the arrow will be indented in.
- **Filled** - When selected, the arrow will be filled in, otherwise it will just be an outline.
- **Chevroned** - When selected, the arrow will be drawn as a simple chevron.
- **Length** - This setting controls the length of the arrow head along the line.
- **Angle** - This setting controls the angle of the arrow, from one side to the other.

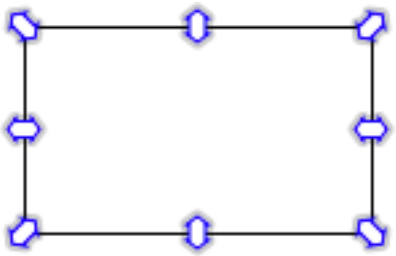
Use these settings to control how arrowheads are drawn.

NOTE: If the arrowhead length is greater than 50% of the length of the line it is on, then the length will be decreased to 50% of the length of the line it is on.

Rectangles

Rectangles can be drawn in several styles and are defined by two anchor points that correspond to a pair of rectangle corners along one of the diagonals as shown in *Figure 4.6*.

Figure 4.6: Rectangle Shape and Anchors



Drawing Rectangles

To draw a rectangle, perform the following steps:

1. Select a rectangle tool by expanding the **Rectangle** group button in the **Shapes** toolbar.
2. Press the mouse down on the **Doodle Board** to set one corner of the rectangle.
3. Drag the mouse to preview the placement of the opposite corner along the diagonal of the rectangle.
4. Release the mouse to set the rectangle.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

Drawing Squares

To draw squares, hold down the *shift* key while dragging the mouse when defining the rectangle to force the width and height to be equivalent.

Moving Rectangles

To move rectangles, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the rectangle so an open hand mouse cursor appears and the rectangle anchor points are drawn as shown in *Figure 4.6*.
2. Press the mouse down and drag to move the rectangle.
3. Release the mouse to finish the move action.

Resizing Rectangles

To resize rectangles, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the rectangle so an open hand mouse cursor appears and the rectangle anchor points are drawn as shown in *Figure 4.6*.
2. Move the mouse pointer over one of the anchor points so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to resize the rectangle.
5. Release the mouse to finish the resize action.

Converting Between Rounded and Non-rounded Rectangles

To change a rectangle into a rounded-rectangle or vice versa, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the rectangle so an open hand mouse cursor appears and the arrow anchor points are drawn as shown in *Figure 4.6*.
2. Right-click on the hovered rectangle and select the **Format Rectangle...** menu item.
3. Scroll to the **Rectangle** section and use the **Rounded** on/off choice to set the rectangle to be rounded or not.

Removing Rectangles

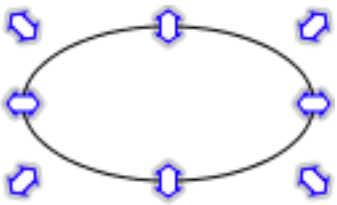
Rectangles can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the rectangle so an open hand mouse cursor appears and the rectangle anchor points are drawn as shown in *Figure 4.4*. Then press the *backspace* or *delete* key.
- Use the eraser tool to hover the mouse pointer over the rectangle so the rectangle anchor points are drawn. Then click with the mouse.

Ovals

Ovals can be drawn in several styles and are defined by two anchor points that correspond to a pair of rectangle corners along one of the diagonals that circumscribes the oval as shown in *Figure 4.7*.

Figure 4.7: Oval Shape and Anchors



Drawing Ovals

To draw an oval, perform the following steps:

1. Select an oval tool by expanding the **Oval** group button in the **Shapes** toolbar.
2. Press the mouse down on the **Doodle Board** to set one corner of the circumscribing rectangle.
3. Drag the mouse to preview the placement of the opposite corner along the diagonal of the circumscribing rectangle.
4. Release the mouse to set the oval.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

Drawing Circles

To draw circles, hold down the *shift* key while dragging the mouse when defining the oval to force the major and minor axes lengths to be equivalent.

Moving Ovals

To move ovals, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the oval so an open hand mouse cursor appears and the oval anchor points are drawn as shown in *Figure 4.7*.
2. Press the mouse down and drag to move the oval.
3. Release the mouse to finish the move action.

Resizing Ovals

To resize ovals, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the oval so an open hand mouse cursor appears and the oval anchor points are drawn as shown in *Figure 4.7*.
2. Move the mouse pointer over one of the anchor points so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to resize the oval.
5. Release the mouse to finish the resize action.

Removing Ovals

Ovals can be removed in a number of ways. You can do the following:

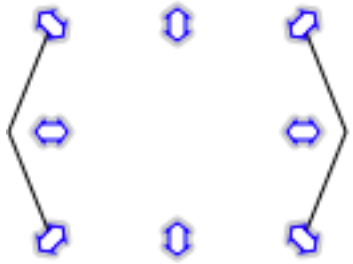
- Use a selection tool to hover the mouse pointer over the oval so an open hand mouse cursor appears and the oval anchor points are drawn as shown in *Figure 4.7*. Then press the *backspace* or *delete* key.
- Use the eraser tool to hover the mouse pointer over the oval so the oval anchor points are drawn. Then click with the mouse.

Brackets

Brackets can be drawn in several styles and are defined by two anchor points that correspond to a pair of rectangle corners

along one of the diagonals that defines the bracket space as shown in *Figure 4.8*.

Figure 4.8: Bracket Shape and Anchors



There are currently 4 bracket styles:

- **Square Brackets** - [ ]
- **Parenthesis** - ( )
- **Curly Brackets** - { }
- **Chevrons** - < >

Drawing Brackets

To draw a set of brackets, perform the following steps:

1. Select a bracket tool by expanding the **Bracket** group button in the **Shapes** toolbar.
2. Press the mouse down on the **Doodle Board** to set one corner of the bracket.
3. Drag the mouse to preview the placement of the opposite corner along the diagonal of the bracket.
4. Release the mouse to set the bracket.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

Drawing Brackets with Equal Width and Height

To draw square brackets, hold down the *shift* key while dragging the mouse when defining the bracket to force the width and height of the bracket content to be equivalent.

Moving Brackets

To move brackets, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the brackets so an open hand mouse cursor appears and the bracket anchor points are drawn as shown in *Figure 4.8*.
2. Press the mouse down and drag to move the brackets.
3. Release the mouse to finish the move action.

Resizing Brackets

To resize brackets, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the brackets so an open hand mouse cursor appears and the bracket anchor points are drawn as shown in *Figure 4.8*.
2. Move the mouse pointer over one of the two end anchor points so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to resize the bracket set.
5. Release the mouse to finish the resize action.

Editing Bracket Lip Protrusion

To change the widths of the current bracket rendering style, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by

emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the brackets so an open hand mouse cursor appears and the arrow anchor points are drawn as shown in *Figure 4.8*.
2. Right-click on the hovered rectangle and select the **Format Bracket...** menu item.
3. Scroll to the **Bracket** section and use the **Wideness** number slider to define how protruded bracket lips are rendered.

Removing Brackets

Brackets can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the brackets so an open hand mouse cursor appears and the bracket anchor points are drawn as shown in *Figure 4.8*. Then press the *backspace* or *delete* key.
- Use the eraser tool to hover the mouse pointer over the brackets so the bracket anchor points are drawn. Then click with the mouse.

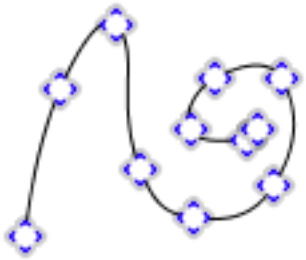
Custom Shapes

In addition to the standard defined shapes previously discussed, ChemDoodle allows you to create custom shapes. Currently there are three types of custom shapes:

- **Pen** - The Pen tool allows you to draw any shape by clicking and dragging an outline.
- **Bezier Curve** - The Bezier Curve tool allows you to draw a bezier curve by defining its control points.
- **Polyline** - The Polyline tool allows you do draw any polygon shape that can be convex or concave.

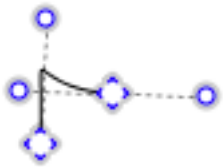
Both pen paths and polylines can be open or closed and are defined by their control points, which the shape will pass through as shown in *Figure 4.9*.

Figure 4.9: Pen and Polyline Control Points



Bezier curves can be open or closed and are defined by a more complex set of control points as shown in *Figure 4.10*.

Figure 4.10: Bezier Control Points



Drawing with the Pen Tool

To draw a custom shape with the **Pen** tool, perform the following steps:

1. Select a Pen tool by expanding the **Custom Shapes** group button in the **Shapes** toolbar.
2. Press the mouse down on the **Doodle Board** to begin drawing.

3. Drag the mouse in an outline of the shape you would like.

4. Release the mouse to set shape.

ChemDoodle will automatically simplify your path for you and generate a cubic interpolation.

Drawing with the Polyline Tool

To draw a custom shape with the **Polyline** tool, perform the following steps:

1. Select the **Polyline** tool by expanding the **Custom Shapes** group button in the **Shapes** toolbar.

2. Press the mouse down on the **Doodle Board** to set the first point.

3. Move the mouse to location you prefer the next point to be placed.

4. Click to place the next point. Points will automatically connect to previous points.

5. Repeat steps 3 and 4 until finished.

6. Click on the first point drawn or double-click the last point to complete the shape and set it.

Moving Pen Paths and Polylines

To move custom shapes, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the custom shape so an open hand mouse cursor appears and the control points are rendered as shown in *Figure 4.9*.

2. Press the mouse down and drag to move the custom shape.

3. Release the mouse to finish the move action.

Modifying Pen Paths and Polylines

You can move the control points that define pen paths and polylines. To do so, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the custom shape so an open hand mouse cursor appears and the control points are drawn as shown in *Figure 4.9*.

2. Move the mouse pointer over one of the control points that you desire to be moved so that control point is filled in with an amber color.

3. Press the mouse down so the control point is filled with a blue color.

4. Drag the control point to move it.

5. Release the mouse to finish.

Drawing with the Bezier Tool

Bezier curves are defined by pairs of control points. There is a main point which the curve passes through, and a second control point that describes the tangent of the line at the point that the curve passes through. To draw a bezier curve, perform the following steps:

1. Select the **Bezier Curve** tool by expanding the **Custom Shapes** group button in the **Shapes** toolbar.

2. Press the mouse down on the **Doodle Board** to set the first point.

3. Drag your mouse to set the paired control point that defines the tangent of the curve at the first point. The further from the first point you make this paired control point, the tighter the curve will hug the first point.

4. Release the mouse to set the paired control point.
5. Move the mouse to location you prefer the next point to be placed that the curve will pass through.
6. Press the mouse down to place the next point. Points will automatically connect to previous points.
7. Drag your mouse to set the paired control point that defines the tangent of the curve at the second point. The further from the second point you make this paired control point, the tighter the curve will hug the second point.
8. Repeat steps 5 through 7 until finished.
9. Press the *escape* key to complete the shape and set it.

Modifying Bezier Curves

You can move the control points that define bezier curves in one of two ways. The first way is by following the same instructions as in the **Modifying Pen Paths and Polylines** section. The second is by using the **Bezier Curve** tool. Perform the following steps:

1. Select the **Bezier Curve** tool by expanding the **Custom Shapes** group button in the **Shapes** toolbar.
2. Move the mouse pointer over the bezier curve that you desire to be modified so that its control points are rendered.
3. Click on the bezier curve so that all of its control points are rendered as shown in *Figure 4.10*.
4. Hover over any of the control points so that an amber color fills the one you wish to move.
5. Press the mouse down and drag the control point to the new desired location.
6. Release the mouse to finish moving the control point.

Deleting Bezier Control Points

Only the control points that have the curve pass through them may be deleted. Deleting one of these control points will also remove the corresponding paired control point. To delete a bezier control point, perform the following steps:

1. Select the **Bezier Curve** tool by expanding the **Custom Shapes** group button in the **Shapes** toolbar.
2. Move the mouse pointer over the bezier curve that you desire to be modified so that its control points are rendered.
3. Click on the bezier curve so that all of its control points are rendered as shown in *Figure 4.10*.
4. Hover over the control point that you wish to remove so that it is filled in with an amber color.
5. Press the *delete* key to delete the control point.

Adding Arrows to Bezier Curves

To add arrows to bezier curves follow the same procedures as discussed for the Arrow shapes earlier in the Chapter. Just right click on the bezier curve after it is hovered, select the **Format Bezier Curve...** menu item, and define the arrow sections to your preference.

Closing and Opening Custom Shapes

To close or open a custom shape, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the

current selection. Perform the following steps:

1. Hover the mouse pointer over the custom shape so an open hand mouse cursor appears and the arrow anchor points are drawn as shown in *Figure 4.9*.
2. Right-click on the hovered custom shape and select the **Format Custom Shape...** menu item.
3. Scroll to the **Path** or **Bezier Curve** section and use the **Close** on/off choice to set if the custom shape path is closed or not.

If closed, the custom shape can be filled in with a desired color.

Removing Custom Shapes

Custom Shapes can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the custom shape so an open hand mouse cursor appears and the custom shape anchor points are drawn as shown in *Figure 4.9*. Then press the *backspace* or *delete* key.
- Use the eraser tool to hover the mouse pointer over the custom shape so the custom shape anchor points are drawn. Then click with the mouse.

Rulers

Rulers measure distances in 2 dimensions and are defined by two anchors placed at their endpoints as shown in *Figure 4.11*. There is also a third midpoint in the middle for controlling the arc angle. This anchor point is discussed in the next section.

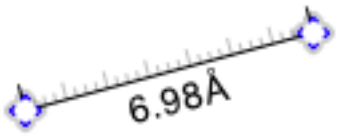


Figure 4.11: Ruler Shape and Anchors

Drawing Rulers at Fixed Angles

To draw a ruler at fixed angles, perform the following steps:

1. Select a **Ruler** tool in the **Shapes** toolbar.
2. Press the mouse down on the **Doodle Board** to set the start point of the ruler.
3. Drag the mouse to preview the placement of the end of the ruler.
4. Release the mouse to set the ruler.

You can also click the mouse to set the start point then move the mouse and click again to set the end point.

By default, rulers will be oriented at fixed angles every 15° starting at 0°.

Drawing Rulers at Non-fixed Angles

To place rulers at non-fixed angles, hold down the *alt* key while dragging the mouse when defining the ruler to break from the fixed chain orientation angles.

Forcing Rulers to be Drawn Vertically and Horizontally

To place rulers oriented vertically or horizontally, hold down the *shift* key while dragging the mouse when defining the ruler. The ruler preview will then automatically orient vertically or horizontally depending on angle from the start point to the current mouse cursor position.

Automatically Measuring Object Width and Height

To measure the width and height of selected objects, perform the following procedure:

1. Select the content to be measured using the selection tools.
2. Select the **Width and Height** menu item in the **Measure>** submenu in the **Content** menu.

Two rulers will be placed to measure the width and height of the selected content.

Automatically Measuring Object Diagonal

To measure the diagonal of selected objects, perform the following procedure:

1. Select the content to be measured using the selection tools.
2. Select the **Diagonal** menu item in the **Measure>** submenu in the **Content** menu.

A single ruler will be placed across the diagonal of the selected content.

Moving Rulers

To move rulers, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the ruler so an open hand mouse cursor appears and the anchor points are drawn as shown in *Figure 4.11*.
2. Press the mouse down and drag to move the ruler.
3. Release the mouse to finish the move action.

Resizing Rulers

To resize rulers, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the ruler so an open hand mouse cursor appears and the ruler anchor points are drawn as shown in *Figure 4.11*.
2. Move the mouse pointer over one of the two end anchor points so that anchor point is filled in with an amber color.
3. Press the mouse down so the anchor point is filled with a blue color.
4. Drag the anchor point to resize the ruler.
5. Release the mouse to finish the resize action.

Showing and Hiding Major and Minor Ticks

To show and hide ruler major and minor ticks, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the ruler so an open hand mouse cursor appears and the ruler anchor points are drawn as shown in *Figure 4.11*.
2. Right-click on the hovered ruler and select the **Format Ruler...** menu item.
3. Scroll to the **Ruler** section and use the **Show Major Ticks** and **Show Minor Ticks** on/off choices to set whether major and minor ticks are visible or not.

Changing the Measurement Unit

To change the ruler's measurement unit, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the

current selection. Perform the following steps:

1. Hover the mouse pointer over the ruler so an open hand mouse cursor appears and the ruler anchor points are drawn as shown in *Figure 4.11*.
2. Right-click on the hovered ruler and select the **Format Ruler...** menu item.
3. Scroll to the **Ruler** section and use the **Unit** drop down selection to select the unit to be displayed.

Removing Rulers

Rulers can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the ruler so an open hand mouse cursor appears and the ruler anchor points are drawn as shown in *Figure 4.11*. Then press the *backspace* or *delete* key.
- Use the eraser tool to hover the mouse pointer over the ruler so the ruler anchor points are drawn. Then click with the mouse.

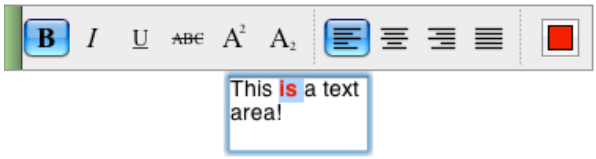
Text Areas

In addition to atom labels, you can also add blocks of text in text area objects. Text areas can have a border and can have a background, and can be resized to any dimension.

To place text areas, click on the **Text Area** tool  in the **Shapes** toolbar. You can place text areas and edit them just as you would **Rectangle** shapes. The text area is resizable and can have a border and background. It will not automatically fit its contained text.

When editing the text area, text format functions will be provided in a toolbar that appears above it as shown in *Figure 4.12*.

Figure 4.12: Editing a Text Area



To edit text areas, use the **Text Area** tool to click on an existing text area, or hover the text area using a selection tool and double-click.

Chapter 5: Editing Content

Overview

The most important feature of graphical editors is access to a robust set of content management tools.

This section introduces the new user to content management tools within ChemDoodle. It covers the following topics:

- Selecting content.
- Duplicating content.
- Editing content.
- Organizing content.
- Grouping content.
- Removing content.

Selecting Content

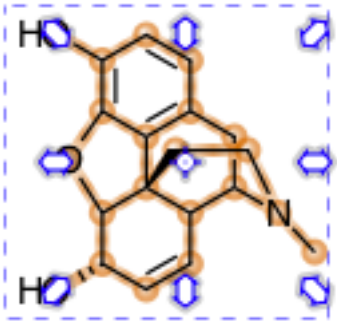
Content can be selected by using any of the selection tools. There are 3 types of selection tools provided in ChemDoodle:

- **Lasso** -  Define an arbitrary boundary that follows the mouse and selects any objects contained within.
- **Rectangular Marquee** -  Define a rectangle that selects any objects contained within.
- **Lasso Only Shapes** -  Define an arbitrary boundary that follows the mouse and selects only shape objects contained within.

These tools can be quite complex to learn, so we suggest you practice with them for a while.

Selected content will show an amber highlight and will be surrounded by an an animated amber outline as shown in *Figure 5.1*.

Figure 5.1: Selected Content



The crawling ants animation can be turned off in the **Preferences** window under the **General** tab.

Selecting Individual Objects

To select an individual object, first select a lasso tool and make sure no content is currently selected. Then hover the object to be selected and click. The single object will then be selected.

Selecting Groups of Objects

To select groups of object, perform the following steps:

1. Select a lasso tool.
2. Click and drag to draw an outline with a lasso or to draw a rectangle with the rectangular marquee to surround all of the objects you would like to select.
3. Release the mouse to select the contained objects.

NOTE: It may be difficult to see the full bounds for some shapes, such as large text

areas with little text in them. If you have trouble selecting a shape, make sure to discover where its bounds are and draw the selection bounds around both anchors.

Select All

To select all content on a page, expand the **Select** submenu in the **Content** menu and press the **All** menu item. The keyboard shortcut to use this function is *ctrl-A* (*command-A* on Mac OS X).

Adding/Removing Individual Objects from a Selection

If a selection has already been made, you can add or remove an individual object from the selection. Hold down the *alt* key and hover the object to be added or removed and click the mouse. If that object was previously selected, it will be removed from the selection, otherwise it will be added to the selection.

Adding/Removing Groups of Objects from a Selection

If a selection has already been made, you can add or remove groups of objects from the selection. Hold down the *shift* key and hover the object to be added or removed and click and drag to draw an outline with a lasso or to draw a rectangle with the rectangular marquee to surround all of the objects you would like to select or deselect. Then release the mouse. Any objects contained within the new boundary will be removed from the selection if they were previously selected, otherwise they will be added to the selection.

Selecting Whole Molecules

Instead of surrounding an entire molecule with the selection tools to select it, the following techniques will allow you to select individual molecules:

- Using a selection tool, hold down both the *alt* and *shift* keys and then click on an atom or bond in the molecule.
- Press the *tab* key to navigate through molecules, selecting one at a time, starting at the last drawn molecule and then navigating through them chronologically.

Selecting Chemical Objects by SMARTS

SMARTS is single line, text-based query system for matching chemical objects, similar to how systems like regular expressions match text. You may find it very convenient to select content in files by SMARTS queries. To do so, perform the following steps:

1. Select the **SMARTS...** menu item in the **Select>** submenu in the **Content** menu.
2. A window will appear prompting you for the SMARTS query. Input your query here and press the **Accept** button.

Any content that matches the SMARTS string will then be selected.

Navigating Through Single Shapes

Instead of surrounding an entire shape with the selection tools to select it or clicking on the shape, you can also press the *tab* key while holding down the *shift* key to navigate through shapes, selecting one at a time, starting at the last drawn shape and then navigating through them chronologically.

Selecting Only Shapes

When figures are highly congested, it may be difficult to select shapes from surrounding structures. In this case, use the **Lasso Only Shapes** tool which will only recognize shapes. The **Lasso Only Shapes** tool works identically to the **Lasso** tool in every other way.

Select the Inverse of the Current Selection

To select the inverse of the current selection on a page, expand the **Select** submenu in the **Content** menu and press the **Inverse** menu item.

Deselecting Objects

To deselect the current selection, perform one of the following actions:

- Move the mouse cursor away from the selection so that the lasso cursor icon appears. Then click the mouse.
- When the mouse cursor is within the current selection boundary, double-click the mouse.
- Press the **Deselect** menu item in the **Content** menu.
- Press the *space* key to deselect the current selection and return to the structure drawing mode.

Reselecting Objects

If you lost the current selection by mistake, you can reselect it by selecting the **Reselect** menu item in the **Content** menu.

Duplicating Content

Content in ChemDoodle can be duplicated on the **Doodle Board** in the current document or between separate documents through copy and paste actions. To have ChemDoodle objects copied and pasted correctly on the **Doodle Board**, make sure to keep **ChemDoodle Collage** enabled in the **Preferences** window under the **Advanced** tab.

Copy and Paste

To duplicate content, perform the following steps:

1. Select the content to be duplicated.
2. Press the **Copy** menu item in the **Edit** menu. The keyboard shortcut to use this function is *ctrl-C* (*command-C* on Mac OS X).
3. Press the **Paste** menu item in the **Edit** menu. The keyboard shortcut to use this function is *ctrl-V* (*command-V* on Mac OS X).

Cut and Paste

To duplicate content and remove the original, perform the following steps:

1. Select the content to be duplicated.
2. Press the **Cut** menu item in the **Edit** menu. The keyboard shortcut to use this function is *ctrl-X* (*command-X* on Mac OS X).
3. Press the **Paste** menu item in the **Edit** menu. The keyboard shortcut to use this function is *ctrl-V* (*command-V* on Mac OS X).

Organizing Content

ChemDoodle provides several tools for laying out content in the document.

Aligning

To align content relative to each other, perform the following steps:

1. Select the content to be aligned.
2. Expand the **Align** submenu in the **Content** menu and press the **Left Edges**, **Horizontal Centers**, **Right Edges**, **Top Edges**, **Vertical Centers** or **Bottom Edges** menu items.

Aligning by Bond

To align an entire molecule by a given bond, perform the following steps:

1. Hover the bond to align the molecule by.

2. Press the *up*, *down*, *left* or *right* arrow keys to align the bond from its first to second constituent atom in the selected direction. This will rotate the entire molecule with the bond.

Centering

To center all content on the page, expand the **Center** submenu in the **Content** menu and press the **All on Page** menu item.

To center selected content on the page, perform the following steps:

1. Select the content to be centered.
2. Expand the **Center** submenu in the **Content** menu and press the **Selection on Page**, **Selection Horizontally** or **Selection Vertically** menu items.

Distributing

To distribute content across the document, perform the following steps:

1. Select the content to be distributed.
2. Expand the **Distribute** submenu in the **Content** menu and press the **Horizontally on Page** or **Vertically on Page** menu items.

To distribute content across the document using a buffer spacing that you provide, perform the following steps:

1. Select the content to be distributed.
2. Expand the **Distribute** submenu in the **Content** menu and press the **Horizontally by Buffer Space...** or **Vertically by Buffer Space...** menu items.
3. Input a buffer space value into the number field that appears.
4. Click the **Accept** button to perform the distribution.

Flipping

To flip content horizontally or vertically, perform the following steps:

1. Select the content to be flipped.
2. Expand the **Flip** submenu in the **Content** menu and press the **Horizontally** or **Vertically** menu items.

Flipping a Bond

You may wish to flip non-symmetrical bonds when you need it to face the other direction, such as when working with wedge bonds. There are a few quick ways to do so:

- Hover over the bond and press the *f* key to flip it.
- Hover the bond, right-click and select **Flip Bond Orientation**.
- Use the bond tool of that bond type and click on the bond after hovering it. ChemDoodle will detect the bond is being set to its current bond type and will instead flip the bond.

Placing in Grid

To place all content in a grid that covers the document, perform the following steps:

1. Select the **Grid All on Page...** submenu in the **Content** menu.
2. In the prompt that appears, select whether you want to specify the grid dimensions by **Columns** or by **Rows** by choosing the corresponding selection from the drop down menu.
3. Input the dimension of the grid in the number field. The other dimension will be automatically calculated based on the number of objects being placed in the grid.
4. Select the **Grid** button.

Stacking

Stacking will place all content on the page starting from the top-left of the document to the bottom-right, such that their visual bounds are separated by a small buffer and that all objects are within the page margins. To stack all content on the page, press the **Stack All on Page** menu item in the **Content** menu.

If content is ever placed outside of the page bounds, red strips will appear at the sides of the page that the content extends from. Click on the red strip to stack all of the content that extends from that side of the page back onto the page.

Framing Content

Content can be automatically framed with various different shapes. To frame objects, perform the following steps:

1. Select the objects to be framed using the selection tools.
2. Expand the **Add Frame>** submenu in the **Content** menu.
3. Select the type of frame to use.

The selected content will then be framed.

Editing Content

The selection area is context sensitive and you can click and drag on the various features of the selection to perform different actions.

Translating

To translate content, or move it on the page, perform the following steps:

1. Select the content to be translated.
2. Hover the mouse cursor over the selection so that an open hand cursor appears.
3. Press the mouse down so the mouse cursor turns into a closed hand cursor.
4. Drag the mouse to translate the content.
5. Release the mouse to finish the translation.

During the translation, the change in x position and change and y position will be displayed below the mouse cursor. You can disable this feedback in the **Preferences** window under the **General** tab.

Translating Horizontally or Vertically

If you hold the *shift* key down while translating will lock the content horizontally or vertically depending on where the mouse pointer is.

Duplicating Content

If you hold the *shift* and *alt* keys down while translating content, you will duplicate that content and it will be locked horizontally or vertically depending on where the mouse pointer is. To remove the lock, release the *shift* and *alt* keys.

Rotating

To rotate content, perform the following steps:

1. Select the content to be rotated.
2. Hover the mouse just outside the edge of the selection border so that the rotation cursor appears.
3. Press the mouse down and drag it to rotate the content.
4. Release the mouse to finish the rotation.

During the rotation, the rotation angle will be displayed below the mouse cursor. You can disable this feedback in the **Preferences** window under the **General** tab.

To more precisely rotate content, perform the following steps:

1. Select the content to be rotated.
2. Expand the **Rotate** submenu in the **Content** menu and press the **90° CW, 90° CCW** or **180°** menu items.

To more precisely rotate content by an arbitrary angle, perform the following steps:

1. Select the content to be rotated.
2. Expand the **Rotate** submenu in the **Content** menu and press the **Arbitrary...** menu item.
3. Enter a degree value in the number field that appears and select whether the rotation should be done clockwise or counterclockwise.
4. Press the **Rotate** button to perform the rotation to the settings you provided.

Moving the Rotation Anchor

Sometimes you may not want to rotate content around its center, as is done by default. For instance, you may desire to rotate structures around an atom. This can be achieved by moving the rotation anchor that is initially found in the center of the selection.

To move the rotation anchor, perform the following steps:

1. Move the mouse over the rotation anchor so that the anchor fills in with an amber color and the mouse cursor changes to a resize cursor.
2. Press the mouse down and drag the rotation anchor to the desired position.
3. Release the mouse to set the new rotation anchor position.

Now all rotations will proceed around the new rotation anchor position.

When moving the rotation anchor, it will automatically lock on to atoms within the selection as you get close to them, aiding you in setting the rotation anchor over atom positions.

Scaling

To scale content, perform the following steps:

1. Select the content to be scaled.
2. Hover the mouse over one of the anchor points in the selection so that the mouse resize cursor appears.
3. Press the mouse down and drag the anchor to scale the content.
4. Release the mouse to finish the scale action.

While scaling, the x scale factor and y scale factor will be displayed below the mouse cursor. You can disable this feedback in the **Preferences** window under the **General** tab.

To preserve the width-to-height ratio while scaling content along the diagonals, just hold down the *shift* key while performing the above steps.

To precisely scale content, perform the following steps:

1. Select the content to be scaled.
2. Press the **Scale...** menu item in the **Content** menu.
3. Select whether to scale the content by dimension or bond length and then specify the rest of the settings.
4. Press the **Scale** button to scale the content to the settings you provided.

Fonts
To change the fonts of atom labels and text based shapes, perform the following steps:

1. Select the atoms and shapes that you would like to change the fonts of.
2. Choose the font family, font size and font style in the **Files + Formatting** toolbar to change the fonts.

Drawing Aids

Drawing guides will help when precision is important. There are several categories of drawing guides, and each have their own benefit. Guides can be enabled and disabled in the **Drawing Aids>** submenu of the **View** menu.

Atom Aids
Two types of aids can be drawn for atoms:

- **Orthogonal** - Will show a horizontal and vertical line through the center of each atom to help with alignment.
- **Circular** - Will show a circle around each atom with radius equal to the current standard bond length to help with distances.

Bond Aids
A single type of aid can be drawn for bonds:

- **Parallel** - Will draw a line through each bond, parallel to its direction to help with extrapolation.

Ring Aids
Rings can be colored in with a different color corresponding to the size of the ring to help with perception.

Molecule Aids
Two types of aids can be drawn for molecules:

- **Bounds** - Will show a rectangle representing the bounds of each molecule to help with placement.
- **Orthogonal** - Will show a horizontal and vertical line through the center of each molecule to help with alignment.

Background Aids
Three types of aids can be drawn on the background:

- **Crosshair** - Will render a crosshair and grid to help with partitioning and aligning objects.
- **Grid** - Will render a grid at an interval that you specify to help with aligning objects.
- **Margins** - Will render the bounds for the margins.

Colors

There are two features in the **Files + Formatting** toolbar for changing the colors of content, the **Color** button and the **Quick Colors** button.

Color Button
The **Color Button** was specifically created in ChemDoodle to make it easy to quickly change the colors of groups of objects. There are eight colors defined the color button:

- Background
- Borders and Lines
- Bonds
- Fill
- Atom Labels
- Identifier Text
- Other Text
- Plots

You may change these colors by clicking the thin rainbow button placed directly to the right of the **Color Button**. All objects drawn after choosing colors will conform to those choices. To change the colors of a group of objects to the current selection of colors, just select them and click the **Color Button**.

The **Color Button** will change its display colors to reflect the current settings. A breakdown of the sections of the **Color Button** is shown in *Figure 5.2*.

Figure 5.2: Color Button Layout

If you wish for a certain fill to be empty and to not be colored, then in the color chooser, click the **Empty Color** button for the desired fills to not be painted.

Quick Colors Button

The **Color Button** is powerful but is certainly not a quick way to change colors. To quickly change colors, just use the **Quick Colors Button**.

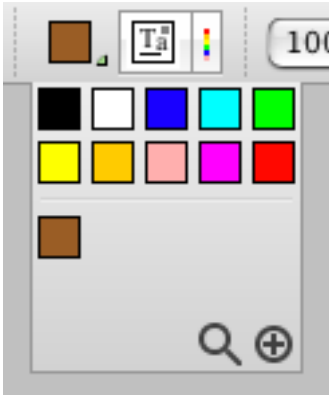
Just selected the content that you would like colors changed for, and press the quick colors button. All of the content will be changed to that color regardless of the content type.

If you click and hover (or drag) over the Quick Colors button, a palette will appear to select a new color. Drag the mouse pointer over one of the preset colors to select it and immediately change the selected content to that color.

You can also add custom colors to the last three rows of the Quick Colors palette. Just release your mouse over the circled plus icon  and release to show a color chooser. Choose the desired color and press the OK button to add it to the palette and change the currently selected content to that color.

The Quick Colors palette is shown in Figure 5.3.

Figure 5.3: The Quick Colors palette.



Color Detection

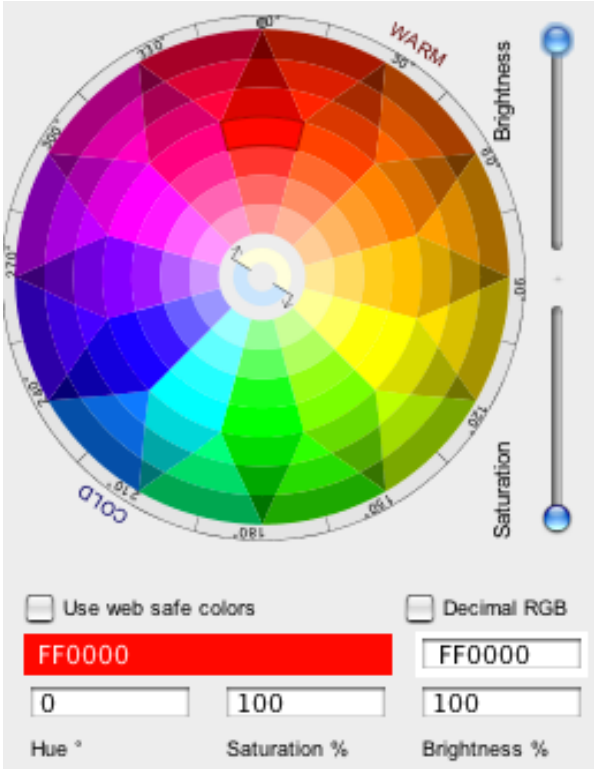
When working with content that uses non standard colors, you may wish to detect what those colors are. To do this, expand the **Quick Colors Button** and release the mouse over the **Detect Color** button  . Then hover over the color in the document you wish to detect and press the mouse down when that color is centered in the cursor. That color will be added to the **Quick Colors Button** for further use.

Color Chooser

The color chooser will be different on all platforms, with different templates to use to pick colors from. However, the ChemDoodle pinwheel color chooser will be present on all

platforms. The pinwheel color chooser is shown in *Figure 5.3*.

Figure 5.3: ChemDoodle's Pinwheel Color Chooser



The color selected can be seen in the preview bar at the bottom, with the hex value shown by default. You can also view the RGB value by enabling the *Decimal RGB* checkbox.

To select a color, just move the mouse pointer over the pinwheel until the color you would like to select is hovered, then click the mouse. You can also use the mouse wheel to scroll through colors.

If the pinwheel appears all black, you will need to increase the *Brightness* setting by moving the *Brightness* slider up. If the pinwheel appears all white, you will need to decrease the *Saturation* setting by moving the *Saturation* slider down.

Modifying the Z-order of Shapes

Occasionally, you may want to change how shapes are z-ordered with respect to each other and with respect to atoms and bonds. Shapes, by default, will always render behind atoms and bonds and will be z-ordered chronologically.

To modify the z-order of a shape, perform the following steps:

1. Hover the shape to change the z-order of.
2. Right-click on the shape.
3. Expand the **Arrange** submenu.
4. Select the **Send Forward**, **Send Backward**, **Send to Front** or **Send to Back** menu item depending on your preference.

To change if a shape is rendered in front of or behind atoms and bonds, perform the following steps:

1. Hover the shape to change the z-order of.
2. Right-click on the shape.
3. Expand the **Arrange** submenu.
4. Select the **Place in Front of Structures** or **Place in Back of Structures** menu item depending on your preference.

Grouping Content

Content in ChemDoodle can be grouped. Once grouped, you will no longer be able to edit the member objects individually. Any transformations performed on the group will affect all member objects.

Grouping can be nested, so groups can be grouped into further groups. Ungrouping is

not recursive, so ungrouping a group containing groups will leave those contained groups intact.

Grouping

To group content, perform the following steps:

1. Select the content to be grouped.
2. Press the **Group** menu item in the **Content** menu.

Ungrouping

To ungroup content, perform the following steps:

1. Select the groups to be ungrouped.
2. Press the **Ungroup** menu item in the **Content** menu.

Removing Content

Removing individual Objects

Individual objects can be removed by using the eraser tool to hover the object and then by clicking to remove it. Additionally, at any time, when an object is hovered, press the *backspace* or *delete* key.

Removing Groups of Objects

Groups of objects can be removed in a number of ways. You can do the following:

- Use a selection tool to select the content to be removed. Then press the *backspace* or *delete* key.
- First select the content to be removed. Then use the eraser tool to click on the **Doodle Board**.
- Select the eraser tool, then press the mouse down and drag over all of the content to be removed. Selected content will be highlighted. Then release the mouse to remove all highlighted objects. Dragging over content that has already been highlighted will de-highlight it.

Chapter 6: Advanced Chemistry and Cheminformatics

Overview

ChemDoodle is powered by an advanced cheminformatics engine to perform several functions for creating graphics, such as ring perception and structure depiction. This engine allows for some very powerful functions to help you create your chemical graphics and to analyze the structures you draw.

This section introduces the new user to advanced structure functionality within ChemDoodle. It introduces the following topics:

- The cheminformatics algorithms implemented in ChemDoodle.
- How to use these functions to perform various advanced tasks.
- How to edit your structures in a more advanced way than described in **Chapter 3**.
- How to take full advantage of the functions provided in ChemDoodle.

Aromaticity

Aromaticity is detected based on the Hückel model. All rings are assumed to be planar. Any appropriately hybridized heteroatoms can be constituents in an aromatic ring.

Toggling between Kekulé and Circle Representations for Aromatics

To toggle between viewing aromatics in Kekulé form (with double bond lines) or with circles, perform the following steps.

1. Open the **Preferences** window.
2. Select the **Rings** tab under the **Visuals** tab.
3. Check or uncheck the *Use Circles* visual specification under the **Aromatics** section based on your preference.

Forcing Aromaticity

In rare cases, ChemDoodle may determine a ring to have no aromatic character when it should be aromatic for some purpose. To force a ring to be recognized as aromatic, change all of the ring bonds to *Resonance* bonds.

Calculating Covalent Bonds

Some chemical input read into ChemDoodle may not include bond topology such as *PDB* and *XYZ* files as well as some output from modeling programs. Instead of having to define the bonds by hand, ChemDoodle contains tools for deducing covalent bonds based on published covalent radii.

To deduce covalent bonds, perform the following steps:

1. Select the atoms that you would like covalent bonds deduced between.
2. Select the **Calculate Covalent Bonds** menu item from the **Structure** menu.

Covalent radii are a best fit from a large number of experimental covalent radii. In some cases, a bond distance from a file may be larger than the distance calculated by adding the corresponding element covalent

radii together and the bond will not be found. To address this, ChemDoodle multiplies all covalent radii by a scalar when deducing bonds. By increasing this multiplier, ChemDoodle will discover bonds at longer distances. You can change the radius multiplier in the **Preferences** window under the **Functions** tab.

Carbon Labels

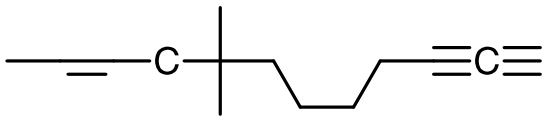
By default, ChemDoodle draws skeleton figures where carbon labels are suppressed. Regardless, it may be necessary to show the carbon label for various reasons and this can be done easily for each atom or globally for all atoms. To affect this globally, change the following visual specification for the document style sheet in the **Preferences** window. For each atom, change the following visual specification in the atom's **Format** window.

The atom *Display Carbon Label* visual specification has 4 options for displaying carbon labels:

- **Always** - always display the "C" for the carbon label.
- **On Lone and Hidden** - only display carbon labels on lone and hidden carbons.
- **On Hidden** - only display carbon labels on hidden carbons. (default)
- **Never** - never display "C" labels.

The default is **On Hidden** and only carbon atoms that are "hidden" between two bonds of the same bond order will have their label displayed as shown in *Figure 6.1*.

Figure 6.1: Hidden carbon labels are shown.



Lone carbons are disconnected atoms and have no bonds attached.

In addition to manually changing this visual specification, there is a quick method provided to show/hide carbon labels. To quickly show individual carbon labels, perform the following steps:

1. Hover the carbon atom with label to be shown.
2. Right-click on the atom and select the **Show Carbon Label** menu item.

To hide the carbon label. Perform the same steps, but instead select the **Hide Carbon Label** menu item.

Terminal Carbon Labels

By default, all terminal carbon atoms will display labels. In some cases, these labels may clutter a diagram. To hide terminal carbon labels, uncheck the **Show Terminal Labels** visual specification in the **Carbons** section in the **Atoms** section in the **Visuals** section of the **Preferences** window.

Chemical Suppliers

Chemical suppliers for the structures you draw can be listed by performing the following steps:

1. Draw the structure you would like to search for.
2. Select the structure with a selection tool.
3. In the **Structure** menu, expand the **Chemical Suppliers** menu item.
4. Select the **Substructure Match** or **Exact Match** menu item depending on whether

you want to search for a substructure or exact match for the selected structure.

5. The ChemExper database will appear in your default browser with a listing of matches. Select the match to view the chemical suppliers.

The *ChemExper* database provides the supplier information and you must abide by their terms of use and any copyrights or disclaimers presented when using their service.

Chemical Warnings

ChemDoodle will check your structures for you and flag any questionable objects.

Warning Types

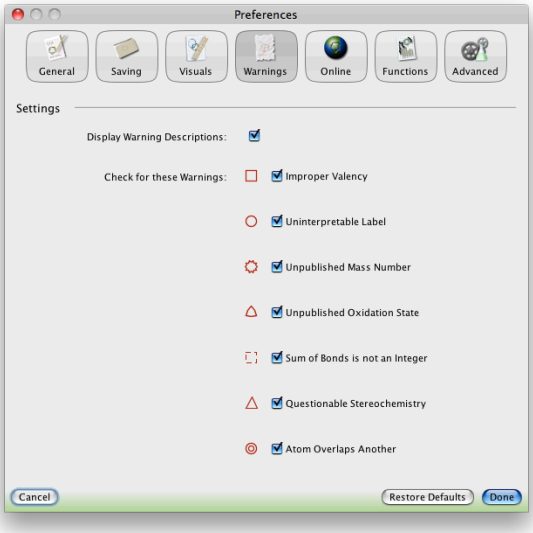
The following warnings are currently implemented:

- **Improper Valency** - It is unlikely that this element can have the current coordination number. Or the atom label is an abbreviation and the valency is overextended.
- **Uninterpretable Label** - ChemDoodle does not understand or interpret the text present in the atom label as chemically relevant.
- **Unpublished Mass Number** - This mass number is not found in ChemDoodle's database of published isotopes for the element.
- **Unpublished Oxidation State** - The oxidation state of this atom is not found in ChemDoodle's database of published oxidation states for the element.
- **Sum of Bonds is not an Integer** - The coordination number of this atom is not a whole number.
- **Questionable Stereochemistry** - The stereochemistry of this atom is questionable.
- **Atom Overlaps Another** - This pair of atoms has the same coordinates and will be perceived as a single atom in graphical output.

Disabling Warnings Globally

These warnings can be disabled individually in the **Preferences** window under the **Warnings** tab as shown in *Figure 6.2*. This tab also contains an option to disable the display of chemical warning explanations at the top-left of the document the warnings are present in.

Figure 6.2: Chemical Warnings



Disabling Warnings for a Single Atom

To disable warnings on a single atom, perform the following steps:

1. Hover the atom with the warning shown to be disabled.
2. Right-click on the atom and select the **Ignore Warnings** menu item.

To reenable warnings for an atom that is ignoring warnings, just right-click on it after hovering it and select the **Check for Warnings** menu item.

Hiding Warnings from Rendering

Chemical warnings will never appear in any image output or printouts.

If the warnings clutter the document while drawing, they can be easily suppressed by selecting the **Hide Warnings** menu item in the **View** menu.

Cleaning Structures

ChemDoodle can generate 2D and 3D coordinates for structures.

Optimizing Structures in 2D

If your structures do not have acceptable or aesthetic coordinates, ChemDoodle can clean them. To clean your structures, perform the following steps:

1. Select the structures to be cleaned.
2. Expand the **Clean** submenu in the **Structure** menu and select the **2D Optimization** menu item.

ChemDoodle employs the published CCG algorithm for cleaning structures. This method is a statistical approach. Therefore, repeated applications of the function may produce different results. If you are not happy with the first result of the function, try it again, something better may be generated.

Distance Geometry Embedding

Distance geometry embedding sets 3D coordinates for a structure based on a regression of its bond distance matrix. This function works best on highly embedded structures such as fullerenes and carbon nanotubes. To use this method, perform the following steps:

1. Select the structures to generate 3D coordinates for by distance geometry embedding.
2. Expand the **Clean** submenu in the **Structure** menu and select the **Distance Geometry Embedding** menu item.

Preserving Stereochemistry

By default, structure cleaning will preserve stereochemical configurations. To disable this, deselect **Clean Retains Stereochemistry** in the **Functions** panel in **Preferences**.

Descriptors

ChemDoodle calculates a large number of molecular descriptors. The descriptors are currently categorized into 4 types: constitutional, topological, physicochemical and ADME.

Constitutional

Constitutional descriptors are based on the makeup of the molecule, such as atom counts and molecular formula. The following constitutional descriptors are provided:

- **Atom Count** - The number of atoms in a molecule.
- **Bond Count** - The number of bonds in a molecule.
- **Degree of Unsaturation** - The sum of all bond orders substracting 1 for each, plus the number of rings.
- **Element Counts** - The number of each element that is present in a molecule.
- **Euler Facet Ring Count** - The count of all Euler facets in a molecule. This is defined as all of the sides of the 3D shape that is created by expanding the 2D structure on a 3D sphere.

- **Exhaustive Ring Count** - The total number of graph cycles present in the molecule.
- **Frèrejacque Number** - The fundamental ring count. Also known as the cyclomatic number or the SSSR count.
- **Frèrejacque Number** - The fundamental ring count. Also known as the cyclomatic number or the SSSR count.
- **Hydrogen Bond Acceptor Count** - Counts the number of atoms with lone pairs capable of hydrogen bonding.
- **Hydrogen Bond Donor Count** - Counts all Nitrogens, Oxygens and Fluorines that have Hydrogens attached.
- **Rotatable Bond Count** - Counts all saturated bonds. Exceptions are *Single* bonds connected to Hydrogens or terminal atoms, *Single* bonds of amides, thioamides, sulphonamides and those connecting two hindered aromatic rings (having at least three ortho substituents).
- **Total Electron Count** - Counts all electrons in a molecule. Takes into account charges.
- **Lightest Isotopic Mass** - Calculates the lightest isotopic mass by summing the lightest isotope for each atom given its element.
- **McGowan Characteristic Volume** - Calculates the vdW volume with McGowan's method.
- **Molecular Mass** - Calculates the molecular mass from atomic masses based on the IUPAC technical reports.
- **Monoisotopic Mass** - Calculates the monoisotopic mass from isotopic masses based on the IUPAC technical reports.
- **Volume as a Sum of Atomic and Bond Contributions** - Calculates the VABC vdW volume.
- **Empirical Formula** - Generates the empirical formula for the molecule. The empirical formula is just the molecular formula, where all element multiplicities have been divided by the greatest common denominator.
- **Molecular Formula** - Generates the molecular formula for the molecule in the form of CxHy... where ... denotes all other elements and their counts in alphabetical order. This is based on the Hill system, so if no carbon atoms are present, the hydrogen count will be in alphabetical order with the rest of the elements.

Topological

Constitutional descriptors are solely based on the connectivity between atoms in a molecule, such as a bond distance matrix. The following topological descriptors are provided:

- **Centric Index** - Calculates the Centric index for the molecule (Bonchev *et al.*).
- **Diameter** - Calculates the longest topological distance in a molecule.
- **Hosoya Index** - Calculates the Hosoya index for the molecule.
- **Molecular Topological Index** - Calculates the Molecular Topological index for the molecule (Schultz *et al.*).
- **Platt Index** - Calculates the Platt index for the molecule.
- **Ring Complexity** - Calculates the Ring Complexity for the molecule.
- **Szeged Index** - Calculates the Szeged index for the molecule.

- **Wiener Index** - Calculates the Wiener index for the molecule.
- **Zagreb Indices** - First and second order calculations are supported. (Z_1, Z_2)
- **Balaban Index** - Calculates the Balaban index for the molecule.
- **Bertz Complexity Index** - Calculates the Bertz Complexity index for the molecule.
- **Branching Index** - Calculates the Branching index for the molecule. The Branching index is equivalent to ${}^1\chi$.
- **Chi Molecular Connectivity Indices** - Indices from zeroth to third order are supported. Both simple and valence models are calculated. (${}^0\chi$, ${}^1\chi$, ${}^2\chi$, ${}^3\chi$, ${}^0\chi_v$, ${}^1\chi_v$, ${}^2\chi_v$, ${}^3\chi_v$)
- **Fraction Molecular Framework** - Calculates the Fraction Molecular Framework (fMF) ratio for the molecule.
- **Harary Index** - Calculates the Harary index for the molecule.
- **Kappa Shape Indices** - Indices from the first to third order are supported. Both simple and alpha models are calculated. (${}^1\kappa$, ${}^2\kappa$, ${}^3\kappa$, ${}^1\kappa_\alpha$, ${}^2\kappa_\alpha$, ${}^3\kappa_\alpha$)
- **Superpendentic Index** - Calculates the Superpendentic index for the molecule.
- **Adjacency Matrix** - Generates a matrix M of size AxA, where A is the number of atoms in the molecule. $M(A_i, A_j)$ equals 1 if there is a bond connecting atoms i and j, and equals 0 otherwise.
- **Bond Distance Matrix** - Generates a matrix M of size AxA, where A is the number of atoms in the molecule. $M(A_i, A_j)$ equals the the number of electrons shared between atoms i and j.
- **Bond Electron Matrix** - Generates a matrix M of size AxA, where A is the number of atoms in the molecule. $M(A_i, A_j)$ equals the shortest bond distance between atoms i and j.
- **Detour Matrix** - Generates a matrix M of size BxA, where B is the number of bonds in the molecule and A is the number of atoms in the molecule. $M(B_i, A_j)$ equals 1 if bond i contains atom j, and 0 otherwise.
- **Incidence Matrix** - Generates a matrix M of size AxA, where A is the number of atoms in the molecule. $M(A_i, A_j)$ equals the longest bond distance between atoms i and j.
- **Laplacian Matrix** - Generates a matrix M of size AxA, where A is the number of atoms in the molecule. $M(A_i, A_j)$ equals 1 if there is a bond connecting atoms i and j, and equals 0 otherwise. M(i,i) equals the number of bonds connected to atom A_i.

Physicochemical

Constitutional descriptors describe the physical or chemical properties of a molecule. These are estimations of their real physical values. The following physicochemical descriptors are provided:

- **Average Molecular Polarizability** - Estimates the average molecular polarizability. Both the average hybrid components (Miller) and average hybrid polarizabilities (Kang) methods are implemented.
- **Critical Pressure** - Estimates the critical pressure (P_c) of a substance based on Joback's method.
- **Critical Temperature** - Estimates the critical temperature (T_c) of a substance based on Joback's method.

- **Critical Volume** - Estimates the critical volume (V_c) of a substance based on Joback's method.
- **Enthalpy of Formation** - Estimates the enthalpy of formation ($\Delta H^0_{f,298}$) of a substance (ideal gas at 298K) based on Joback's method.
- **Enthalpy of Fusion** - Estimates the enthalpy of fusion (ΔH_f) of a substance based on Joback's method.
- **Enthalpy of Vaporization** - Estimates the enthalpy of vaporization (ΔH_{vb}) of a substance (at T_b) based on Joback's method.
- **Gibbs Energy of Formation** - Estimates Gibbs energy of formation ($\Delta G^0_{f,298}$) of a substance (ideal gas, unit fugacity, at 298K) based on Joback's method.
- **Heat Capacity** - Estimates the heat capacity(C^0_p) of a substance (ideal gas) based on Joback's method.
- **Lipophilicity, logP** - Estimates the octanol/water partition coefficient (logP) of a substance. The NC+NHET, AlogP98, and XlogP v2.0 (Wang) algorithms are implemented.
- **Liquid Viscosity** - Estimates the liquid viscosity (η_L) of a substance (at 298K) based on Joback's method.
- **Molar Refractivity** - Estimates the molar refractivity of a substance. Both the CMR3 and AMR algorithm are implemented.
- **Normal Boiling Point** - Estimates the normal boiling point (T_b) of a substance based on Joback's method.
- **Normal Freezing Point** - Estimates the normal freezing point (T_f) of a substance based on Joback's method.
- **Topological Polar Surface Area** - Estimates the topological polar surface area (TPSA) of a molecule with the algorithm developed by Ertl *et al*.

ADME

Descriptors that rank bioactivity of drugs (ADME stands for absorption, distribution, metabolism, and excretion):

- **Bioavailability Score** - Calculates the bioavailability score (Martin).
- **Egan Violations Count** - Calculates the number of violations to Egan's rules.
- **Lipinski's Rule of 5 Violations Count** - Counts the number of violations to Lipinski's rule of 5.
- **Veber Violations Count** - Calculates the number of violations to Veber's rules.

Flattening Atomic Coordinates

In cases where imported chemical data contains 3D coordinates, you can set all the z-coordinates to 0 by selecting that content and choosing the **Flatten** menu item in the **Content** menu.

Fragmentation

ChemDoodle contains several functions for fragmenting molecules with various results. The fragmentation functions can be found in the **Content** toolbar 

.

There are three fragmentation functions:

- **Molecular Weight** - 

The molecules will be fragmented and each fragment will have a molecular weight assigned.
- **Synthesis** -  The molecules will be fragmented and each fragment will be set as

a reactant in a synthetic reaction leading to the original molecules.

- **Retrosynthesis -**  The molecules will be fragmented and each fragment will be set as a product in the retrosynthetic reaction resulting in the original molecules.

To fragment a molecule or group of molecules, perform the following steps:

1. Select the desired fragmentation function in the **Content** toolbar.
2. Press the mouse down and drag over all the bonds to be removed, defining how the molecule is fragmented.
3. Release the mouse to complete the function.

Formal Charges

While you can place charges on atoms manually, ChemDoodle can also guess the formal charges for a structure. To have ChemDoodle guess formal charges for a structure, perform the following steps:

1. Select the atoms for which formal charges are to be guessed.
2. Choose the **Place Formal Charges** menu item in the **Structure** menu.

Glassware Clipart

Figures for glassware setups can be created by using the glassware clipart library within ChemDoodle.

To build glassware setups, perform the following steps:

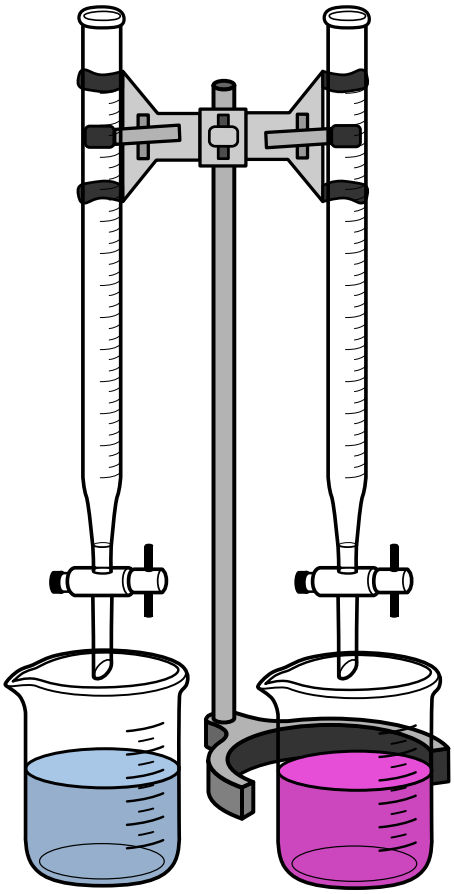
1. Click on the **Laboratory Glassware** button in the **Shapes** toolbar.
2. In the window that appears, select a glassware piece that you would like to place into your figure.
3. Press the mouse down on the current document and drag to place it where you prefer the piece to be placed. Hold down the *shift* key to flip the template horizontally while placing.
4. Release the mouse to set the glassware piece.
5. Repeat steps 2-4 until your figure is complete.

It may prove necessary to be conscious of the order in which you place the glassware pieces in the figure, in order to show some piece over another.

Keep in mind that each template is a complete image, and it is not possible to show one piece in between the front and back of another piece. However, you may export your figure to be post-edited in vector editing software (such as Adobe Illustrator) to achieve this effect.

All glassware clipart is governed by the same visual specifications that other shapes are. So you can change the stroke thickness and the colors of the various components in the clipart as shown in *Figure 6.3*.

Figure 6.3: A glassware setup with altered colors.



Flipping Glassware

To flip the clipart graphics, just hold down the *shift* key while placing them. The preview will then show you the flipped graphic.

You can also manually edit whether a clipart is flipped or not by right-clicking on it with nothing selected, selecting the **Format Clipart...** menu item and then changing the *Flip* on/off choice in the Clipart section.

Tubing

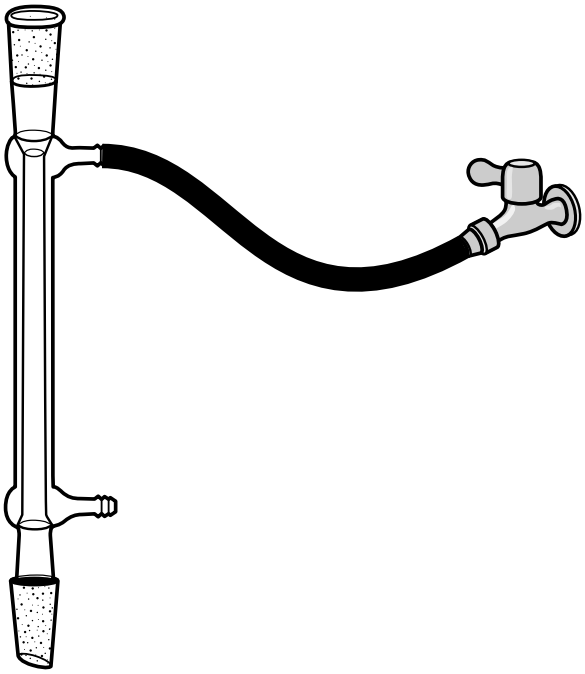
You may wish to connect pieces of glassware via tubing. A good technique for doing this is by using the **Bezier Curve** tool to draw the path of the tubing, and then increasing the stroke width of the path to the desired thickness.

One method for doing so is as follows:

1. Select the **Bezier Curve** tool in the **Shapes** toolbar.
2. Press the mouse down in the middle of the outlet in the glassware figure where the first tubing connection will be made.
3. Drag the mouse out in the direction that the first outlet faces. The longer you drag out the control point, the longer the curve will be straight at that point.
4. Press the mouse down in the middle of the outlet in the glassware figure where the second tubing connection will be made.
5. Drag the mouse out in the direction that the second outlet faces. The longer you drag out the control point, the longer the curve will be straight at that point.
6. Edit the bezier curve if necessary, or press the *escape* key to finish drawing the curve.
7. Hover the curve using a selection tool and right-click, selecting the **Format Bezier Curve...** menu item.
8. In the **Strokes** section of the settings window that appears, change the **Thickness** setting to 10 pixels.
9. Select the **Done** button to close the settings window.

Your completed figure will then contain a nice smooth curve connecting the outlets that represents tubing as shown in *Figure 6.4*.

Figure 6.4: Glassware figure containing tubing



Graph Reduction

To reduce molecule graphs, perform the following steps:

1. Select the structure with the graphs you would like to be reduced.
2. Expand the **Graph Reduction** submenu in the **Structure** menu and select the preferred reduction method.

Reduce 0° (Lone)
Will remove all selected atoms that have no bonds attached.

Reduce 1° (Terminals)
Will remove all selected atoms that have only 1 bond attached to them. This process will stop after the first iteration.

Repeatedly Reduce 1°
Will remove all selected atoms that have only 1 bond attached to them. This process will continue until it has pruned all terminal chains from the selection.

Reduce 1° + 0°
Will remove all selected lone and terminal atoms.

Reduce 2° (Chains)
Will remove all chains from a molecule, leaving single bonds connecting any remaining 3° atoms.

Reduce 2° + 1° + 0°
Will remove all lone, terminal and chain atoms, leaving a simplified core that represents the embedded ring structure of a graph.

Hydrogens

Hydrogens do not need to be drawn on structures as they are implicitly declared. At any time, Hydrogens can be added to a structure as text in atom labels or as atoms with bonds attached.

Implicit Hydrogen Rendering
By default, implicit hydrogens are automatically rendered on any element labels that are visible.

To disable the auto-rendering of implicit hydrogens, uncheck the **Show Implicit Hydrogens** visual specification in the **Hydrogens** section of the **Atom** section of the **Visuals** tab in the **Preferences** window.

You can also disable the auto-rendering of implicit hydrogens for a specific atom by performing the following steps:

1. Hover the atom with implicit hydrogens to remove.
2. Right-click on the atom.
3. Select the **Hide Implicit Hydrogens** menu item.

This will stop the auto-rendering of implicit hydrogens on that atom. To restore the

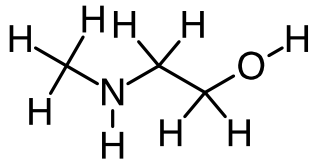
implicit hydrogen auto-rendering, just follow the same steps as above, but choose the **Show Implicit Hydrogens** menu item.

Adding Hydrogens as Atoms

To add hydrogens to a structure as atoms as shown in *Figure 6.5*, perform the following steps:

1. Select the structure to add hydrogens to.
2. Expand the **Add/Remove Hydrogens** submenu in the **Structure** menu and select the **From Selection** menu item.

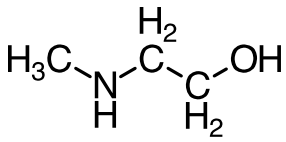
Figure 6.5: Hydrogens added as atoms



Adding Hydrogens as Text

To add Hydrogens as text into atom labels as shown in *Figure 6.6*, change the **Add as** setting in the **Hydrogens** section in the **Preferences** window, under the **Visuals** tab, under the **Atoms** tab to *Text*. Now when using the **Add/Remove Hydrogens** functions, hydrogens will be explicitly added as text.

Figure 6.6: Hydrogens added as text



Defining when Hydrogens are Added to Carbons

You can modify how hydrogens are added to carbon atoms: whether they are always added, only added to unsaturated carbons or never added to carbons. These options are presented in the **Preferences** window, under the **Visuals** tab, under the **Atoms** tab in the **Carbons** section.

IUPAC Naming

Currently only generating a structure from an IUPAC name is supported.

Name to Structure

To parse an IUPAC name and generate a chemical structure, perform the following steps:

1. Select the **Parse IUPAC Name...** menu item from the **Structure** menu.
2. In the prompt that appears, input the IUPAC name and select the **Accept** button.

The generated structure will then be placed in the document.

Kekulé Structures

ChemDoodle contains a function for assigning *Double* bonds to a structure such that pi electron delocalization is maximized. Both frames of *Single* bonds and substructures consisting of only *Resonance* bonds can be affected.

Kekulizing a Single Bond Frame

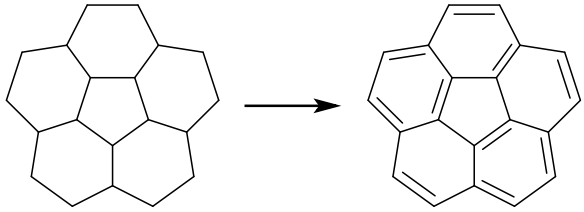
To easily draw Kekulé structures, you may begin by just drawing a *Single* bond frame. This way, ChemDoodle can optimally assign *Double* bonds to the structure. If there are other bond types present, ChemDoodle will not Kekulize the structure. However, the **Saturate** function in the **Structure** menu will change all bond types to *Single* bonds.

To Kekulize a structure of only *Single* bonds, perform the following steps:

1. Select the structure containing only *Single* bonds to be Kekulized.
2. In the **Structure** menu, select the **Kekulize** menu item.

For example, corannulene is generated from a Kekulization of a *Single* bond frame in *Figure 6.7*.

Figure 6.7: Kekulizing a Single bond frame to generate corannulene.



Kekulizing a Substructure of Resonance Bonds

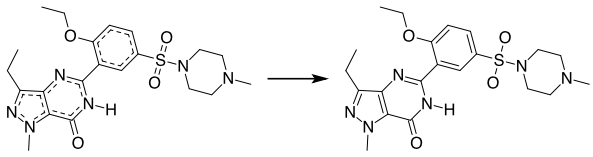
In some cases, structures may be read in with *Resonance* bonds. It may be necessary to present a Kekulé structure instead of the resonance model. When Kekulizing a structure with *Resonance* bonds, only those *Resonance* bonds will be affected.

To Kekulize a substructure of *Resonance* bonds, perform the following steps:

1. Select the structure containing the substructure of *Resonance* bonds to be Kekulized.
2. In the **Structure** menu, select the **Kekulize** menu item.

For example, the aromatic rings in Viagra are Kekulized in *Figure 6.8*.

Figure 6.8: Kekulizing the aromatic rings in the resonance model for Viagra.



Delocalizing a Kekulé Structure

You can also perform the reverse reaction and delocalize a Kekulé structure. Do this by selecting the content to delocalize and select the **Delocalize** menu item in the **Structure** menu.

Label Expansion

Atom labels can be much more than just an element symbol. They may contain implicit hydrogens or chemical shorthand notations or abbreviations. ChemDoodle can expand these condensed labels to their all atom models.

Expanding Labels

To expand labels, perform the following steps:

1. Select the atoms with labels to be expanded using any of the selection tools.
2. Select the **Expand Labels** menu item in the **Structure** menu.

Implicit Hydrogens

Implicit hydrogens can be presented as text in an atom label. They may be added automatically, can be added manually using the **Atom Label** tool or globally using the **Add/Remove Hydrogens** function with the appropriate visual specifications set.

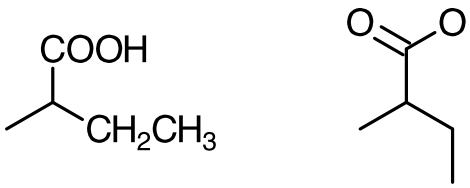
When expanded, implicit hydrogens are ignored. So the label *NH2* will become a *N* label when expanded.

Condensed Labels

Chains and functional groups may be denoted with a condensed label. For instance, a carboxy group may be denoted by a *COOH* atom label or an ethyl group may be denoted by *CH2CH3*.

When expanded, condensed labels will be replaced by the all atom model of the fragment as shown in *Figure 6.9*.

Figure 6.9: Left a molecule with condensed atom labels; right the corresponding expanded structure.



Several constructs are supported by the condensed interpreter in ChemDoodle:

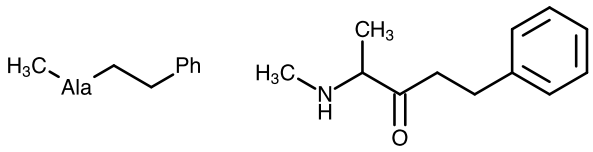
1. **Linear Chains** - Stringing elements together will place them in a chain, so *CCCC* or *CH2CH2CH2CH3* denotes a n-butyl group.
2. **Multiple Attachments** - Using parenthesis will denote multiple attachments, so the label *C(CH3)3* will denote a t-butyl group.
3. **Single and Double Bonds** - If no bonds are placed between elements, then *Single* bonds are used to connect them. The **-** (minus) character will also specify a *Single* bond connection and the = (equals) character will specify a *Double* bond connection. Therefore, *CC* and C-C both specify an ethyl group while C=C will specify an vinyl group.

Abbreviations

In addition to condensed formulas, abbreviations can be used to define fragments in atom labels. For instance, the *Ph* abbreviation defines a phenyl group. All supported abbreviations are listed in the **Symbols** widget in the *Abbreviations* section.

When expanded, abbreviations will be replaced by the all atom model they define as shown in *Figure 6.10*.

Figure 6.10: Left a molecule with abbreviations; right the corresponding expanded structure.



ChemDoodle can only expand abbreviations that represent discrete molecules, monovalent or divalent fragments. ChemDoodle will attempt to interpret abbreviations properly based on their valency. For instance, the *CO2* abbreviation with a valency of 0 is a carbon dioxide molecule while that same label with a valency of 2 denotes a ester group.

Adding Custom Abbreviations

Custom abbreviations can be added by performing the following steps:

1. Select the **Add New...** menu item in the **Abbreviations** submenu of the **Structure** menu.
2. Type the abbreviation label to be used in atom labels in the *Abbreviation Label* text field.
3. Type the full name of the abbreviation in the *Full Description/Name* text field.
4. Provide the **SMILES** string for the full atom model of the abbreviation in the *SMILES for Abbreviation* text field. If the valency of the abbreviation is greater than 0, then the attachment atom is the first atom defined by the **SMILES** string. If the abbreviation is divalent, then the last atom defined in the **SMILES** string will be used as the second attachment atom.
5. Select the valency of the abbreviation using the *Valency* drop down selection.
6. Press the **Add** button to add the new abbreviation.

ChemDoodle will update to recognize the added abbreviation and when used, that

abbreviation will be expanded to the **SMILES** string defined.

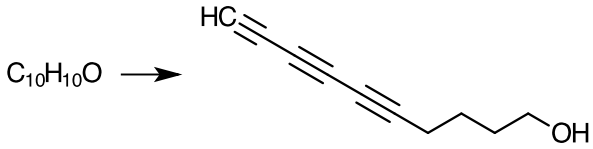
Mixing Condensed Notations and Abbreviations

Abbreviations and condensed notations can be combined. So the atom label *CPh3* will denote a triphenylmethyl group.

Molecular Formulas

Sometimes you may intend to input a molecular formula into an atom label, to calculate a molecular weight, for instance. If a molecular formula is input, then ChemDoodle will associate that atom with an isomer of the molecular formula, as best as it can as shown in *Figure 6.11*. So your calculations of weight will be correct, but other calculations will have to be met with scrutiny. For accurate calculations, make sure to draw a correct structure or structural formula.

Figure 6.11: ChemDoodle expands a molecular formula to an isomer all atom model as best as it can.

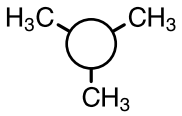


Newman Projections

To build graphics for Newman Projections, perform the following steps:

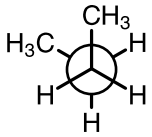
1. Draw a 2-methylpropane structure.
2. Hover the central atom and right-click.
3. Select the **Show Carbon Label** menu item.
4. Again, hover the central atom and right-click.
5. Select the **Format Atom...** menu item.
6. In the **Elements** section, select the **Use Circles** checkbox, make sure **Coloring** is set to *User Chosen* and **Radius Convention** is set to *Constant*, and then set the **Constant Radius** to the preferred size. You will now see a black circle appear over the central carbon.
7. Still in the **Atom Settings** window, under the **Colors** section, change the **Text Color** to white. You should now see a figure just like *Figure 6.12*.

Figure 6.12: A half completed Newman Projection.



8. Click on the **Done** button exit the **Atom Settings** window.
9. Draw a second 2-methylpropane structure.
10. Rotate the second structure to the desired torsion for the Newman Projection.
11. Using a lasso tool, move the second drawn structure over the first to complete the Newman Projection.

Figure 6.13: A finished Newman Projection.



You can then edit the terminal labels to display the structure desired as is shown in *Figure 6.13*. It may be convenient to save a copy of this structure as a file for later use.

Ring Perception

Rings are cycles of atoms and are important, because ChemDoodle uses them to define graphics such as which direction double

bonds face and calculations such as aromaticity detection. There are several published algorithms to define rings in structures producing different ring sets.

Supported Ring Sets

Currently, ChemDoodle can perceive the following sets:

- **Smallest Set of Smallest Rings** - The smallest set of smallest rings (SSSR) is the standard for defining ring sets in flat 2D structures.
- **Euler Facet Rings** - The Euler facet ring set is better than the SSSR at defining essential rings in 2D depictions of 3D structures. It is defined by all the rings that make up the faces of a 3D object when the 2D chemical graph is placed on a 3D sphere.
- **Hanser (All) Rings** - Every last graph cycle in selected structures.

Exploding Ring Sets

Ring sets can be exploded from the structure. In other words, they will be laid out around the structure to show the rings and where they are contained. To explode ring sets, perform the following steps:

1. Select the structures with the rings to be exploded.
2. Expand the **Rings** submenu in the **Structure** menu and select the **Explode Smallest Set of Smallest Rings**, **Explode Euler Facet Rings** or **Explode Hanser (All) Rings** menu items.

In very complex structures, the exploded ring diagram will be highly overlapped. Just stack the rings (in the **Content** menu) to view them all clearly.

Performance Considerations

If dealing with heavily embedded structures, such as zeolites or MOFs, the algorithms may become very cpu intensive. In these cases, you can disable deep searching for rings by selecting **Ring Search Cutoff** in the **Functions** panel in **Preferences**.

Sequence Tool

ChemDoodle provides a tool for generating sequence structures for common polymer types. The following polymer types are supported:

1. Three Letter Amino Acid Sequence

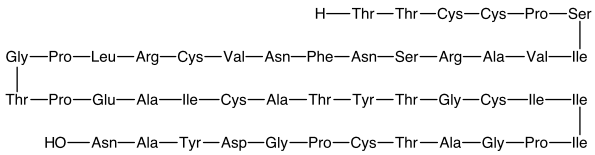
To generate sequences, use the **Sequence** tool 

in the **Shapes** toolbar. To draw a sequence, perform the following steps:

1. Click on the current document where you want the sequence to originate from. The endpoints of the sequence will appear. For amino acid sequences, a water molecule will appear.
2. A single atom will be surrounded by a blue circle; this is the appending atom. All changes to the sequence append directly to this atom. You can hover over other atoms and click to set a new appending atom.
3. Use the keyboard to type the one letter hotkeys for the residues in the sequence set. For instance, pressing the *A* key will append an *Alanine* residue, and pressing the *R* key will append an *Arginine* residue.

Sequences will automatically wrap to stay within the margins of the current document as shown in *Figure 6.14*.

Figure 6.14: A wrapped sequence for Crambin.



Use this tool to easily create macromolecular structures, and to quickly calculate properties such as weights and isotopic distributions.

Stereochemistry

The stereochemistry of chiral centers and double bonds can be determined by selecting the **Stereochemistry** functions located in the **Structure** menu. An **Attribute** object will be associated with the stereocenter to denote the stereochemical configuration. Several conventions can be used. Centers can be forced into a particular configuration in addition to determining the configurations based on the 2D layout.

Chiral Centers

Cahn-Ingold-Prelog (CIP) priority rules are used to resolve *rectus* (R) and *sinister* (S) enantiomers.

Forcing a configuration will interchange the protruding and recessed bonds, if necessary. If only single bonds are present, then the appropriate wedge bonds will be placed when a configuration is forced.

Double Bonds

CIP priority rules are used to resolve *entgegen* (E) or *zusammen* (Z) configurations around double bonds. The less systematic cis/trans conventions can also be used to define olefin enantiomers. The E/Z system will work for any double bond presented, while the cis/trans conventions will not return results in ambiguous cases.

Forcing **Double** bond stereochemistry will flip both substituents on one atom's side of the double bond through the double bond axis, if necessary.

Resolving Stereochemistry

To resolve stereochemistry for structures, perform the following steps:

1. Select the structures or parts of structures with stereocenters to be resolved with the selection tools.
2. Expand the **Stereochemistry>** submenu in the **Structure** menu.
3. Choose the appropriate Assign menu item to resolve stereocenters of that type.

You may also access these functions through the right-click menu.

Forcing Stereochemical Configurations

To force a stereochemical configuration on an atom or bond, perform the following steps:

1. Hover the atom or bond on which the configuration will be forced.
2. Right-click on the hovered object.
3. If that object is a potential stereocenter, then the **Stereochemistry>** submenu will be present. Expand this submenu.
4. Choose the appropriate Force menu item to force the configuration.

Structure Perspective

Even though ChemDoodle generates graphics for structures in two dimensions, the underlying structures are defined in three dimensions.

ChemDoodle will read in 3D coordinates from all chemical files and provides functions for rotating structures in 3D.

NOTE: While ChemDoodle has some 3D editing features, it is not a molecular modeler and is not the appropriate choice to build 3D coordinates for structures.

To rotate structures in 3D, perform the following steps:

1. Select the structures to be rotated in 3D using the selection tools.
2. Select the **Rotate in 3D** tool  in the **Content** toolbar.
3. Click the mouse down and drag to rotate the structure in 3D.
4. Release the mouse to finish the action.

By default, mouse movements while rotating structures in 3D will rotate the structure around the x and y axes based on horizontal and vertical movement respectively. You can also set the 3D rotations to be defined by a quaternion trackball in the **Preferences** window under the **General** tab.

Just like when rotating structures in 2D, there will also be a rotation anchor present during 3D rotation. Before selecting the 3D rotation tool, you can move the rotation anchor to a helpful position than the center, such as over atom positions. This makes it easy to rotate structures around atoms in 3D space.

Unique IDs

IDs can be automatically added as attributes for atoms and bonds. To do so, just select the appropriate choice in the **Unique IDs>** submenu in the **View** menu.

Zero Order/Ionic Bonds

In some cases, a molecule may contain ionic bonds or you may wish to associate two atoms that are not connected with a covalent bond.

ChemDoodle contains a zero/ionic bond order specifically for these cases. You can use this bond order by selecting the **Zero/Ionic** bond type button  in the **Bonds** toolbar. Any atoms connected with this bond type will be spatially linked and can be sent to cheminformatics algorithms such as molecular formula generation and structure cleaning.

Note: Most filetypes have no concept of a zero order bond, so saving these bond types and loading them into other applications may not produce desired results.

Chapter 7: Reactions

Overview

Reactions can be drawn in ChemDoodle using structures and arrow shapes. Almost any type of reaction or mechanism can be drawn. ChemDoodle also contains tools for explicitly defining reactions for various purposes.

This section introduces the new user to reactions within ChemDoodle. It covers the following topics:

- How to draw reactions.
- How to draw mechanisms.
- What types of arrows can be drawn.
- How to build and define reactions and reaction schemes.
- How to edit reactions.
- How to clean reactions.

Drawing Reaction Arrows

Reaction arrows are created from basic arrow shapes. Instructions for drawing arrow shapes are provided in *Chapter 4*.

Arrow Types

Many different types of arrows can be easily created using the **Arrows** toolbar described in *Chapter 2*. This section briefly goes over the different styles and presets.

Arrowhead Styles

Arrowhead styles can be set to both the start and end of the arrow. Several arrowhead styles (half-heads) can be flipped over the arrow axis. The following arrowhead styles are provided:

- **Full Indented -** ➤
- **Full -** ►
- **Unfilled Full Indented -** ➢
- **Unfilled Full -** ▻
- **Chevron -** ➢
- **Half Indented -** ➤
- **Half -** ►
- **Unfilled Half Indented -** ➤
- **Unfilled Half -** ►
- **Hook -** ➤

Changing Arrowhead Lengths and Angles

Both the arrowhead length and angle can be changed to match any look. To change the arrowhead length and angle, perform the following steps:

1. Hover the arrow containing the arrowhead to be edited.
2. Right-click on the arrow and select the **Format Line...** menu item.
3. Scroll down to the **Reaction** section in the **Format Line** window that appears.
4. In the **Arrow at Start** and **Arrow at End** sections, use the **Length** and **Angle** sliders to edit the arrowheads.

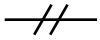
Quickly Toggle Arrowheads

Instead of opening the shape settings window, you can easily toggle default arrowheads on the ends of objects that support arrowheads by hovering the object and pressing the *left*

arrow (to toggle start) or *right arrow* (to toggle end) keys.

Connector Styles

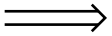
A connector is the line that connects the start and end arrows, if any. The following connector styles are provided:

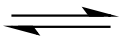
- **Solid -**
- **Dashed -**
- **Wavy -**
- **Doubled -**
- **No Go (cross) -** 
- **No Go (slash) -** 
- **Rearrangement -** 

Special Arrow Presets

Many different types of arrows can be drawn with **Arrows** toolbar. The following describes how these tools build common arrow types.

Reaction Arrow - A reaction arrow is the default style and is drawn with no start arrow, a **Full Indented** end arrow and a **Solid** connector.

Retrosynthetic Arrow -  A retrosynthetic arrow can be drawn with no start arrow, a **Chevron** end arrow and a **Doubled** connector. The default arrowhead angle and length is not aesthetic for this type of arrow, so use the retrosynthetic preset in the presets group button to quickly access this type.

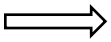
Equilibrium Arrow -  An equilibrium arrow can be drawn with a **Half Indented** start arrow, a **Half Indented** end arrow and a **Doubled** connector. The double line spacing can be edited in the arrow's visual specifications.

Resonance Arrow - A resonance arrow can be drawn with a **Full Indented** start arrow, a **Full Indented** end arrow and a **Solid** connector.

Electron Pair Shift -  A shift of an electron pair can be drawn with no start arrow, a **Full Indented** end arrow and a **Solid** connector. Then select the appropriate arc angle for the figure.

Single Electron Shift -  A shift of a single electron can be drawn with no start arrow, a **Half Indented** end arrow and a **Solid** connector. Then select the appropriate arc angle for the figure.

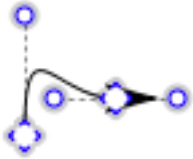
Photon - A photon can be drawn with a **Full** end arrow and a **Wavy** connector.

Bold -  A bold arrow can be drawn with no start arrow, an **Unfilled Full** end arrow and a **Doubled** connector. The default arrowhead angle and length is not aesthetic for this type of arrow, so use the retrosynthetic preset in the presets group button to quickly access this type.

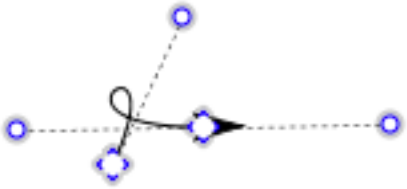
Bezier Arrow Ideas

In addition to straight and arced arrows, some pretty complex arrow shapes may be drawn with the bezier tools. The following are a few ideas. Just mimic the location of the control points to match them.

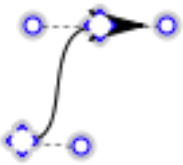
The Chute Arrow



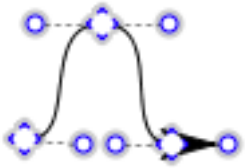
The Loop Arrow



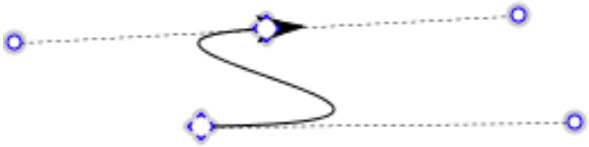
The Escalator Arrow



The Hump Arrow



The Zigzag Arrow



Building Reactions

Reaction figures can be drawn by placing structures next to arrow shapes to describe reaction schemes. This method will create a visual diagram for the reaction, but underlying semantics will not exists. In other words, there is no formal definition of the reaction reactants or products.

To address this, ChemDoodle provides a reaction building system to explicitly define reactions and reaction schemes.

Implicitly

To implicitly define a reaction, perform the following steps:

1. Draw the arrow you would like to represent the reaction arrow.
2. Draw any reactants and place them to the left of the arrow shape.
3. Draw and products and place them to the right of the arrow shape.
4. Select the arrow shape and all reactants and products using the selection tools.
5. Press the **Build Implied Reaction** menu item in the **Reaction** menu to define the reaction.

All structures with midpoints to the left of the arrow shape's midpoint will be defined as reactants in the reaction while all structures with midpoints to the right of the arrow shape's midpoint will be defined as products in the reaction.

Explicitly

To explicitly define a reaction, first select the arrow shape you would like to represent the reaction arrow using the selection tools. Then press the **Edit Reaction…** menu item in the **Reaction** menu open the **Edit Reaction** window for that selected arrow, as shown in *Figure 7.3*.

The **Edit Reaction** window is a drag and drop interface. All molecules in the current document are displayed in the bottom tray, while the left and right trays correspond to the

constituent reactants and products respectively. Just drag and drop molecules from the bottom tray into the other two to set up the reaction. Once a molecule has been placed, it will be grayed out in the bottom tray and no longer selectable. You can transfer a placed molecule between the products and reactants by dragging the molecule between the side trays. You can remove a molecule from the reaction completely by dragging and dropping it back in the bottom tray.

Press the **Done** button in the **Reaction Builder** window to set the reaction.

Adding Reaction Conditions

To add reaction conditions above and below the reaction arrow, first select the arrow shape you would like to add conditions to using the selection tools. Then press the **Edit Reaction…** menu item in the **Reaction** menu open the **Edit Reaction** window for that selected arrow, as shown in *Figure 7.3*.

The **Edit Reaction** window contains two text editors for adding text above and below the reaction arrow. Click on a text area and type to add text. You can format the text using the text formatting tools above the text areas.

Use the **Symbols** widget to input characters into the reaction condition text areas that are not present on the keyboard.

Press the **Done** button in the **Reaction Builder** window to set the reaction.

Adding Plus Symbols

After building a reaction, plus symbols will automatically be added at the midpoints between the constituent reactants and products. This feature can be turned off in the **Preferences** window under the **Visuals** tab under the **Reactions** tab as shown in *Figure 7.2*. Just uncheck the **Automatically Place Pluses** option.

If you want to add your own symbols, just use **Text Area** objects. **Text Area** objects are discussed in *Chapter 4*.

Dissolving Reactions

To dissolve a built reaction, just select the arrow the reaction is defined by with a selection tool, then select the **Dissolve Reactions** menu item in the **Reaction** menu.

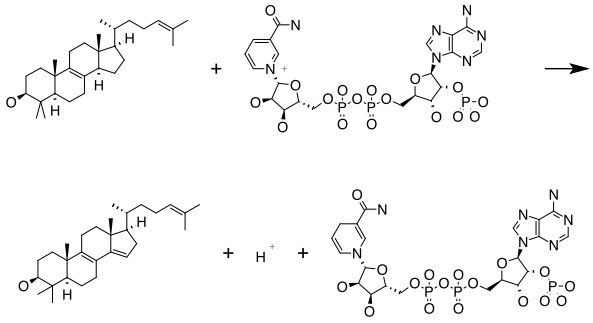
Cleaning Reactions

To clean a reaction, perform the following steps:

1. Define the reaction implicitly or explicitly using the instructions in the previous section.
2. Select the arrow shape of the reaction you would like to clean using the selection tools.
3. Press the **Clean** menu item in the **Reaction** menu to clean it.

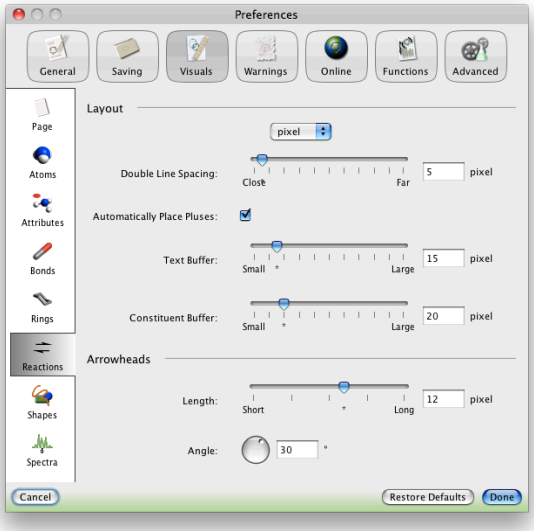
The reaction arrow will be horizontally leveled and resized to its text adhering to the *Text Buffer* visual specification. Then the reaction arrow and constituent molecules will be aligned according to their vertical centers and distributed horizontally with a buffer space. The entire reaction is then centered horizontally. If the reaction is too wide for the document, the reactants and arrow are then stacked above the products so that both groups are mutually centered as shown in *Figure 7.1*.

Figure 7.1: A wide reaction that has been stacked.



The settings for determining how reactions are laid out can be set in the Preferences window under the **Visuals** tab under the **Reactions** tab as shown in *Figure 7.2*.

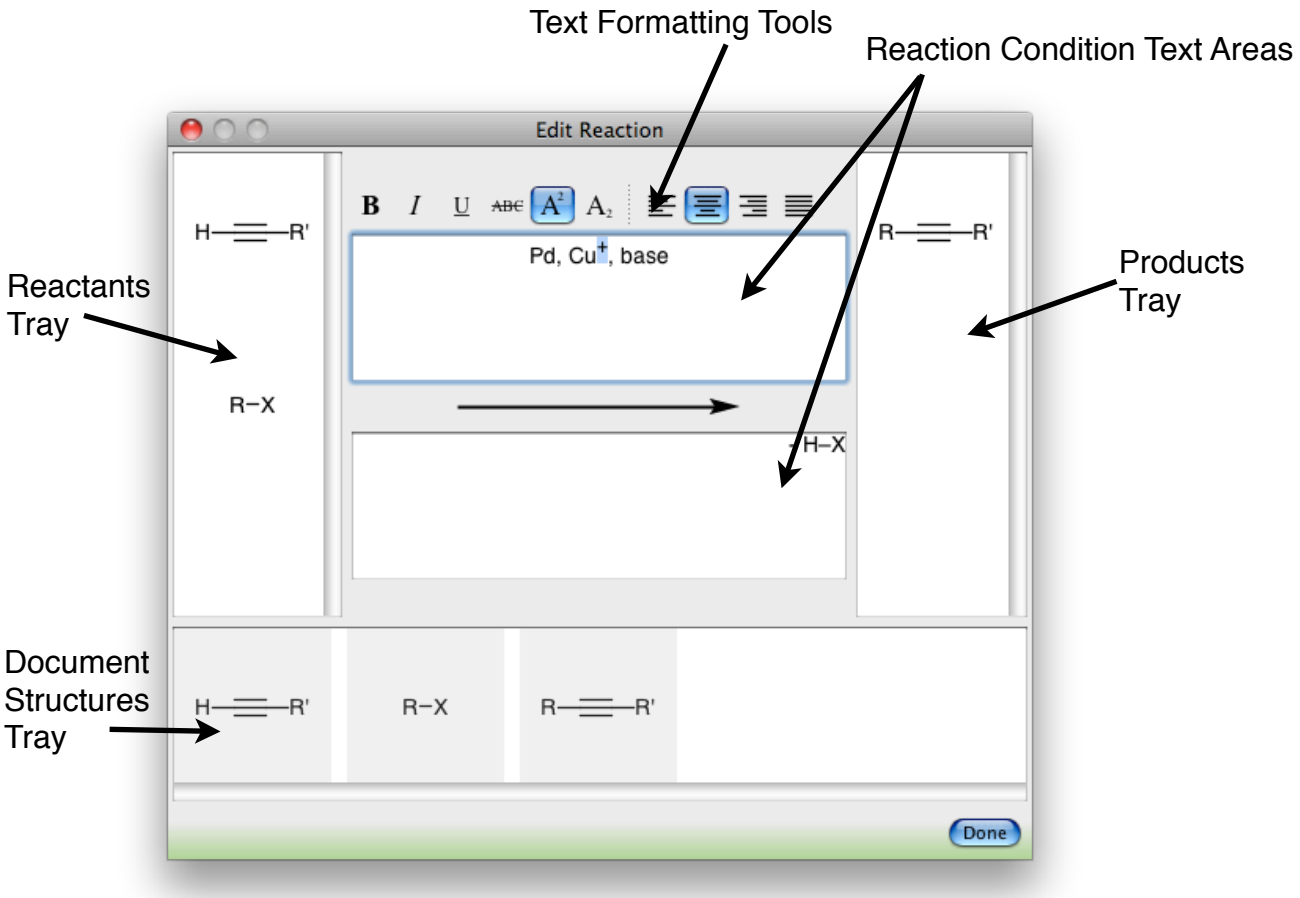
Figure 7.2: Reaction Visual Specifications



You can adjust the double line spacing for equilibrium arrows, decide whether or not pluses should be automatically drawn, set the text buffer for conditions text and the buffer between constituent reaction objects. You can also set the default settings for arrowheads.

ChemDoodle can clean multiple reactions at the same time, but currently can only properly clean discrete reactions. Cleaning complex reaction schemes with a given molecule defined in several different reactions may not produce desired results.

Figure 7.3: Edit Reaction Window



Chapter 8: Spectra

Overview

ChemDoodle understands several spectroscopy and spectrometry techniques. These spectra can be loaded and edited to create graphics.

This section introduces the new user to spectra within ChemDoodle. It covers the following topics:

- What types of spectra are supported.
- How to load spectra.
- How to save spectra.
- How to simulate spectra.
- How to edit spectra.

Inserting Spectra

Spectra can be read in from the *JCAMP-DX* format which is the standard defined by *IUPAC*. The currently supported *JCAMP* formats are for nuclear magnetic resonance spectroscopy (NMR), infrared spectroscopy (IR), mass spectrometry (MS) and chemical structures.

To insert spectra from *JCAMP* files, perform the following steps:

1. Select the **Open...** menu item in the **File** menu.
2. In the file chooser that appears, change the format filter on the bottom to *IUPAC JCAMP-DX*.
3. Find the *JCAMP* file on your computer and select it with the file chooser.
4. Press the **Open** button at the bottom-right of the file chooser to load the spectrum.

The spectrum will be loaded and displayed in the center of a new document.

Spectra Types

Both continuous and discontinuous spectra are supported. An example of NMR input is shown in Figure 8.1. An example of IR input is shown in Figure 8.2. An example of MS input is shown in figure 8.3.

Figure 8.1: An NMR spectrum loaded from a JCAMP file.

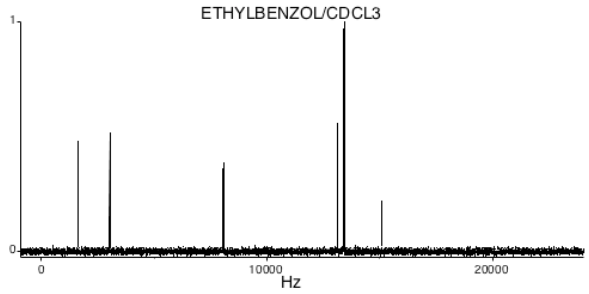


Figure 8.2: An IR spectrum loaded from a JCAMP file.

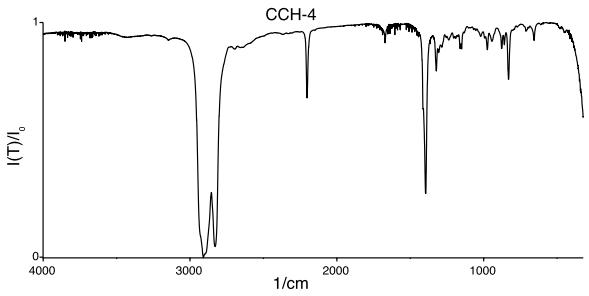
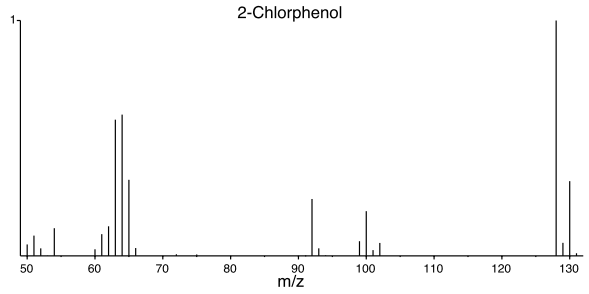


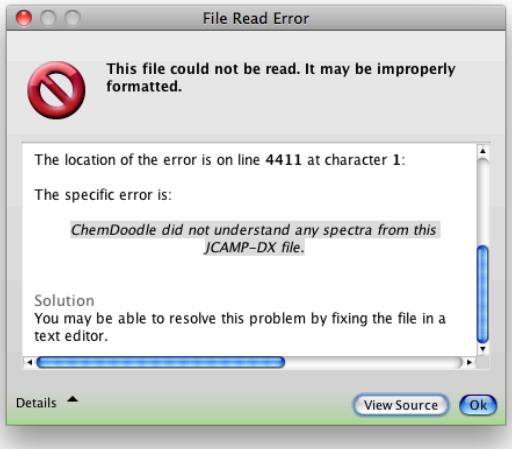
Figure 8.3: An MS spectrum loaded from a JCAMP file.



Uninterpretable Spectra

There are many different ways to represent *JCAMP* data. Therefore, ChemDoodle may not be able to understand a *JCAMP* file. If ChemDoodle was not able to interpret any spectra from the *JCAMP* file, you will see the message shown in *Figure 8.4*. Please send us the *JCAMP* file if you see this issue so that we may improve our compatibility with the format.

Figure 8.4: ChemDoodle could not understand the spectrum in the JCAMP file.



Saving Spectra

ChemDoodle can output spectra in the following formats:

1. ChemDoodle Documents {*.icl*, *.icxml*}
2. IUPAC JCAMP-DX {*.jdx*, *.dx*}

Be very careful when overwriting spectra to formats other than the ChemDoodle Document. ChemDoodle only reads and writes the information that is relevant to the display of its graphics, and other data will be lost. If saving 3rd party spectra files for any reason, always save them as a new file.

Simulating Spectra

ChemDoodle can simulate spectra for various techniques. Currently the following techniques are implemented:

- ^{1}H Nuclear Magnetic Resonance Spectroscopy
- ^{13}C Nuclear Magnetic Resonance Spectroscopy
- Mass Spectrum Parent Peak

To simulate spectra, perform the following steps:

- Select a the chemical structure you would like to simulate a spectrum for using the selection tools.
- In the **Spectrum** menu, hover over the **Generate** submenu to view available techniques.
- Click on the technique you would like to use.

The generated spectrum will then appear on the **Doodle Board**. Some very intense simulations may take a few seconds to complete.

Editing Spectra

Moving Spectra

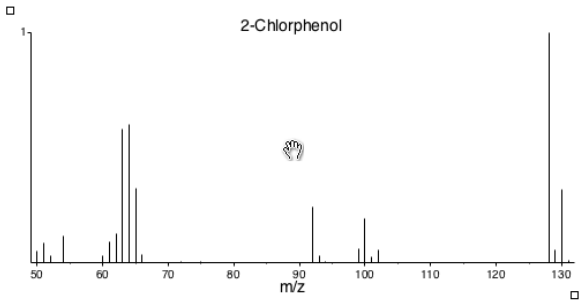
To move spectra, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the spectrum so an open hand mouse cursor appears and the two spectrum anchor points are drawn as shown in *Figure 8.5*.

2. Press the mouse down and drag to move the spectrum.

3. Release the mouse to finish the move action.

Figure 8.5: Hovering over the spectrum will display its anchor points.



Resizing Spectra

To resize spectra, use a selection tool, either the lasso or the rectangular marquee. Make sure that no content is currently selected by emptying the current selection. Perform the following steps:

1. Hover the mouse pointer over the spectrum so an open hand mouse cursor appears and the two spectrum anchor points are drawn as shown in *Figure 8.5*.

2. Move the mouse pointer over one of the two anchor points so that anchor point is filled in with an amber color.

3. Press the mouse down so the anchor point is filled with a blue color.

4. Drag the anchor point to resize the spectrum.

5. Release the mouse to finish the resize action.

Removing Spectra

Spectra can be removed in a number of ways. You can do the following:

- Use a selection tool to hover the mouse pointer over the spectrum so an open hand mouse cursor appears and the two spectrum anchor points are drawn as shown in *Figure 8.5*. Then press the *backspace* or *delete* key.

- Use the eraser tool to hover the mouse pointer over the spectrum so the two spectrum anchor points are drawn. Then click with the mouse.

- Select the spectrum using any of the selection tools. Then press the *delete* or *backspace* key.

Expanding the Perspective

Expanding the spectrum will fit the entire range and domain of the plot to the display rectangle. Perform the following steps.

1. Use the selection tools to select any number of spectra.

2. Click on the **Expand Perspective** menu item in the **Spectrum** menu.

All selected spectra will have their perspectives expanded.

Editing the Perspective

Editing the perspective will allow you to modify how the plot fits in the viewing rectangle and will also allow you to edit the axes and title. These functions are presented in the **Spectrum Edit** window as shown in *Figure 8.8*.

To change the plot domain, click and drag the sliders presented directly under the spectrum. The sliders display, from left to right, the minimum domain cutoff, the magnitude of the domain, and the maximum domain cutoff. You can also change the plot domain by clicking and dragging on the main spectrum panel. Click on the placement where you would like the domain to begin, then drag to where you would like the domain to end and

release the mouse. A dotted grey line will display while dragging to show you the new domain. Additionally, holding the *shift* key while dragging on the spectrum will translate the domain of the spectrum.

To change the range scale, click and drag the vertical slider directly to the right of the spectrum. You can also change the range scale by using the mouse scroll gesture on the main spectrum panel. Scroll up to increase the range scale and scroll down to decrease the range scale.

To expand the perspective, double-click on the main spectrum panel.

Changing the Title

To change the title of the spectrum, in the **Spectrum Edit** window shown in *Figure 8.8*, click on the **Title** text field located at the bottom-left and type in the desired title.

Changing the Axes

There are several options for editing the axes.

X-axis options are presented in the **X Axis** section of the **Spectrum Edit** window shown in *Figure 8.8*. You can choose to show or hide it by clicking the **Show** check box. You can choose whether to flip the domain or not by clicking the **Flip** check box. You can adjust the increments for the major and minor tick spacings using the **Major Tick Spacing** and **Minor Tick Spacing** drop down selections. The values in the drop down selections are exponents for base 10. You can change the title of the X-axis by clicking on the **Unit** text field and typing the desired title.

Y-axis options are presented in the **Y Axis** section of the **Spectrum Edit** window shown in *Figure 8.8*. You can choose to show or hide it by clicking the **Show** check box. The **Baseline Bump** check box will positively offset the plot by a small value. You can adjust the increment for the major tick spacing using the **Tick Spacing** drop down selection. The values in the drop down selection are exponents for base 10. You can change the title of the Y-axis by clicking on the **Unit** text field and typing the desired title.

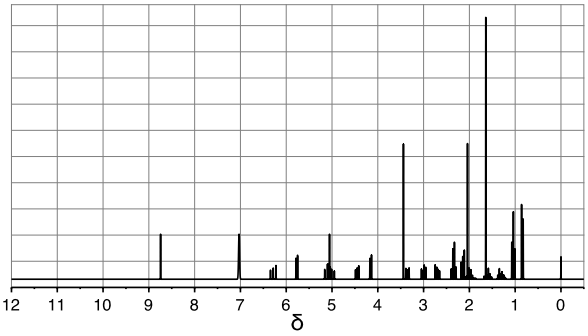
Showing Grids

Grids can be displayed by performing the following steps:

1. Hover the spectrum to display the grid over.
2. Right-click on the spectrum and select the **Format Spectrum...** menu item.
3. Scroll down to the **Grid** section and select the **Show Grid** checkbox.

The color and thickness of the grid lines can also be set in this format window. A grid appears as shown in *Figure 8.6*.

Figure 8.6: A grid is displayed over a spectrum.



Showing Integration Lines

Integration lines can be displayed by performing the following steps:

1. Hover the spectrum to display the integration line over.
2. Right-click on the spectrum and select the **Format Spectrum...** menu item.
3. Scroll down to the **Integration Line** section and select the **Show for NMR Spectra** checkbox.

The color and thickness of the integration line can also be set in this format window. While intended for NMR spectra, integration lines can be added to any plot if desired. An integration line appears as shown in *Figure 8.7*.

Figure 8.7: An integration line is calculated over an NMR multiplet.

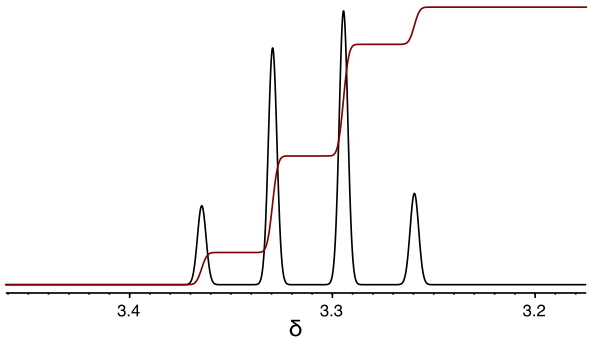
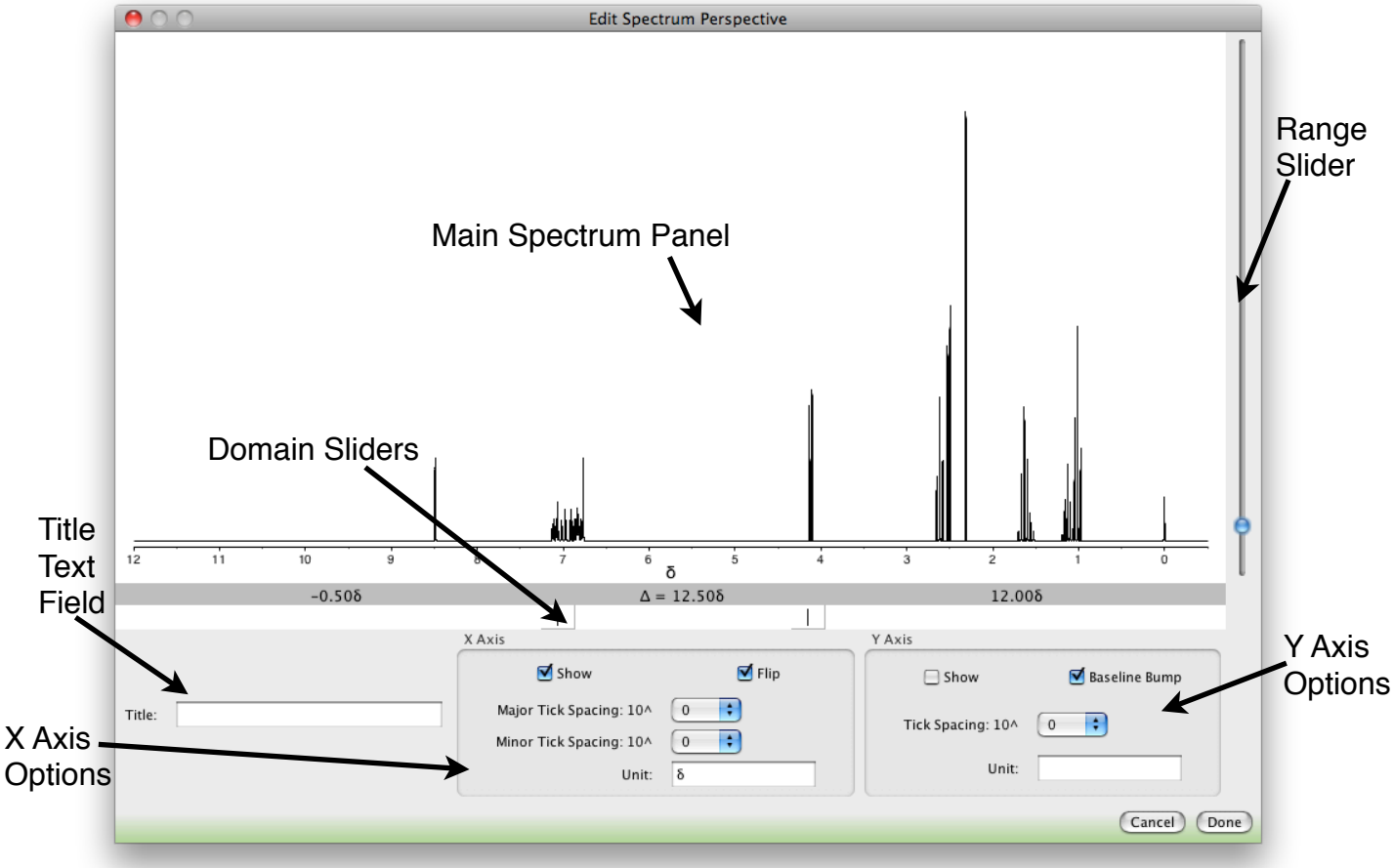


Figure 8.8: The Spectrum Edit Window



Chapter 9: Visual Specifications

Overview

All graphics in ChemDoodle are fully customizable. Visual specifications for the graphics can be defined for the entire document, groups of objects or individual objects.

This section introduces the new user to ChemDoodle document settings and visual specifications. It covers the following topics:

- What are document settings, visual specifications and style sheets.
- How to create and install custom *Chemical Document Settings* files.
- Which graphic specifications can be customized.
- How to customize the graphics of your figures.

Document Settings

Document settings are the variables that determine how graphics are rendered in a document. They are also called visual specifications when referring to an individual object. All together, they form the document's style sheet.

Style Sheets

Style sheets can be named when creating formatted documents. The creation of formatted documents is discussed in *Chapter 1*.

In addition to creating or conforming ChemDoodle documents to the preset style sheets, you can create your style sheets in *ChemDoodle Document Settings* files that can be used later. In the **Preferences** window, under the **Visuals** tab, under the **Page** tab, there is a **Create Chemical Document Settings File** button at the bottom of the options. Just perform the following steps to create a new *ChemDoodle Document Settings* file with your completed style sheet:

1. Go through the all of the tabs under the **Visuals** tab in the **Preferences** window and set all of the values in the options to the preferred values.
2. Click on the **Create Chemical Document Settings File** button in the **Preferences** window under the **Visuals** tab under the **Page** tab.
3. A new window will appear. Type in the name of the *ChemDoodle Document Settings* file.
4. Choose three fonts to cascade through. This is important because different operating systems have different font sets and you may have selected a font not accessible on another operating system if you want to use it on that operating system. *Serif* and *SansSerif* will always be defined on all operating systems, so select those fonts in the third option as wild cards.
5. Press the **Ok** button to save the *Chemical Document Settings* file.

All *Chemical Document Settings* files are saved to the *presets* folder in the *ChemDoodleSettings* folder located in your operating system's standard *Documents* folder. Any functions for using *ChemDoodle Document Settings* files or for conforming documents will now list the new style sheet.

If you want to use *Chemical Document Settings* files provided by other users of ChemDoodle, just copy their file into the *presets* folder in the *ChemDoodleSettings* folder located in your operating system's standard *Documents* folder. If you have ChemDoodle open while copying the file, close and restart it. They copied style sheet will then be accessible in ChemDoodle.

Setting the Default Document Settings

When you globally change the visual specifications for a document, ChemDoodle will ask you if you would like the changed settings to become the new default settings. There are two cases when this happens:

1. After opening the **Preferences** window and changing visual specifications.
2. After conforming a document using the **Conform Document...** menu item in the **Edit** menu.

Just click **Yes** to set the changed settings as the default settings. Now when a new document is opened, the current default settings will be used to define the graphics.

Alternatively, you may answer **No** to the question, and later, if you decide to indeed use the current document settings as the default document settings, then select the **Save Document Settings...** menu item in the **Window** menu.

Restore the Original Default Document Settings

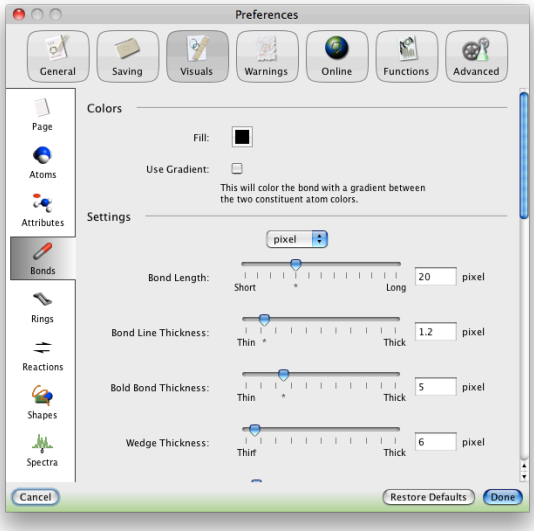
To restore the original default document settings, open the **Preferences** window and click the **Restore Defaults** button at the bottom of the window. Then close the window and select **Yes** when asked to set the current settings as the new default settings.

Individual Settings

Setting Types

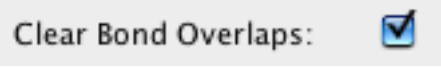
All visual specifications provided in ChemDoodle are listed in the **Preferences** window under the **Visuals** tab as shown in *Figure 9.1*.

Figure 9.1: Visual Specifications

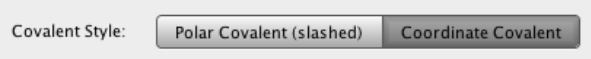


Each visual specification consists of a title to the left and a component to the right. These components include:

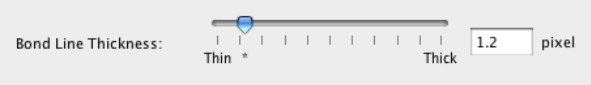
- **On/Off Choices** - Click the check box to choose whether the specification is used or not. For example, the following check box will enable or disable the **Clear Bond Overlaps** visual specification.



- **Single Option Choices** - Choose one of the options from a group exclusively to define it as the value to use for the specification. For example one option can be chosen from the following group set to determine the value for the **Covalent Style** specification.



- **Number Sliders** - Define a number value by clicking and dragging the slider or by explicitly typing the value in the text field. Some number components will be associated with a dimension drop down selection to easily set values in other units, such as centimeters instead of pixels. For example, slide the slider or type a value into the text box of the following number component to define the value for the Bond Line Thickness specification.



NOTE: Some number components define angles, and an angle swivel will be provided instead of a slider. Click and drag to the angle you want on the swivel to set the angle.

- **Color Buttons** - Click on color buttons and use the color selection window that appears to select a new color. For example, the following color button will determine bond line color.

All objects drawn after changing the visual specifications in the **Preferences** window will conform to the new specifications. All visual specifications are listed in the following sections.

Page

Colors

Background - A color button for the background color of the document.

Dimensions

Page Size - A specialized component for setting the page size. Set the width and height by typing in the text boxes or select a standard size from the drop down selections. The button to the left of the text fields will swap the width and height.

Ångströms / Bond Length - A number slider for setting the ratio between Ångströms and the **Bond Length** specification in pixels. This specification is useful when finding covalent bonds and when reading in files with Ångström coordinates.

Margins

Top - Type in the value for the top page margin.

Left - Type in the value for the left page margin.

Bottom - Type in the value for the bottom page margin.

Right - Type in the value for the right page margin.

Atoms

Colors

Text - A color button for the text color of atom labels.

Labels

Buffer Space - A number slider to set the amount of whitespace between atom text and the bonds connected to that atom.

Vertical Alignment - A number slider to control the baseline for rendering text relative to the center of the atom.

Token Stacking - A single option choice to set whether atom labels will stack all tokens, stack only the second token or will never stack tokens.

Stack Lone/Terminal - An on/off choice to set whether lone and terminal atoms will stack their label tokens.

Horizontal Spacing - A number slider to set the horizontal whitespace between each label token.

Vertical Spacing - A number slider to set the vertical whitespace between each label token.

Subscript Reduction - A number slider to set the size of subscript font relative to the atom label font.

Subscripts Shift - A number slider to set the magnitude of the offset from the atom label font baseline to draw subscripts from.

Superscript Reduction - A number slider to set the size of superscript font relative to the atom label font.

Superscript Shift - A number slider to set the magnitude of the offset from the atom label font ascent to draw superscripts from.

Hydrogens

Add as - A single option choice to determine if Hydrogens are added as text to labels or as atoms with bonds attached.

Add to Carbons - A single option choice to set how Hydrogens add to Carbons; Hydrogens can always add to Carbons, can only add to unsaturated Carbons or will never add to Carbons.

Show Implicit Hydrogens - An on/off choice to set whether implicit hydrogens are automatically rendered or not.

Carbons

Display Carbon Labels - A single option choice to set if Carbon labels display always, only on lone and hidden Carbons, only on hidden Carbons, or never show.

Hidden Carbon Angle - An angle number slider for setting the hidden Carbon angle. The hidden Carbon angle is the deviation from 180° between bonds on a Carbon atom that only has 2 bonds attached to it.

Show Terminal Labels - An on/off choice to set whether terminal carbon labels are displayed or not.

Elements

Use Circles - An on/off choice for controlling if element labels are rendered as text or as circles.

Coloring - A single option choice for determining whether user chosen colors, *CPK* colors, *Jmol* colors, or *PyMOL* colors are used for element labels.

Radius Convention - A single option choice to control if circles are rendered with a constant radius, the atomic radius of their element, the covalent radius of their element or the van der Waals radius of their element.

Constant Radius - A number slider to set the constant radius to render element atom circles with.

Border Width - A number slider to set the width of the circle outlines when atoms are rendered as circles.

Attributes

Colors

Fill/Text - A color button for the text color of attribute labels and graphics.

Logistics

Allowed Distance - A number slider to control the maximum distance an attribute can be translated away from the object it defines.

Text

Font Size Reduction - A number slider to control the font size reduction of attribute text from its defined font. This is so attribute text is smaller than the text of the object is associated with.

Charges

Surround with a Circle - An on/off choice to set whether charges are rendered with a circle around them.

Radicals

Diameter - A number slider to set the diameter of rendered electrons.

Separation - A number slider to set the separation distance between electrons or electrons and charges in paired attributes such as electron pairs and radical cation symbols.

Bonds

Colors

Fill - A color button for the bond line color.

Use Gradient - An on/off choice for rendering bonds with a gradient between the constituent atom colors.

Split Color - An on/off choice for rendering bonds that will split the bond color between the constituent atom colors.

Settings

Bond Length - A number slider to define the optimal length for bonds. This affects anything that depends on bond length including drawing bonds and cleaning structures.

Bond Line Thickness - A number slider to define the width of bond lines.

Bold Bond Thickness - A number slider to define the width of bold bonds.

Wedge Thickness - A number slider to define the width of the wide end of wedge bonds.

Unsaturated Spacing (Absolute) - A number slider to define the spacing between bond lines in higher order bonds.

Unsaturated Spacing (Relative) - A number slider to define the spacing between bond lines in higher order bonds, but relative to the length of the bond.

Clip Angle - An angle number slider to define the angle at which non-symmetrical double bonds will clip the second bond line.

Hash Width - A number slider to define the width of hashes in bonds rendered with a hash.

Hash Spacing - A number slider to define the width the spacing between hashes in bonds rendered with a hash.

Hash Offset - A number slider to define the translation from the origin of hashes in bonds rendered with a hash.

Arrow Length - A number slider to define the arrowhead length of covalent bonds.

Arrow Angle - An angle number slider to define the arrowhead angle of covalent bonds.

Wavy Length - A number slider to define the amplitude of wavy bonds.

Zigzag Length - A number slider to define the amplitude of zigzag bonds.

Stroke

Style - A drop down selection to set the default bond stroke style.

Texture - A number slider for setting the magnitude of texture in stroke styles. For instance, a higher number will cause *Bristle* strokes to look more bristled.

Bond Ends - A single option choice to set how bond ends are rendered; with no cap, a round cap or a square cap.

Options

Join Bond Connections - An on/off choice to define whether the rendering engine will merge bonds end together for more aesthetic graphics.

Double Bond Asymmetry - A single option choice to set when double bonds will be rendered asymmetrically; always, when between 2 Carbons, only in rings or never.

Heteroatom Retraction - An on/off choice that defines whether asymmetric double bonds will retract the second line from an atom or not based on that atom being a heteroatom.

Terminal Retraction - An on/off choice that defines whether terminal double bonds will retract the second line from a terminal atom or not.

Unsaturated Spacing - A single option choice for setting whether unsaturated bonds are rendered with an absolute spacing or with a relative spacing between bond lines. Changing this specification will place the corresponding visual specification in the **Settings** section.

Even Hashes - An on/off choice to determine if the **Hash Width** and **Hash Offset** specifications only affect **Bold Dashed** and **Recessed** bonds.

Clear Bond Overlaps - An on/off choice to determine if an overlapped bond will erase the section of overlap.

Overlap Clear Width - A number slider to define the length of the bond that is erased when overlapped.

Covalent Style - A single option choice to set if covalent bonds are rendered as **Polar Covalent** bonds with a slash in the stroke, or as **Coordinate Covalent** bonds.

Indent Arrow Bond - An on/off choice to set if covalent bond arrowheads are indented.

Rings

Fused

Favor Aromatics - An on/off choice to force double bonds in fused systems to face aromatic rings over non-aromatic rings.

Double Bond Orientation - A single option choice to determine if double bonds in fused ring systems will face larger rings or smaller rings.

Aromatics

Use Circles - An on/off choice to render aromatics with a circle instead of in Kekulé form.

Circle Radius - An number slider to define the diameter of the aromatic circle relative to the dimensions of the ring.

Reactions

Layout

Double Line Spacing - A number slider to define the spacing between the lines in equilibrium arrows.

Automatically Place Plusses - An on off choice to set whether reactions automatically place plusses between constituent reactants and products.

Text Buffer - A number slider to define the buffer between the text set as the reaction conditions and the ends of the associated arrow when the text is centered. This value times 2 will determine the default length that arrows without associated text are cleaned to when cleaning reactions.

Constituent Buffer - A number slider to define the spacing between reaction constituents when cleaning reactions.

Arrowheads

Length - A number slider to define the arrowhead length of arrow shapes.

Angle - An angle number slider to define the arrowhead angle of arrow shapes.

Shapes

Colors

Borders and Lines - A color button for the lines and borders of shapes.

Fill - A color button for the fill color of shapes.

Text - A color button for the text color of shapes.

Settings

Shapes Add - A single option choice to set whether shapes are drawn in front of atoms or behind atoms.

Strokes

Thickness - A number slider to define the width of solid strokes in shapes.

Hash Width - A number slider to define the width of hashes in shapes rendered with a hash.

Hash Spacing - A number slider to define the width the spacing between hashes in shapes rendered with a hash.

Hash Offset - A number slider to define the translation from the origin of hashes in shapes rendered with a hash.

Shadows

Translation - A number slider to define the distance from the shape the shadow should be rendered.

Angle - An angle number slider to define the angle in relation to the shape to place the shadow.

Opacity - A number slider to define the transparency of shadows.

Brackets

Wideness - A number slider to define the width of bracket lips relative to the standard size.

Orbitals

Length Multiplier - A number slider to define the default extent of orbitals in bond lengths. So if the length multiplier is 1, then all

orbitals placed will have a length of 1 bond length.

Stroke Shaded Lobes - An on/off choice to set whether shaded lobes in orbitals will also be outlined.

Paths

Close - An on/off choice to set if paths are closed by default.

Rectangles

Rounded Arc Width - A number slider to define the width of the corner arcs in rounded rectangles.

Rounded Arc Height - A number slider to define the height of the corner arcs in rounded rectangles.

Rulers

Show Major Ticks - An on/off choice to set if major ticks are shown in rulers.

Close - An on/off choice to set if minor ticks are shown in rulers.

Unit - A drop down selection to set the default units of ruler objects.

Spectra

Colors

Plots - A color button for the spectrum plots.

Grids - A color button for the spectrum grids.

Integration Lines - A color button for the spectrum integration lines.

Plot Strokes

Thickness - A number slider to define the width of solid strokes in spectrum plots.

Hash - An on/off choice to render spectrum plots with a hashed stroke.

Hash Width - A number slider to define the width of hashes in spectrum plots rendered with a hash.

Hash Spacing - A number slider to define the width the spacing between hashes in spectrum plots rendered with a hash.

Hash Offset - A number slider to define the translation from the origin of hashes in spectrum plots rendered with a hash.

Grids

Show - A on/off switch to set whether spectrum grids are shown by default.

Thickness - A number slider to define the line thickness of spectrum grids.

Integration Lines

Show - A on/off switch to set whether spectrum integration lines are shown by default.

Thickness - A number slider to define the line thickness of spectrum integration lines.

Editing Visual Specifications

For Single Objects

To edit the visual specifications of a single object, perform the following steps:

1. Switch to a selection tool and make sure the current selection is empty.
2. Hover the mouse pointer over the object of which the visual specifications are to be changed.
3. Right-click on the object and select the **Format Object...** menu item or double-click on the object.

4. Change the visual specifications in the window that appears. You will see the graphics update in real-time on the **Doodle Board**.
5. Click the **Done** button in the window to set the changes.

You can also press the Cancel button to cancel all changes.

For a Group of Objects

To edit the visual specifications of a group of objects, perform the following steps:

1. Switch to a selection tool.
2. Select all of the content of which the visual specifications are to be changed.
3. Open the **Preferences** window and click on the **Visuals** tab.
4. Change all the visual specifications in the **Visuals** tab to your preference. You will see the graphics update in real-time on the **Doodle Board**.
5. Click the **Done** button in the **Preferences** window to set the changes.

You can also press the Cancel button to cancel all changes.

Conforming a Group of Objects to the Current Style Sheet

To conform a group of objects to the current style sheet, perform the following steps:

1. Switch to a selection tool.
2. Select all of the content of which the visual specifications are to be changed.
3. Press the **Conform to Document Settings** menu item in the **Content** menu.

All content will conform to the visual specifications defined in the document's style sheet. This function will also change fonts and scale structures to match the defined bond length.

Conforming the Entire Document to a Different Style Sheet

To conform the entire document to a different style sheet, perform the following steps:

1. Press the **Conform Document...** menu item in the **Edit** menu.
2. In the window that appears, choose the style sheet you prefer from the drop down selection.
3. You will be asked if you would like to conform atom text by changing fonts; choose **Yes** or **No**.
4. If the bond length has changed, you will be asked if you would like the structures to be scaled to match the new value; choose **Yes** or **No**.

The entire document will now conform to your choice of style sheet.

3D Graphics

ChemDoodle is a tool for generating 2D graphics. However, ChemDoodle handles 3D input and you can create orthographic 2D scenes of your 3D data. That being said, with all of the bond types and atom labels showing, the figure may not be very aesthetic. To create better looking 2D orthographic scenes of your 3D data, perform the following suggestions.

- Change all bonds to plain single bonds, and include double bonds if necessary.
- Change the visual specifications to show all atoms as circles instead of as text labels.
- Change the visual specifications to render atoms with their Jmol colors.

- Increase the bond line width visual specification.
- Change the visual specifications to render bonds with a gradient between their constituent atoms.
- Increase the bond overlap buffer visual specification to clearly show bond overlaps.

We have provided a sample style sheet to quickly create 2D orthographic scenes from 3D data that can be accessed when creating a formatted document or conforming a given document as is described in the previous section called **Orthographic 3D Scene**.

Bond Stroke Styles

ChemDoodle provides several bond stroke styles to casually style your structures for presentations, posters and more casual media. To change bond stroke styles, select the bonds to be changed with a selection tool and use the **Stroke** toolbar.

The default bond line stroke width is 1.2 pixels. This is not sufficient to see some stroke styles and the value will need to be increased. Other stroke styles, such as the **Brush** style, will not display well for really short bonds and structures rendered with those styles should be expanded.

The following bond stroke styles are currently provided:

- **Basic** - 
- **Bristle** - 
- **Brush** - 
- **Calligraphy** - 
- **Charcoal** - 
- **Scribble** - 
- **Wobble** - 

Advanced Document Rendering

The graphics defined by ChemDoodle are always exact and based on very precise coordinates. However, the screen that you use to display ChemDoodle and bitmap images that are output will need to define the graphics in a much less precise resolution. Algorithms have been developed to minimize the perception of this loss of resolution and ChemDoodle provides full access to control how the graphics are rendered. Note that scalable vector graphics are also exact and based on precise coordinates and are therefore resolution-less. The following settings will only affect the display of graphics on your computer monitor and the output of bitmap graphics; scalable vector graphics will not be affected.

Advanced document rendering settings can be defined in the **Preferences** window under the **Advanced** tab.

Anti-Aliasing

Anti-aliasing controls whether or not the geometry rendering methods will attempt to reduce aliasing artifacts along the edges of shapes. Anti-aliasing is enabled by default.

A typical antialiasing algorithm works by blending the existing colors of the pixels along the boundary of a shape with the requested fill paint according to the estimated partial pixel coverage of the shape. This function reduce the appearance of jagged edges. *Figure 9.2* is a structure rendered without anti-aliasing enabled, while *Figure 9.3* is a structure rendered with anti-aliasing enabled.

Figure 9.2: Anti-aliasing is disabled.

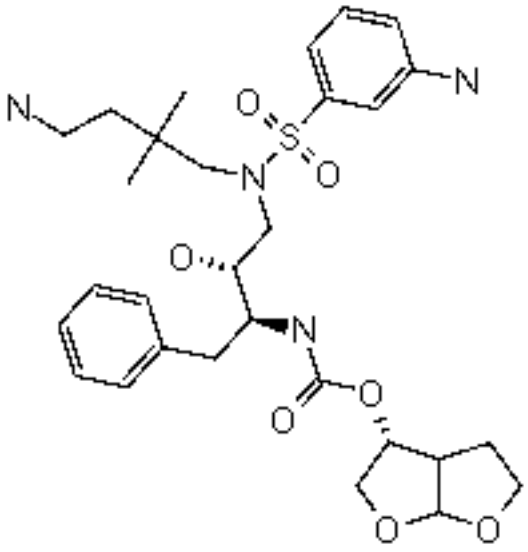
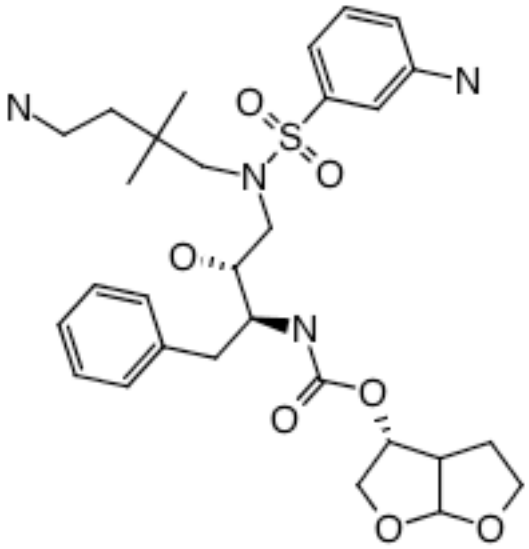


Figure 9.3: Anti-aliasing is enabled.



Font Fractional Metrics

Font fractional metrics controls whether the positioning of individual character glyphs takes into account the sub-pixel accuracy of the scaled character advances of the font or whether such advance vectors are rounded to an integer number of whole device pixels. This hint only recommends how much accuracy should be used to position the glyphs and does not specify or recommend whether or not the actual rasterization or pixel bounds of the glyph should be modified to match. Font fractional metrics are disabled by default to produce better graphics for bitmap images and for the computer screen. In ChemDoodle, this property does not affect printing. Since printing is usually with a high resolution device, ChemDoodle will always enable font fractional metrics for printer rendering.

Rendering text to a low resolution device like a screen will necessarily involve a number of rounding operations as the high quality and very precise definition of the shape and metrics of the character glyphs must be matched to discrete device pixels. Ideally the positioning of glyphs during text layout would be calculated by scaling the design

metrics in the font according to the point size, but then the scaled advance width will not necessarily be an integer number of pixels. If the glyphs are positioned with sub-pixel accuracy according to these scaled design metrics then the rasterization would ideally need to be adjusted for each possible sub-pixel origin.

Unfortunately, scaling each glyph customized to its exact subpixel origin during text layout would be prohibitively expensive so a simplified system based on integer device positions is typically used to lay out the text. The rasterization of the glyph and the scaled advance width are both adjusted together to yield text that looks good at device resolution and has consistent integer pixel distances between glyphs that help the glyphs look uniformly and consistently spaced and readable.

This process of rounding advance widths for rasterized glyphs to integer distances means that the character density and the overall length of a string of text will be different from the theoretical design measurements due to the accumulation of a series of small differences in the adjusted widths of each glyph. The specific differences will be different for each glyph, some being wider and some being narrower than their theoretical design measurements. Thus the overall difference in character density and length will vary by a number of factors including the font, the specific device resolution being targeted, and the glyphs chosen to represent the string being rendered. As a result, rendering the same string at multiple device resolutions can yield widely varying metrics for whole strings.

When font fractional metrics are enabled, the true font design metrics are scaled by the point size and used for layout with sub-pixel accuracy. The average density of glyphs and total length of a long string of characters will therefore more closely match the theoretical design of the font, but readability may be affected since individual pairs of characters may not always appear to be consistent distances apart depending on how the sub-pixel accumulation of the glyph origins meshes with the device pixel grid. Enabling this hint may be desirable when text layout is being performed that must be consistent across a wide variety of output resolutions. Specifically, this hint may be desirable in situations where the layout of text is being previewed on a low resolution device like a screen for output that will eventually be rendered on a high resolution printer or typesetting device.

When disabled, the scaled design metrics are rounded or adjusted to integer distances for layout. The distances between any specific pair of glyphs will be more uniform on the device, but the density and total length of long strings may no longer match the theoretical intentions of the font designer. Disabling this hint will typically produce more readable results on low resolution devices like computer monitors.

Dithering

Dithering controls how closely to approximate a color when storing into a destination with limited color resolution. Dithering is enabled by default

Some rendering destinations may support a limited number of color choices which may not be able to accurately represent the full spectrum of colors that can result during rendering operations. For such a destination, dithering controls whether rendering is done with a flat solid fill of a single pixel value

which is the closest supported color to what was requested, or whether shapes will be filled with a pattern of colors which combine to better approximate that color.

Rendering Algorithm

This setting provides a high level recommendation as to whether to bias algorithm choices more for speed or quality when evaluating tradeoffs. This hint could be consulted for any rendering or image manipulation operation, but decisions will usually honor other, more specific settings in preference to this setting. The rendering algorithm is set to *Quality* by default.

Alpha Interpolation Algorithm

The alpha interpolation setting is a general setting that provides a high level recommendation as to whether to bias alpha blending algorithm choices more for speed or quality when evaluating tradeoffs. The alpha interpolation algorithm is set to *Quality* by default.

This setting controls the choice of alpha blending calculations that sacrifice some precision to use fast lookup tables or lower precision SIMD instructions. This hint could also control whether or not the color and alpha values are converted into a linear color space during the calculations for a more linear visual effect at the expense of additional per-pixel calculations.

Color Rendering Algorithm

The color rendering algorithm controls the accuracy of approximation and conversion when storing colors into a destination image or surface. The color rendering algorithm is set to *Quality* by default.

When a rendering or image manipulation operation produces a color value that must be stored into a destination, it must first convert that color into a form suitable for storing into the destination image or surface. Minimally, the color components must be converted to bit representations and ordered in the correct order or an index into a color lookup table must be chosen before the data can be stored into the destination memory. Without this minimal conversion, the data in the destination would likely represent random, incorrect or possibly even unsupported values. Algorithms to quickly convert the results of rendering operations into the color format of most common destinations are well known and fairly optimal to execute.

Simply performing the most basic color format conversion to store colors into a destination can potentially ignore a difference in the calibration of the color space of the source and destination or other factors such as the linearity of the gamma correction. Unless the source and destination color space are identical, to correctly perform a rendering operation with the most care taken for the accuracy of the colors being represented, the source colors should be converted to a device independent color space and the results then converted back to the destination color space. Furthermore, if calculations such as the blending of multiple source colors are to be performed during the rendering operation, greater visual clarity can be achieved if the intermediate device independent color space is chosen to have a linear relationship between the values being calculated and the perception of the human eye to the response curves of the output device.

Stroke Control

Stroke control defines whether a rendering implementation should or is allowed to modify the geometry of rendered shapes for various purposes. Stroke control is set to *Best Compromise* by default.

Some implementations may be able to use an optimized platform rendering library which may be faster than traditional software rendering algorithms on a given platform, but which may also not support floating point coordinates. Some implementations may also have sophisticated algorithms which perturb the coordinates of a path so that wide lines appear more uniform in width and spacing.

If an implementation performs any type of modification or "normalization" of a path, it should never move the coordinates by more than half a pixel in any direction.

When stroke control is set to *Normalize*, geometry will be altered to improve uniformity or spacing of lines and overall aesthetics. The compromise is that geometry will be offset to fit to the pixel resolution of the rendering device. A consequence is that lines that are parallel may not appear exactly parallel, such as in double bonds.

When stroke control is set to *Pure*, geometry will be left unmodified and rendered with sub-pixel accuracy. There will be noticeable lightness and bolding in straight lines that are vertical or horizontal.

Figure 9.5 shows a rectangle and structure displayed with stroke control set to *Pure*, while *Figure 9.6* shows the same objects with stroke control set to *Normalize*.

Figure 9.5: A structure and rectangle rendered with stroke control set to Pure. Notice the bolding and blurring of the horizontal and vertical lines.

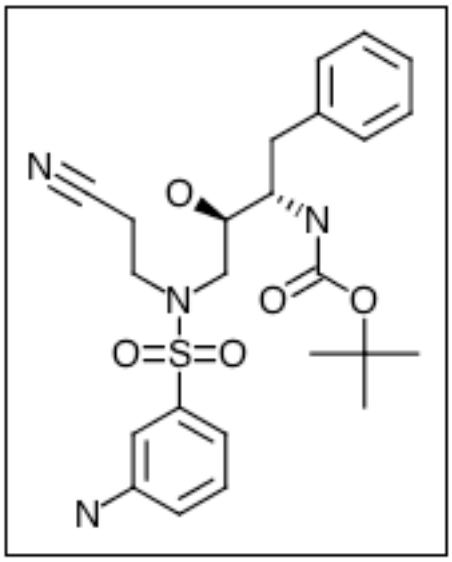
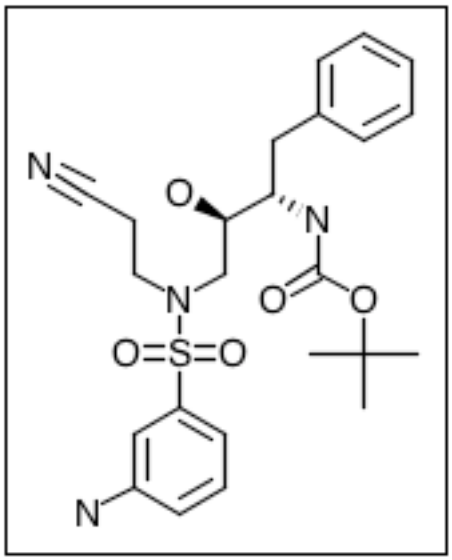


Figure 9.6: A structure and rectangle rendered with stroke control set to Normalize. Notice that parallel lines are not preserved.



For even better graphics, a third option is provided called *Best Compromise*. This option will use pure stroke control for all chemical structures. All other shapes will first be analyzed for vertical and horizontal lines, and any found will be rendered with normalized stroke control while the rest of the graphics will be rendered with pure stroke control.

Image Scaling

Image scaling controls how image pixels are filtered or resampled during an image rendering operation. This will have noticeable affects on images that are not rendered in their natural scale. The image scaling algorithm is set to *Progressive Bilinear* by default.

Implicitly images are defined to provide color samples at integer coordinate locations. When images are rendered upright with no scaling onto a destination, the choice of which image pixels map to which device pixels is obvious and the samples at the integer coordinate locations in the image are transferred to the pixels at the corresponding integer locations on the device pixel grid one for one. When images are rendered in a scaled, rotated, or otherwise transformed coordinate system, then the mapping of device pixel coordinates back to the image can raise the question of what color sample to use for the continuous coordinates that lie between the integer locations of the provided image samples. Interpolation algorithms define functions which provide a color sample for any continuous coordinate in an image based on the color samples at the surrounding integer coordinates.

Progressive Bilinear is better than *Bicubic* which is better than *Bilinear* which is better than *Nearest-Neighbor* at producing reasonable graphics of stretched or shrunken bitmap images. The better the algorithm used, the worse the runtime will get.

Chapter 10: Sharing Information

Overview

ChemDoodle has advanced functions for interacting with other applications on your computer. This is essential for inputting graphics into word processors or for transferring chemical data into modeling applications.

This section introduces the new user to ChemDoodle's system clipboard capabilities. It covers the following topics:

- Introducing the system clipboard.
- How to copy data and graphics from ChemDoodle into other applications.
- How to copy data and graphics from other applications into ChemDoodle.
- What types of data can be transferred.
- What image formats are supported.
- How to save images.
- How to insert images.
- How to take advantage of round trip editing.

The System Clipboard

The system clipboard is a construct of the operating system that contains data for sharing between applications. Only one application can place data on the system clipboard at a time. Other applications can then see that data and load it. This system forms the basis for copy and paste functionality. ChemDoodle will place a wide range of chemical and graphic data on the system clipboard as well as associate that data with the correct *MIME* types for other applications to use.

MIME Types

A *MIME* type is an identifier to define the data it is associated with. For example, a structure can be represented in *MDL MOLFile* format. The *MDL MOLFile* format is a plain text format and can be associated with the *MIME* type, *text/plain*. However, this is a very generic description and other applications will only recognize it as plain text, rather than as a chemical structure. Therefore a different *MIME* type is associated with this data, *chemical/x-mdl-molfile*, to define it as a structure in the *MDL MOLFile* format. In this manner, other applications will recognize this data as a chemical.

ChemDoodle follows the *MIME* standards put forth by the *Chemical MIME Project* (http://www.ch.ic.ac.uk/chemime/). This should be regarded as the standard, however, many chemical software developers do not follow these rules, thereby causing issues when transferring data between chemical applications.

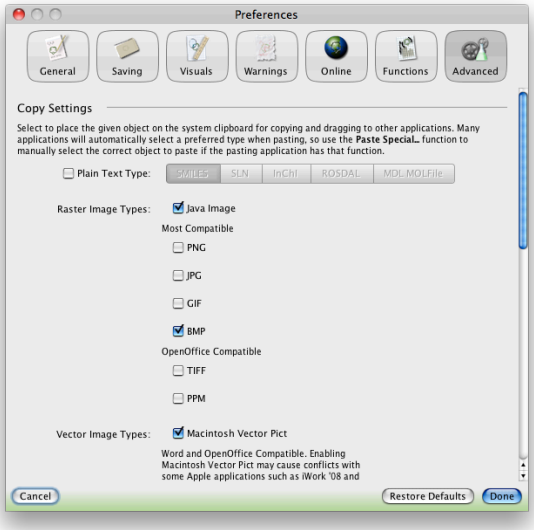
Additionally, since many items can be present on the system clipboard at once, applications may paste a certain data type by default that may not be the data you want to paste. For instance, *Microsoft Word* can paste both text data types and image data types. If both are present on the system clipboard, *Microsoft Word* will automatically select the text data type when pasting, even if you wanted the image to be pasted. There can even be different image types, confusing the situation further.

Therefore, ChemDoodle allows you to define how data and which data is placed on the system clipboard to work with the applications that you use.

Clipboard Settings

ChemDoodle can transfer data to almost any application that has been created. But it is impossible for ChemDoodle to determine which data should be transferred. Therefore, you need to set the appropriate **Copy Settings** to make sure any ambiguities are resolved with the application you are pasting to. Copy Settings can be set in the **Preferences** window under the **Advanced** tab as shown in *Figure 10.1*. These settings will allow you to explicitly control what data ChemDoodle will transfer to other applications.

Figure 10.1: Copy Settings



There are three main types of data that may be transferred:

- **Text Types** - Contains a line or lines of text that will be interpretable by other applications. Some chemical formats are also listed here to be pasted as text into other applications. All text data will be interpreted as text by other applications and any chemical significance will be lost. Only one text data type will be placed on the system clipboard at a time.
- **Image Types** - This group contains both bitmap and vector images. Bitmap images are not scalable in resolution. Vector images are much more versatile and will remain crisp and clear regardless of resizing or transformation. Bitmap and vector images are discussed in detail in the next section.
- **Chemical Types** - Chemical types include structure information. Only chemical programs will see these.

Therefore, to work with other applications, first decide what type of data you would like to transfer and what types of data the other application accepts. Then set the appropriate copy settings to continue.

Scalable Vector Graphics

There are two types of images, bitmap and vector. Bitmap images are traditional images and define a rectangle of pixels and their colors, while vector images define drawing instructions for recreating it. When resizing, the bitmap will become blurry, pixelated and lose its quality while the vector image will remain crisp and clear. *Figure 10.2* shows a bitmap image of a structure, while *Figure 10.3* shows a vector image of the same structure. Both were created by ChemDoodle. Try zooming in on both images using your PDF reader and you can see the difference in quality for yourself.

Figure 10.2: A Bitmap Image

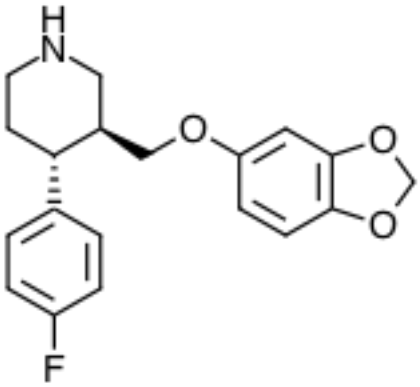
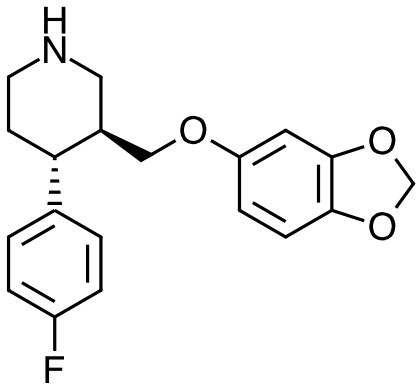


Figure 10.3: A Vector Image



Bitmap images will suffer from this issue with any change of resolution, including printing to a printer. Because of this, we recommend you insert vector images into your documents. The only downside to using vector graphics is that some programs may not support them. ChemDoodle compatibility with 3rd party applications is discussed in *Appendix C*.

If you must use a bitmap image, then ChemDoodle provides high resolution options (such as scaling and DPI control) for a few bitmap formats as discussed in the **Image Output Options** section later in this chapter.

Copying Data to Other Applications

Using the Copy Function

To copy data from ChemDoodle into other applications, perform the following steps:

1. Determine which data you would like to transfer and the types of data that the other application can accept and configure the copy settings in the **Preferences** window under the **Advanced** tab accordingly.
2. Select the objects on the **Doodle Board** that you would like to copy using the content selection tools.
3. Click on the **Copy** menu item in the **Edit** menu or press its menu accelerator keyboard shortcut which is *ctrl-C* (*command-C* on Mac OS X).
4. Use the paste function present in the other application to paste the content. If the other application has a **Paste Special...** function, you may use that to specify which data type to paste.

Using the Copy As Function

The copy as functions are preset shortcuts for placing certain data forms on the system clipboard without changing the data types to be copied in the **Advanced** tab of the **Preferences** window.

Just select the content in the document to be copied and then select one of the menu items in the **Copy As...** submenu of the **Edit** menu. The most popular data types are supported. These functions will place both text and chemical data on the system clipboard for maximum compatibility with 3rd party applications. No image data will be placed on the system clipboard.

Pasting Data from Other Applications

To paste data from other applications into ChemDoodle, perform the following steps:

1. Use the copy function present in the other application.
2. Click on the **Paste** menu item in the **Edit** menu or press its menu accelerator keyboard shortcut which is *ctrl-V* (*command-V* on Mac OS X) to paste the highest priority data to the **Doodle Board**.

Where Content is Pasted

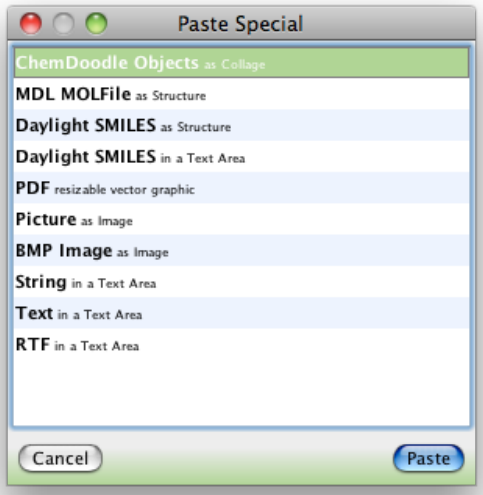
The pasted content will be located according to the following rules:

1. If your mouse pointer is hovering over the document, the center of the pasted content will be located at the mouse pointer.
2. If the mouse pointer is not hovering over the document, and the lasso is active, then the pasted content will appear to the bottom-right of the lassoed content.
3. If the mouse pointer is not hovering over the document and the lasso is inactive, then the pasted content will appear at the top left of the document.

Paste Special...

Since an application can place different data types on the system clipboard, the data that ChemDoodle pastes may not always be the desired type. In general, ChemDoodle pastes chemical data over images and images over text. If you would like to paste alternate data, click on the **Paste Special...** menu item in the **Edit** menu. A window will appear listing all ChemDoodle compatible data as shown in *Figure 10.4*. Just select the list item you would like to paste and press the **Paste** button.

Figure 10.4: Paste Special Window



Pasting Text as Chemical Data

Sometimes it may be necessary to handle text data from the system clipboard. For instance, a chemical application may paste the *MOLFile* format in plain text, or you may be copying a *SMILES* string from a web browser. ChemDoodle provides a **Paste Text as Chemical** function to conveniently handle this.

To paste text content from another application as chemical data, perform the following steps:

1. Use the copy function present in the other application to place the text on the system clipboard.
2. Expand the **Paste Text As Chemical...** submenu in the **Edit** menu.
3. Depending on the type of data being represented by the text, select the appropriate menu item in the submenu to paste.

Using this method, any of the line notations that ChemDoodle understands can be pasted as chemical data. Additionally, there is a

XYZ-Like Data menu item for pasting text as chemical data in an XYZ-like format. This option will automatically scan the text to extract atom labels and positions. The final menu item is **Guess Chemical Format**. This will detect the chemical format of the text data on the system clipboard and paste the chemical data accordingly, which is perfect for ASCII or XML data types, such as *MOLFiles* or *CML*. This function will alert you if not chemical format could be associated with the text data.

Chemical Format Compatibility

ChemDoodle supports one of the largest chemical format libraries in the industry and can interpret various chemical formats for input to and output from other chemical applications. Chemical formats are discussed in detail in *Appendix B*.

Image Format Compatibility

ChemDoodle supports the input and output of a wide range of bitmap and vector images.

Supported Input Formats

ChemDoodle can read the following bitmap image formats:

- Joint Photographic Experts Group {.jpg, .jpeg, .jpe, .jfif, .jfi, .jif}
- Microsoft Bitmap {.bmp, .dib}
- Tagged Image File Format {.tiff, .tif}
- Wireless Bitmap {.wbmp}
- CompuServ Graphics Interchange Format {.gif}
- Portable Network Graphics {.png}
- UNIX Portable PixMap {.ppm, .pnm, .pbm, .pgm}
- Photoshop Document {.psd}

ChemDoodle can read the following vector image formats:

- Adobe Portable Document Format {.pdf}
- Web Scalable Vector Graphics {.svg, .svgz}

Supported Output Formats

ChemDoodle can write the following bitmap image formats:

- CompuServ Graphics Interchange Format {.gif}
- Joint Photographic Experts Group {.jpg, .jpeg, .jpe, .jfif, .jfi, .jif}
- Microsoft Bitmap {.bmp, .dib}
- Portable Network Graphics {.png}
- Tagged Image File Format {.tiff, .tif}
- UNIX Portable PixMap {.ppm, pnm, pbm, pgm}
- Wireless Bitmap {.wbmp}

ChemDoodle can write the following vector image formats:

- Adobe Portable Document Format {.pdf}
- Encapsulated Postscript {.eps, .epi, .epsi, .epsf}
- Macintosh Vector Pict {.pict}
- OpenDocument Graphics {.odg}
- Web Scalable Vector Graphics {.svg, .svgz}
- Windows Enhanced Metafile {.emf}

Importing Chemical Content from Images

ChemDoodle will automatically embed chemical data in certain image formats. When these images are inserted into ChemDoodle, they will be checked for chemical information and that chemical information will be loaded if found.

ChemDoodle embeds chemical information into the following image formats:

- Adobe Portable Document Format {.pdf}
- Encapsulated Postscript {.eps}
- OpenDocument Graphics {.odg}
- Web Scalable Vector Graphics {.svg}

Exporting the Document to an Image

To export all of the objects in the current document to an image, perform the following steps:

1. Select the **Save As Image...** menu item from the **File** menu.
2. A file chooser will appear. Select the location you would like to have the document saved in and type in a name for the file if you do not like the default name. You do not need to type in an extension as ChemDoodle will do this for you.
3. After you are satisfied with a location and name, select the image type of the image to be exported.
4. After selecting the file type to be used, press the **Save** button to export your document as an image.
5. If options are available, a window will be shown to allow you to set the options. Define the settings to your preference and then click the **Done** button.

Exporting only Certain Objects to an Image

To export specific objects in the current document to an image, perform the following steps:

1. Use a selection tool to select the objects to be exported to an image.
2. Select the **Save Selection As Image...** menu item from the **File** menu.
3. A file chooser will appear. Select the location you would like to have the document saved in and type in a name for the file if you do not like the default name. You do not need to type in an extension as ChemDoodle will do this for you.
4. After you are satisfied with a location and name, select the image type of the image to be exported.
5. After selecting the file type to be used, press the **Save** button to export the selected objects to an image.
6. If options are available, a window will be shown to allow you to set the options. Define the settings to your preference and then click the **Done** button.

Image Output Options

There are several options that you can define for output images. Some options are only available for bitmap or vector types, while some options will be available for both.

Image Border Buffer

You can control the image border buffer, or the amount of space surrounding the graphics in an image, by changing the **Border Buffer** setting in the **Preferences** window under the **Advanced** tab. The default image border buffer is 3 pixels.

Image Scale (bitmap only)

This setting will determine the scale of the output image. The larger the scale, the larger the output image. Vector graphics can be rescaled at any time, and therefore this setting is only available for bitmap images. You will need to scale bitmap images to a larger size if you want to use a higher resolution, but retain the same dimensions.

Resolution (bitmap only)

This setting will instruct printers and other renderers how to scale the image. The higher the DPI setting, then the crisper the image will look, but the smaller it will appear. By default, the DPI setting is 300dpi. Currently, only the *JPEG* and *PNG* output support this option. Vector graphics are resolution-less, and therefore this setting is only available for bitmap images.

Transparency (bitmap only)

If the bitmap image type supports transparency, this option will be available.

Render Text as Shapes (PDF)

In vector graphics, text is output as shapes, so they are no longer recognized as text by other applications. If you prefer to preserve the characters for editing in other applications, then select this option. Note that the font you use for the text must be present on the system that you open the PDF in, or the font you used will be replaced with something similar, but not identical.

Inserting Images

For any of the image formats that ChemDoodle can read, you can import files of that format into your documents. To do so, perform the following steps:

1. Select the **Insert Image...** menu item in the **File** menu.
2. In the file chooser that appears, navigate to and select the image you would like to insert.
3. Select the **Open** button to insert the image.

If you selected an image file type that is not understood by ChemDoodle, a message will appear to notify you of the issue.

In addition to inserting images via the **File** menu, you may also simply drag compatible images from your file system or from other applications on the **Doodle Board**.

Round Trip Editing

Round trip editing is a very advanced feature for allowing ChemDoodle content to transfer between applications by embedding it into images. In most cases, ChemDoodle will automatically perform this embedding for you. Through round trip editing, you can copy ChemDoodle content into your word processor for instance, and then later copy that content back into ChemDoodle for re-editing.

> *NOTE: Make sure you always save your drawings and figures in a ChemDoodle Document and never rely on a third party application to save your ChemDoodle data. That third party application may change how it works and you may lose your data!*

Support

Round trip editing requires that both ChemDoodle and the application you are inserting the ChemDoodle content into work together. Currently, ChemDoodle supports round trip editing with any applications that understand Object Linking and Embedding (OLE) on Windows, that preserve PDF

comments on Mac OS X, or with OpenOffice on Linux. This covers a large number of applications that most scientists use, however there will always be that one application it does not work with. We are actively working to expand the range of applications ChemDoodle can provide round trip editing functionality with.

Windows

Setup

No additional setup is required for round trip editing on Windows. The OLE server is automatically registered when ChemDoodle is installed.

Clipboard Settings

By default, in Advanced Preferences, OLE is enabled. OLE is required to be enabled for round trip editing to work on Windows.

Procedure

Round trip editing is very simple on Windows. Just copy in ChemDoodle and paste into the receiving application. To edit the content, copy the embedded object from the receiving application and paste back into ChemDoodle to recover the objects. Once you have finished editing, again copy in ChemDoodle and paste back into the receiving application to replace the original object.

Some applications may not paste the OLE object by default. In this case, make sure to use a provided **Paste Special** function in the receiving application to choose the OLE object.

Not all applications on Windows support OLE, and round trip editing is not possible with those applications.

Mac OS X

Setup

No additional setup is required for round trip editing on Mac OS X.

Clipboard Settings

By default, in Advanced Preferences, PDF is enabled. PDF is required to be enabled for round trip editing to work on Mac OS X.

Procedure

Round trip editing is very simple on Mac OS X. Just copy in ChemDoodle and paste into the receiving application. To edit the content, copy the image from the receiving application and paste back into ChemDoodle to recover the objects. Once you have finished editing, again copy in ChemDoodle and paste back into the receiving application to replace the original image.

Some applications may not paste the PDF by default. In this case, make sure to use a provided **Paste Special** function in the receiving application to choose the PDF.

Not all applications on Mac OS X preserve PDF comments, and round trip editing is not possible with those applications.

Workaround for iWork Pages

iWork Pages corrupts PDF comments, so round-trip editing will fail directly from Pages. There are two workarounds for this:

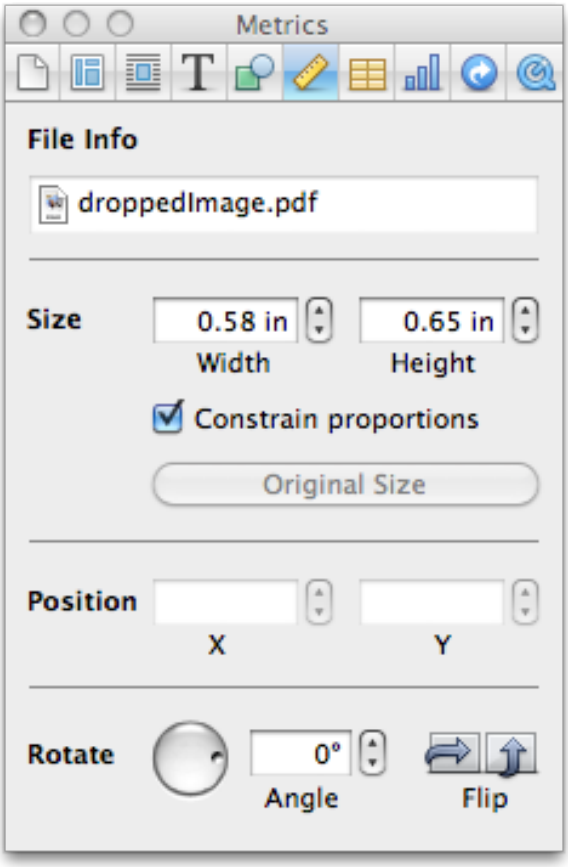
1. Copy the figure from Pages into Keynote and then copy in Keynote and paste into ChemDoodle to recover the data.
2. Use the Inspector to retrieve the unaltered PDF directly from Pages.

To perform the second procedure, please follow these steps:

1. When working with figures pasted into Pages from ChemDoodle, open the Inspector by clicking on the **Inspector** button in Pages top toolbar. 

2. In the **Inspector**, click on the **Metrics** icon  , and then click on the ChemDoodle figure so that *droppedImage.pdf* appears as in *Figure 10.5*.
3. Drag the *droppedImage.pdf* onto the Doodle Board in ChemDoodle to recover the data.

Figure 10.5: Inspector showing the droppedImage.pdf ChemDoodle embedded object.



Linux

Forward

Round trip editing on Linux is only possible with OpenOffice/LibreOffice and other variants and *only* on Linux. We did our best to provide as simple a procedure as possible, but given the lacking state of these projects, there are some inconveniences to deal with. We will do our best to continue to improve this procedure, but your help is required to submit issues to the OpenOffice/LibreOffice development teams and urge them to improve their software and APIs.

Setup

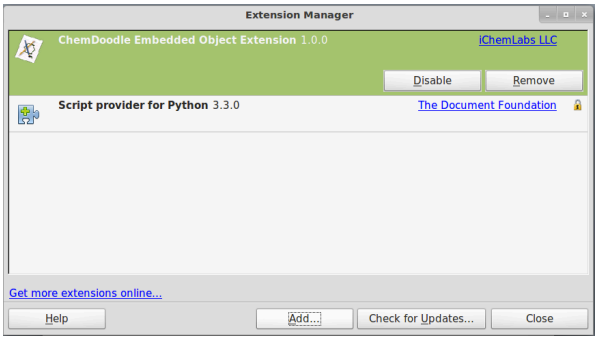
Round trip editing on Linux requires that the user install our ChemDoodle OpenOffice plugin. The plugin is named *ChemDoodle.oxt* and can be found in the *resources* folder in the *ChemDoodle* installation folder.

To install the plugin, perform the following steps:

1. Launch OpenOffice/LibreOffice.
2. In the **Tools** menu, select **Extension Manager...**
3. Click the **Add...** button.
4. In the file chooser that appears, locate the *ChemDoodle.oxt* file in the *resources* folder and select it.

If the plugin is successfully registered, it will appear in the **Extension Manager** as shown in *Figure 10.6*.

Figure 10.6: The Extension Manager with the ChemDoodle plugin properly registered



Clipboard Settings

In Advanced Preferences, both **PNG (720dpi)** and **ChemDoodle Collage** are required to be enabled for round trip editing to work on Linux. Other raster image types should be disabled.

Procedure

To insert a ChemDoodle object into OpenOffice/LibreOffice, perform the following steps:

1. Ensure the clipboard settings are correct as stated above.
2. Select the content you wish to copy and use a copy function in ChemDoodle.
3. In the Office application you want to insert the object into, open the **Object** submenu in the **Insert** menu and select **OLE Object...** (*Figure 10.7*)
4. In the window that appears, select **ChemDoodle Embedded Object** and select the **OK** button. (*Figure 10.8*)

Figure 10.7: The OLE Object... menu item

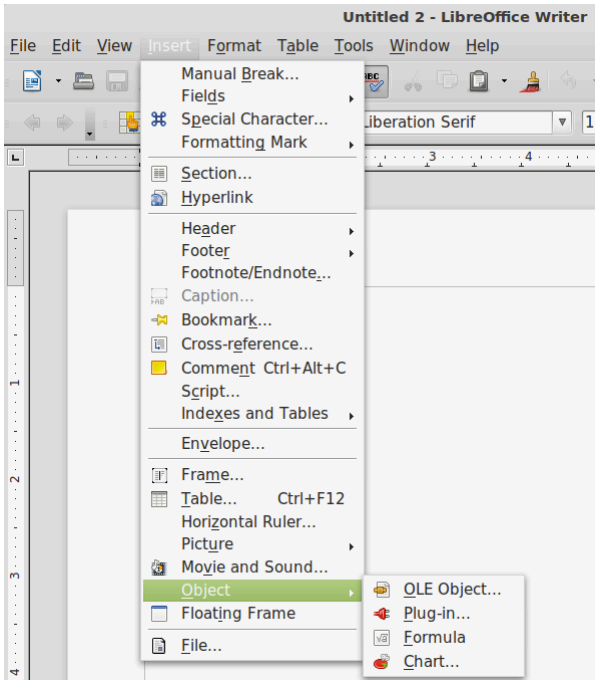
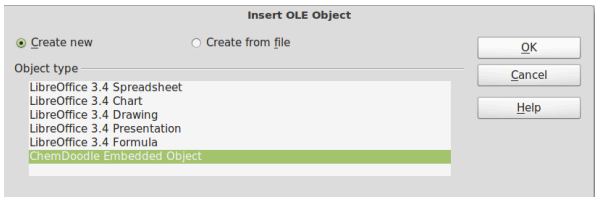


Figure 10.8: Selecting the ChemDoodle Embedded Object to insert



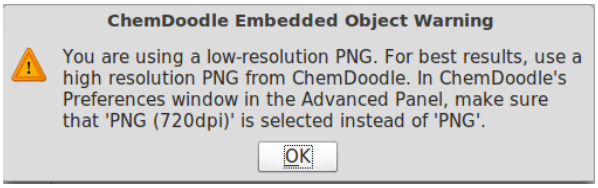
To edit the inserted ChemDoodle object, perform the following steps:

1. Select the inserted ChemDoodle object that you wish to edit, and *double-click* on it.
2. Use a copy function with the ChemDoodle object still selected.
3. In ChemDoodle, use a paste function to paste the ChemDoodle Objects.
4. Edit the content.
5. Reselect the content and follow the procedure for inserting the ChemDoodle object into OpenOffice/LibreOffice above to replace the previous object.

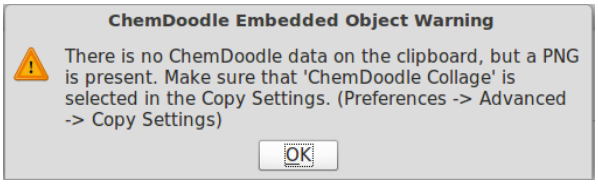
Troubleshooting

Common error boxes may appear, troubleshoot them as follows.

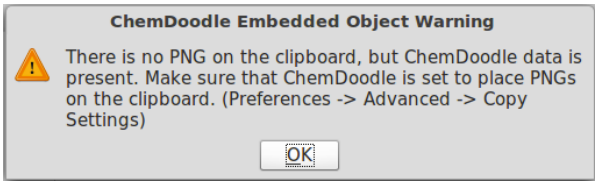
The following warning means that you should enable the *PNG (720dpi)* option and disable the *PNG* option in Advanced Preferences for the best quality images.



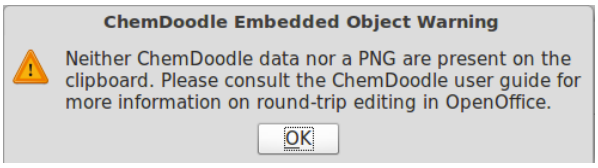
The following warnings means that you should enable *ChemDoodle Collage* in Advanced Preferences.



The following warning means that *PNG (720dpi)* needs to be enabled in Advanced Preferences.



The following warning means you need to read the **Clipboard Settings** section above again.



Other Issues

Why is a bitmap image used instead of a vector graphic?

OpenOffice/LibreOffice does not support vector graphics through their Embedded Object insertion. Please contact the appropriate Office development teams to urge them to improve this. For now, we use a 720 dpi image so print quality will still be excellent.

Why can't I paste the object directly between Office applications?

This is apparently a bug in OpenOffice/LibreOffice, please contact the appropriate Office development teams to urge them to fix this.

Why do I have to double click the object to round trip it?

This is just what OpenOffice/LibreOffice requires to execute the object. Please contact the appropriate Office development teams to urge them to improve this.

Why can't I just paste the object? Why do I need to go through the menu to insert it?

Implementing direct pasting of the object exhibits many inconsistencies which make it unsuitable for regular use. This is something we are trying to work around. Please contact the appropriate Office development teams to urge them to fix this.

Printing

The document can be printed from ChemDoodle. In most cases, this procedure is identical to other applications you use on your operating system. You can define settings, preview, and print.

Page Setup

By selecting the **Page Setup...** menu item in the **File** menu, you will be able to set the printer settings. The window that appears will be identical to the same window that appears

in other applications on your operating system. Here, you can determine which printer to print to and set up the page orientation.

Flipping the Page Orientation

In some cases, you may desire that your document is printed in landscape mode. To do this, perform the following steps:

1. Select the **Page Setup...** menu item in the **File** menu.
2. In the window that appears, find the appropriate setting for page orientation, and change it to landscape.
3. Press the confirm button in the window to save your settings and close it.
4. A question will appear asking if you would like to swap the width and height of ChemDoodle. If this is appropriate for your document, select **Yes**, otherwise, select **No**.

It is important that the direction that the printer prints your document, and the size of your document are distinct. Printing in landscape mode only means that the printer prints your content at a 90 degree angle. It does not alter your document in any way. So in some cases, you may want to flip the dimensions of your document and reorient your figures such that they will better fit on a landscape orientation.

This procedure gives you the most control over your documents, by allowing you to control the dimensions of your document and separately to control the orientation that your document is printed to the printer.

Print Preview

To preview your document before you print, select the **Print Preview** menu item in the File menu. Click the **Ok** button to the bottom right when you are finished to close the preview. Only the content that should appear in the printing will appear in the preview, no warnings, highlights or other interface decorations will be present.

Printing a Document

To print a document, perform the following steps:

1. Select the **Print...** menu item in the **File** menu.
2. In the window that appears, confirm or change any available settings.
3. Press the **Print** button to print your document.

Appendix A: Managing ChemDoodle

Overview

The chapters in this user guide explain how to use ChemDoodle to draw and work with chemical figures. There are other functions for managing the application itself.

This section shows the new user how to manage ChemDoodle. It covers the following topics:

- Updating ChemDoodle.
- Deactivating and restoring ChemDoodle.
- Using your iChemLabs account.
- Making use of provided media and resources.

Application and File Icons

You may wish to associate file icons and application icons with ChemDoodle if ChemDoodle does not already do this for you, such as on Linux. In the *resources* folder in the main *ChemDoodle* installation folder, operating system specific graphics will be provided for ChemDoodle and recognized chemical file types. Use you operating system's documentation to associate those icons with the application and file types.

Updating ChemDoodle

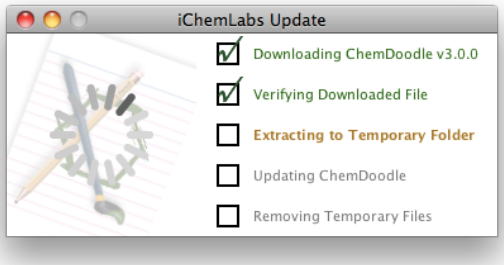
ChemDoodle will check for official iChemLabs updates and will automatically update to the latest available version for you if you allow it to do so.

To check for updates, just click the **Check For Updates** menu item in the **Help** menu. If no update is available, you will see a confirmation message stating that your copy of ChemDoodle is up to date. If there is an update available, you will see an **Update Available** window appear listing all the changes introduced by the update. Just click the **Update** button to proceed. ChemDoodle will close to perform the update, so make sure to save your files before continuing.

> *NOTE: You must have administrator privileges to update ChemDoodle. If you see a message stating that you cannot update because you do not have the necessary permissions, please double check that you ran ChemDoodle as administrator (on Windows for instance) or contact your system administrator to help you.*

The auto-updater will then open. It will download the latest ChemDoodle updates, verify the contents with our server, and then proceed to update ChemDoodle. The updater can be seen in *Figure A.1*. It may take several minutes to complete. After the updater completes, it will notify you that it is ready and that ChemDoodle will be reopened. Just click the **Ok** button to close the updater and continue. Your version of ChemDoodle has now been updated. Enjoy!

Figure A.1: The iChemLabs Updater



By default, ChemDoodle will automatically check for updates while loading. You can disable this feature in the **Preferences** window under the **Online** tab. You may always manually check for updates by using the menu item mentioned above.

Windows Administrator Privileges

A common issue on Windows Vista/7+ is to enable administrator privileges for ChemDoodle to update. If ChemDoodle states that you do not have the necessary administrator privileges on these platforms, perform the following steps:

1. Exit ChemDoodle.
2. Locate the ChemDoodle icon (shortcut or actual application).
3. Right-click on the icon and select **Run as administrator**.
4. Accept the security request.

You will then be able to update ChemDoodle.

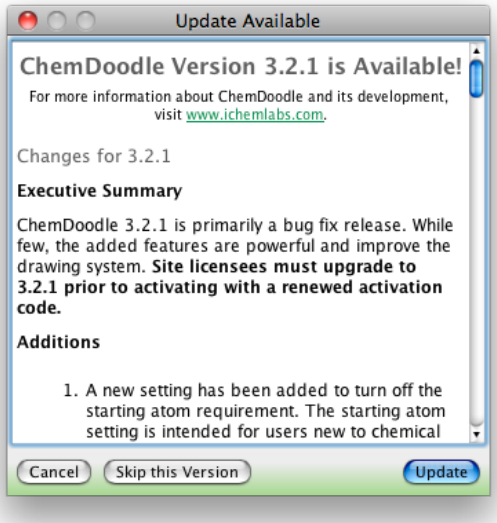
If this process does not work, you will need to consult with a system administrator to update ChemDoodle.

Skipping Updates

If you wish to ignore the current update, when the **Update Available** window is displayed, just select the **Skip this Version** button as shown in *Figure A.2*. You will no longer be notified that this update is available. You will still be notified of subsequent updates, which you may also skip.

To obtain an update that was skipped, select the **Check For Updates** menu item in the **Help** menu.

Figure A.2: The Update Available window with the Skip this Update button.



Purchasing Upgrades

Major version upgrades to ChemDoodle must be purchased. When a major version upgrade becomes available, you will still be presented with the **Update Available** window. However, instead of an **Update** button, a **Purchase Upgrade** button will be presented. Click on the **Purchase Upgrade** button to be directed to the upgrade purchase page. After purchasing the upgrade, again check for updates. The **Update** button will then be showing and you may proceed with the update as described in the previous sections.

Moving your Activated Copy to a New Computer

At some point, you may want to switch to a different computer. Your purchased

ChemDoodle activation code is restricted by the number of computers ChemDoodle is activated on. Therefore, we provide you the ability to deactivate ChemDoodle and reactivate it on a new computer. To begin, just click the **Deactivate ChemDoodle** menu item in the **Help** menu.

NOTE: When deactivating ChemDoodle and switching to a new computer, your custom preferences and other user settings will be lost. If you have settings files (templates, chemical document settings), those can be copied to the new ChemDoodleSettings folder that will appear after ChemDoodle is activated on the new computer.

Once the deactivation procedure has begun, it cannot be cancelled. Make sure you record your activation code, which will be displayed in the **Details** section of the deactivation confirmation message, so you can use it again. You should also have a record of your code from the email receipt you received upon purchasing it.

Once you accept the confirmation message, ChemDoodle will close and your copy will be deactivated. You may now use your activation code to activate ChemDoodle on a new computer.

Preparing for a System Restore

If you do anything to your system that will remove or eliminate the ChemDoodle license file, such as performing a system restore or installing your operating system from scratch, you will need to first deactivate your copy of ChemDoodle. Instructions for deactivating ChemDoodle can be found in the previous section.

Using iChemLabs Cloud Services

With an iChemLabs account, you have the ability to save files online so you can open them anywhere or send them to other iChemLabs applications as well as access relevant cloud services from within ChemDoodle.

You may log into your iChemLabs account at anytime in ChemDoodle by choosing the **Sync with Online Account...** menu item in the **File** menu. The login window will also have an option to link your iChemLabs account with your copy of ChemDoodle. If selected, ChemDoodle will automatically log into your iChemLabs account while it starts up. You can then change these settings at any time in the **Preferences** window under the **Online** tab.

All customers receive a free account to use this feature. Your username is the email address your activation code is associated with, and your password is the last 4 characters of your activation code. The password must be either in all uppercase or all lowercase.

Currently, the following iChemLabs applications integrate with your iChemLabs account:

- ChemDoodle
- ChemDoodle Mobile

Appendix B: Chemical File Types

Overview

ChemDoodle can currently read and write 24 different chemical file types. This section discusses the following issues:

- What chemical file types are supported.
- ChemDoodle's adherence to third party file type specifications.
- The extent of support for third party chemical file types.
- Warnings about saving your documents in a format other than the ChemDoodle Document format.
- How to annotate your files.
- How to use ChemDoodle's file conversion tool.

Adherence to Third Party Specifications

File formats implemented in ChemDoodle strictly follow their published specifications. ChemDoodle does not take liberties with their rules or inject ChemDoodle-only content into them. All file format objects and properties are mapped as closely as possible to objects and properties in ChemDoodle. Thorough implementation details are also provided in the following sections. Specification references can be found by selecting the **References** menu item in the **Help** menu.

ChemDoodle will try to interpret all 3rd party files as best as possible, so if you do find a file that doesn't read well, please send it to us so we can improve our compatibility.

Be Careful Saving 3rd Party Formats

ChemDoodle does its best to preserve the data it reads in from third party formats, however it may not be perfect as those formats may have been intended for systems that are very different from ChemDoodle. For instance, one program may define a charge by placing a text box near an atom, while ChemDoodle defines a charge by associating a charge attribute with that atom. When read, ChemDoodle may decide to convert that text box to a charge attribute, thereby changing the data that is in the file.

That being said, it is very important that you carefully consider whether to allow ChemDoodle to save over 3rd party data files as ChemDoodle may not retain all essential information that the other program requires. When saving 3rd party files, ChemDoodle will display this warning as a reminder before allowing you to continue. These warnings can be disabled in the **Preferences** window under the **Saving** tab.

Instead, we recommend that you first save a copy of that file to edit, instead of saving over files created in other applications.

Testing 3rd Party File Type Output

If you are unsure about whether your document will be saved in its entirety to a 3rd party format, first check with this documentation. If you are still concerned, save a test file in ChemDoodle, close the

document you just saved, and then reopen the file in ChemDoodle. If some content is missing or any object properties have changed in some way, then the format you are trying to save to does not support those objects and/or properties or ChemDoodle does not yet support the output of those objects and/or properties for that format.

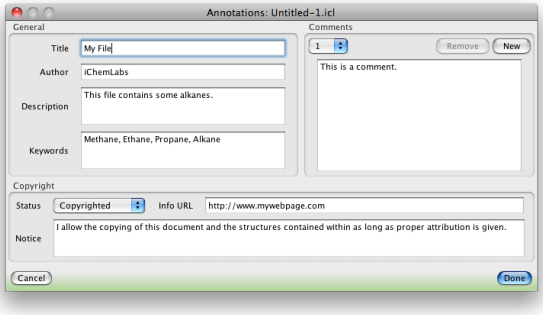
Supported Chemical File Types

1. ChemDoodle Documents (*.icl*)
2. ChemDoodle Javascript Data (*.cwc.js*)
3. ACD/ChemSketch Document (*.sk2*)
4. Beilstein ROSDAL (*.ros*)
5. CambridgeSoft ChemDraw Exchange (*.cdx*)
6. CambridgeSoft ChemDraw XML (*.cdxml*)
7. CHARMM CARD File (.crd)
8. ChemAxon Marvin Document (*.mrv*)
9. Chemical Markup Language (*.cml*)
10. Daylight SMILES (*.smi*, *.smiles*)
11. IUPAC InChI (*.inchi*)
12. IUPAC JCAMP-DX (*.jdx*, *.dx*)
13. ISIS Sketch File (*.skc*)
14. ISIS Sketch Transportable Graphics File (*.tgf*)
15. MDL MOLFiles, both V2000 and V3000 connection tables (*.mol*, *.mdl*)
16. MDL RXNFiles, both V2000 and V3000 connection tables (*.rxn*)
17. MDL RDFiles (*.rdf*, *.rd*)
18. MDL SDFiles (*.sdf*, *.sd*)
19. Molinspiration JME String (*.jme*)
20. RCSB Protein Data Bank Files (*.pdb*, *.ent*)
21. Schrödinger MacroModel (*.mmd*, *.mmod*)
22. Schrödinger Maestro (*.mae*)
23. Standard Molecular Data (*.smd*)
24. Tripos Mol2 (*.mol2*, *.ml2*, *.sy2*)
25. Tripos Sybyl Line Notation (*.sln*)
26. XYZ Files (*.xyz*)

File Annotations

Annotations can be read and written to files where possible. Each document has its own set of annotations. To view previously defined annotations, edit them or create your own, select the **Annotations...** menu item in the **File** menu. Then edit the fields shown in *Figure B.1*.

Figure B.1: File Annotations Window

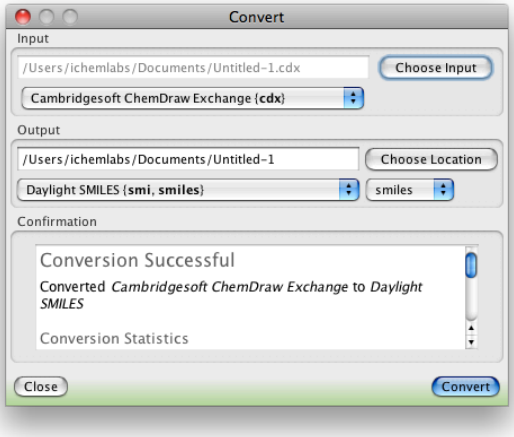


All data associated with a file will be saved in ChemDoodle Documents. Other users that open your annotated ChemDoodle Documents files will be able to easily access them. Other file types may be able to save annotations as well, read their documentation in the following sections for the extent of annotation functionality.

File Conversion Tool

ChemDoodle contains robust functionality for easily and quickly converting files between different formats. This tool is accessed by clicking the **Convert...** menu item in the **File** menu and is shown in *Figure B.2*. Unlike other chemical conversion utilities, ChemDoodle converts all document objects and properties in addition to just atoms and bonds; this including shapes, fonts, colors, annotations, document settings, etc.

Figure B.2: Chemical File Conversion Utility



Perform the following steps to convert a file:

1. Choose a recognized input file with the file chooser that appears after clicking the **Choose Input** button. Use the file format filter at the bottom of the file chooser to select different file formats.
2. Choose the location to store the output by clicking the **Choose Location** button or by manually typing in the path to the file. You can change the name of the output file this way.
3. Choose an output format and extension from the drop down selection below the output location.
4. Click the **Convert** button.

When complete, ChemDoodle will display statistics about the conversion or any issues encountered.

iChemLabs ChemDoodle Documents

About
The ChemDoodle Document format is the native ChemDoodle format. Everything created in ChemDoodle can be stored in a ChemDoodle Document.

Versions
- any

Extensions
- .icl
- .icxml

Format
XML

Annotations
All annotations are saved.

Document Settings
All document settings are stored.

Options
- **Embed Images** - Embedding images will result in larger save files, but the documents will open on other computers without needing to first find the images. If there are pasted images in a document (rather than loaded from a file), allow the embedding of images to save them properly.

iChemLabs ChemDoodle Javascript Data

About
The ChemDoodle Javascript Data format is a Javascript file containing JSON data for native objects that can be handled by the ChemDoodle Web Components.

Versions
- any

Extensions
- .cwc.js

Format
Javascript with JSON

Annotations
No annotations are saved.

Document Settings
No document settings are stored.

Options
Currently, there are no options.

ACD/ChemSketch Document

About
This is a binary format for storing chemical figures and is the main format for the ACD/ChemSketch application. Non-chemical objects are not yet supported. Most chemical objects and properties that are mutually inclusive between ChemSketch and ChemDoodle are supported.

Version
2+

Extensions
- .sk2

Format
Binary

Annotations
No annotations are stored.

Document Settings
Styles for objects are stored but there is no global style sheet.

Options
Currently, there are no options.

Supported Formats
- ACD_ChemSketch_2_0_DocumentFormat
    - DocumentDescriptionFormat
        - PageDescriptionFormat
        - PictureFormat
            - StyleListFormat
                - BaseGraphStyleFormat
                - PenStyleFormat
                - FontStyleFormat
                - AtomStyleFormat
                - BondStyleFormat
            - ObjectsListFormat
                - MoleculeFormat
                - AtomDataFormat
                - BondDataFormat
        - PageInfoDescriptionFormat
    - EnvironmentDescriptionFormat

Notes
- Most mutually inclusive chemical objects between ChemSketch and ChemDoodle are supported.
- Shapes are not yet supported.
- There is a serious issue with how superatoms are stored in ChemSketch files that renders them impossible to recover. In these cases, ChemDoodle will replace the superatom with a Carbon atom.
- All bond types are mapped to the closest supported bond type.

Beilstein ROSDAL

About
Beilstein ROSDAL is a chemical line notation format. ROSDAL stands for **R**epresentation **O**f **S**tructure **D**escription **A**rranged **L**inearly. The documentation on this format is quite sparse and most programs will not support it.

Version
Unknown

Extensions
- .ros

Format
Line Notation, plain text

Annotations
No annotations are stored.

Document Settings
No document settings are stored.

Options
Currently, there are no options.

Notes
- All non-elemental atom labels are converted to Carbon labels.
- All bond types are mapped to the closest supported bond type.
- Line notation formats do not contain coordinates. They will have to be generated by the application that reads the ROSDAL file.
- Shapes will not be stored.
- ROSDAL shorthands, charges and stereochemical bonds are supported.
- Based on the sparse documentation, ROSDAL is completely implemented in ChemDoodle.

CambridgeSoft ChemDraw Files

About
CDX Files

This is a binary format for storing chemical figures. Non-chemical objects are supported. Most objects and properties that are mutually inclusive between ChemDraw and ChemDoodle are supported. This is a common format for manuscript submission, but we recommend that you use CDXML instead as CambridgeSoft suggests it.

CDXML Files

ChemDraw XML files are identical to their CDX counterparts, except they are XML format instead of binary. We recommend that you use CDXML for manuscript submission if ChemDoodle Documents are not an option.

Version
8+

Extensions
- cdx
- cdxml

Format
CDX is binary while CDXML is XML

Annotations
No annotations are stored.

Document Settings
Most document settings are stored.

Options
Currently, there are no options.

Supported Objects and Properties
- kCDXProp_CreationProgram
- kCDXProp_Name
- kCDXProp_PrintMargins

- kCDXProp_ChainAngle
- kCDXProp_BondLength
- kCDXProp_BoldWidth
- kCDXProp_LineWidth
- kCDXProp_MarginWidth
- kCDXProp_HashSpacing
- kCDXProp_FractionalWidths
- kCDXProp_InterpretChemically
- kCDXProp_BondSpacing
- kCDXProp_LabelStyle
- kCDXProp_MacPrintInfo
- kCDXProp_ColorTable
- kCDXProp_FontTable
  - kCDXObj_Page
    - kCDXProp_BoundingBox
    - kCDXProp_HeightPages
    - kCDXProp_WidthPages
    - kCDXObj_Fragment
      - kCDXObj_Node
        - kCDXProp_2DPosition
        - kCDXProp_3DPosition
        - kCDXProp_Node_Element
        - kCDXProp_Atom_Isotope
        - kCDXProp_Atom_Charge
        - kCDXProp_Atom_Radical
        - kCDXProp_Atom_ShowStereo
        - kCDXProp_Atom_CIPStereochemistry
        - kCDXProp_IgnoreWarnings
        - kCDXProp_Atom_ShowStereo
        - kCDXObj_Text
          - kCDXProp_Text
          - kCDXProp_RotationAngle
      - kCDXObj_Bond
        - kCDXProp_Bond_Begin
        - kCDXProp_Bond_End
        - kCDXProp_Bond_Order
        - kCDXProp_Bond_Display
        - kCDXProp_Bond_Display2
        - kCDXProp_ForegroundColor
        - kCDXProp_BoldWidth
        - kCDXProp_LineWidth
        - kCDXProp_HashSpacing
        - kCDXProp_BondSpacing
        - kCDXProp_Bond_ShowStereo
        - kCDXProp_Bond_CIPStereochemistry
- kCDXObj_Graphic
  - kCDXProp_BoundingBox
  - kCDXProp_Graphic_Type
  - kCDXProp_ForegroundColor
  - kCDXProp_LineWidth
  - kCDXProp_BoundingBox
  - kCDXProp_Arrow_Type

- kCDXProp_Arrow_HeadSize
- kCDXProp_SupersededBy
- kCDXObj_Arrow
  - kCDXProp_ForegroundColor
  - kCDXProp_ArrowShaftSpacing
  - kCDXProp_ArrowheadTail
  - kCDXProp_ArrowheadHead
  - kCDXProp_Arrow_HeadSize
  - kCDXProp_Tail3D
  - kCDXProp_Head3D
- kCDXProp_Arc_AngularSize
- kCDXProp_CornerRadius
- kCDXProp_Rectangle_Type
- kCDXProp_BoldWidth
- kCDXProp_Center3D
- kCDXProp_MajorAxisEnd3D
- kCDXProp_MinorAxisEnd3D
- kCDXProp_Oval_Type
- kCDXProp_Orbital_Type
- kCDXProp_Bracket_Type
- kCDXObj_BracketedGroup
  - kCDXObj_BracketAttachment
    - kCDXProp_Bracket_GraphicID
- kCDXProp_Symbol_Type
- kCDXObj_Text
  - kCDXProp_BoundingBox
  - kCDXProp_2DPosition
  - kCDXProp_LineStarts
  - kCDXProp_Text
- kCDXObj_EmbeddedObject
  - kCDXProp_BoundingBox
  - kCDXProp_ForegroundColor
  - kCDXProp_GIF
  - kCDXProp_TIFF
  - kCDXProp_PNG
  - kCDXProp_JPEG
  - kCDXProp_BMP
  - kCDXProp_RotationAngle
- kCDXProp_EndObject

Notes

- Most mutually inclusive objects between ChemDraw and ChemDoodle are supported.
- All bond types are mapped to the closest supported bond type.
- ChemDraw formats do not use Unicode characters, which has become the standard. Upon read, ChemDoodle will convert Symbol font characters to their corresponding unicode characters, however, the reverse is not done. Greek characters (and other non-Latin Unicode characters) may not be displayed correctly in ChemDraw for this reason.

CHARMM CARD File

About
CHARMM CARD files describe cartesian coordinates for molecules. These files are typically used with the CHARMM software.

Version
c36b2

Extensions
- .crd

Format
ASCII, plain text

Options
Currently, there are no options.

Annotations
No annotations are stored.

Document Settings
No document settings are stored.

Notes
- All non-elemental atom labels are converted to Carbon labels.
- Shapes will not be stored.
- All coordinates are in Ångströms and are centered around the origin.

ChemAxon Marvin Documents

About
Marvin Documents extend chemical markup language with additional objects and properties representing the graphical abilities of ChemAxon products.

Version
5.3.2

Extensions
- .mrv

Format
XML

Annotations
Inherits CML annotations.

Document Settings
No document settings are stored.

Options
Inherits CML options.

Supported Tags and Attributes
*inherits *CML* objects and properties

- MDocument
  - MChemicalStruct
  - MTextBox
    - MField
    - MPoint
      - x
      - y
  - MEllipse
    - thickness
    - lineColor
    - MPoint

        - x
        - y
    - MRectangle
        - thickness
        - lineColor
        - MPoint
            - x
            - y
    - MRoundedRectangle
        - thickness
        - lineColor
        - arcWidth
        - arcHeight
        - MPoint
            - x
            - y
    - Bracket
        - thickness
        - lineColor
        - type
        - MPoint
            - x
            - y
    - MPolyline
        - thickness
        - lineColor
        - type
        - headLength
        - tailLength
        - arcAngle
        - MPoint
            - x
            - y
    - MTextBox
        - MField
        - MPoint
            - x
            - y

Notes

- Most mutually inclusive objects between MarvinSketch and ChemDoodle are supported.
- All bond types are mapped to the closest supported bond type.
- Output is always in arrays.
- Inherits CML notes.

Chemical Markup Language

About
Chemical Markup Language stores a wide range of chemical objects and properties utilizing XML protocol. It is only a secondary format, most useful for embedding chemical content in webpages.

Versions
- 2
- 1 *(Read-only)*

Extensions
- .cml

Format
XML

Annotations

If provided, annotations are read and written with the logically corresponding attributes in the metadataList element: dc:creator, dc:date, dc:description, dc:rights, dc:title.

Document Settings
No document settings are stored.

Options
- **Dimension**: Either 2 dimensions can be save with coordinates in pixels (for drawings), or 3 dimensions can be saved with coordinates in Ångströms (for exact structural coordinates).
- **Arrays**: You may store all atoms and bonds as arrays to save space. Child objects of atoms and bonds will be excluded.

Supported Tags and Attributes
- cml
    - list
        - metadataList
            - metadata
                - name
                - content
    - molecule
        - formula
            - title
        - atomArray
            - atom
                - id
                - elementType
                - formalCharge
                - isotope
                - x2
                - y2
                - xy2
                - x3
                - y3
                - z3
                - xyz3
        - bondArray
            - bond
                - id
                - atomRefs2
                - order
                - bondStereo

Notes
- All non-elemental atom labels are converted to Carbon labels. "Du", "Dummy" and "R" are allowed.
- All bond types are mapped to the closest supported bond type.

- Shapes will not be stored.
- All 2D coordinates are in pixels.
- All 3D coordinates are in Ångströms and are centered around the origin.
- CML array formats can be read and written.
- The older version 1 format of CML can also be read, but it cannot be written.

Daylight SMILES

About
Daylight SMILES is a chemical line notation format. SMILES stands for **S**implified **M**olecular **I**nput **L**ine **E**ntry **S**pecification.

Version
4.9

Extensions
- .smi
- .smiles

Format
Line Notation, plain text

Options
- **Output Aromaticity**: If selected, then an aromatic model will be imposed on the output SMILES string with lower case letters, such that a Kekulé structure of benzene will be output as *c1ccccc1* instead of *C1=CC=CC=C1*.
- **Kekulize Input**: If selected, input data that contains aromatic information will be Kekulized and that aromatic information will be lost.

Annotations
No annotations are stored.

Document Settings
No document settings are stored.

Notes
- All non-elemental atom labels are converted to Carbon labels.
- Isotopes and charges are handled.
- All bond types are mapped to the closest supported bond type.
- Line notation formats do not contain coordinates. They will have to be generated

by the application that reads the SMILES file.

- Shapes will not be stored.

IUPAC InChI

About

IUPAC InChI is a unique and unambiguous chemical line notation format. InChI stands for **In**ternational **Ch**emical **I**dentifier. It is quickly becoming a standard identifier in databases.

Version
1.02

Extensions
- .inchi

Format
Line Notation, plain text

Annotations
No annotations are stored.

Document Settings
No document settings are stored.

Options
- **Auxiliary Information**: Include the auxiliary information with each InChI string.
- **InChI Key**: Include a unique InChI key with each InChI string.

Notes
- All non-elemental atom labels are converted to Carbon labels.
- All bond types are mapped to the closest supported bond type.
- InChI files do not contain coordinates unless they are provided in an Auxiliary information string. They will have to be generated by the application that reads the InChI file.
- Shapes will not be stored.

- ChemDoodle utilizes JNI-InChI, which is a wrapper around the official IUPAC source for generating InChI files.

IUPAC JCAMP Data

About
JCAMP is primarily for storing spectroscopic data, but can also store low resolution chemical structure data. The supported techniques are mass spectrometry, infrared spectroscopy, nuclear magnetic resonance spectroscopy and ion mobility spectrometry. JCAMP data stands for the **J**oint **C**ommittee on **A**tomic and **M**olecular **P**hysical data. While spectra and chemical structures are read, currently only chemical structures are written, but support for spectra output will be provided in the future.

Versions
- **IR** - 4.24
- **MS** - 5.00
- **NMR** - 5.00
- **Chemical Structures** - 3.7

Extensions
- .jdx
- .dx

Format
Plain text

Annotations
If provided, annotations are read and written from appropriate records. Title, author and copyright status are supported.

Document Settings
No document settings are stored.

Options
- **Convert Hz to PPM**: If enabled and an NMR spectrum is read in with Hz as the x-unit, ChemDoodle will automatically convert the domain to ppm.

Supported Records

- TITLE
- JCAMP-CS
- ORIGIN
- OWNER
- MOLFORM
- ATOMLIST
- BONDLIST
- DATE
- TIME
- CHARGE
- RADICAL
- MAX_RASTER
- XY_RASTER_FACTOR
- XY_RASTER

Notes

- Spectra are read, but not written. Be careful not to overwrite your data.
- All non-elemental atom labels are converted to Carbon labels.
- All bond types are mapped to the closest supported bond type.
- Shapes will not be stored.
- This format is typically for the storage of spectra, but chemical structures can be included.

MDL ISIS Sketch Files

About

SKC Files

This is the default format for storing chemical drawings in ISIS Sketch and Symyx Draw. Non-chemical objects are supported. All objects and properties that are mutually inclusive between ISIS Sketch and ChemDoodle are supported. This format was designed to be platform dependent (for some unknown reason), so SKC files written on Windows will not work on Macs and vice versa. However, ChemDoodle can recognize all SKC files and will correctly read them regardless of what platform they were generated on. You may choose which SKC output format to use if necessary.

TGF Files

ISIS Sketch transportable graphics files are identical to their SKC counterparts, except they are ASCII format instead of binary. Symyx seems to have discontinued support for this format, so most applications will probably not read them.

Version

4

Extensions

- .skc
- .tgf

Format

SKC is binary, TGF is plain text

Annotations

No annotations are stored.

Document Settings

No document settings are stored.

Options

- **SKC Binary Output Format**: ISIS Sketch SKC files are platform dependent, as per MDL's specification. SKC files written on Windows will not work on Macs and vice versa. You may modify how the files are saved with this setting. Upon read, ChemDoodle will determine which format is used, and report any problems.

Supported Blocks and Properties

- rect
  - Obj_coords
  - Pen_width
  - Pen_style_token
  - Fill_style
  - Transparent
  - Pen_RGB2Color
  - Fill_RGB2Color
  - Pen_widthUnit
  - RxnAtch
- rounded_rect
  - Obj_coords
  - Roundrect_curve
  - Pen_width
  - Pen_style_token
  - Fill_style
  - Transparent
  - Pen_RGB2Color
  - Fill_RGB2Color
  - Pen_widthUnit
  - RxnAtch
- line
  - Obj_coords
  - Pen_width
  - Pen_style_token
  - Fill_style
  - ArrowDir
  - ArrowStyle
  - ArrowSize
  - Transparent
  - Pen_RGB2Color
  - Fill_RGB2Color
  - Pen_widthUnit
  - RxnAtch
- polygon
  - Poly_points
  - Poly_smoothed
  - Pen_width
  - Pen_style_token
  - Fill_style
  - Transparent
  - Pen_RGB2Color
  - Fill_RGB2Color
  - Pen_widthUnit
  - RxnAtch
- ellipse
  - Obj_coords
  - Pen_width
  - Pen_style_token

    - Fill_style
    - Transparent
    - Pen_RGB2Color
    - Fill_RGB2Color
    - Pen_widthUnit
    - RxnAtch
- arc
    - Obj_coords
    - Arc_endpts
    - Pen_width
    - Pen_style_token
    - Fill_style
    - ArrowDir
    - ArrowStyle
    - ArrowSize
    - Transparent
    - Pen_RGB2Color
    - Fill_RGB2Color
    - Pen_widthUnit
    - RxnAtch
- spline
    - Poly_points
    - Poly_smoothed
    - Pen_width
    - Pen_style_token
    - Fill_style
    - Transparent
    - Pen_RGB2Color
    - Fill_RGB2Color
    - Pen_widthUnit
    - RxnAtch
- text
    - MDLEdittext
    - Obj_coords
    - Pen_width
    - Pen_style_token
    - Fill_style
    - Transparent
    - Pen_RGB2Color
    - Fill_RGB2Color
    - Pen_widthUnit
    - RxnAtch
- subsketch
    - Begsketch
    - Endsketch
    - Totobjs
- mol
    - Begsketch
    - Endsketch
    - RxnAtch
- rxnarrow
    - Obj_coords
    - Pen_width
    - Pen_style_token
    - Fill_style
    - ArrowDir

    - ArrowStyle
    - ArrowSize
    - Transparent
    - Pen_RGB2Color
    - Fill_RGB2Color
    - Pen_widthUnit
    - RxnAtch
- bracket_rect
    - Obj_coords
    - Roundrect_curve
    - Pen_style_token
    - Transparent
    - Pen_RGB2Color
    - Fill_RGB2Color
    - Pen_widthUnit
    - RxnAtch
- circ_arc
    - Obj_coords
    - Arc_endpts
    - Pen_width
    - Pen_style_token
    - Fill_style
    - ArrowDir
    - ArrowStyle
    - ArrowSize
    - Transparent
    - Pen_RGB2Color
    - Fill_RGB2Color
    - Pen_widthUnit
    - RxnAtch
- smooth_spline
    - Poly_points
    - Pen_width
    - Pen_style_token
    - Fill_style
    - Transparent
    - Pen_RGB2Color
    - Fill_RGB2Color
    - Pen_widthUnit
    - RxnAtch
- bond
    - Bond_atoms
    - Bond_type
    - Bond_stereo_type
    - Fill_style
    - Bond_hash_spacing
    - Bond_bond_spacing
    - Bond_crossed
    - Bond_alt_stereo
    - Pen_width
    - Pen_RGB2Color
    - Pen_widthUnit
    - RxnAtch
- atom
    - Atom_coords
    - Atom_zcoord

- Atom_type
- Atom_symbol
- Atom_chg
- Atom_rad
- Atom_msdif
- Font
- Pen_RGB2Color
- Atom_margin_width
- RxnAtch

Notes

- All mutually inclusive objects between ISIS Sketch and ChemDoodle are supported.
- All bond types are mapped to the closest supported bond type.

MDL Connection Table Files

About

MOL Files

MOL files have become one of the most popular formats for storing chemical information, especially in drawing programs. It typically stores only a single molecule. It consists of a header followed by an MDL connection table. All connection table formats follow ASCII standards.

SD Files

A SD (structure-data) file stores any number of molecules and other annotations. SD files are simply concatenated MOL files with additional data records.

RXN Files

RXN file is a very popular format for storing a single discrete chemical reaction. If consists of connection tables for the reactants and products.

RD Files

A RD (reaction-data) file stores any number of reactions and molecules and other annotations. RD files are simply concatenated RXN and MOL files with additional data records.

Versions

- v3000
- v2000
- v1000 *(Read only)*

Extensions

- .mol
- .mdl
- .sdf

- .sd
- .rxn
- .rdf
- .rd

Format
ASCII, plain text

Annotations
Only a title and the first comment is stored in the header if provided (80 characters each max). All annotations are stored as data records in SD files. Since the data headers are not specifically standardized, other programs will probably not be able to read them, but anyone can view the file in a text editor to see the information.

Document Settings
No document settings are stored.

Options
- **Bond Length Conversion**: Coordinates are in bond lengths. When saving, coordinates can be converted using the standard bond length (30px) or the currently selected bond length.
- **Force v3000 Connection Tables**: v2000 connection tables are standard and used by default; V3000 connection tables must be and will be automatically used if a connection table contains more than 999 atoms.
- **Output Hydrogen Counts**: If this option is selected, the query values for Hydrogen counts will be provided in both v2000 and v3000 connection tables..

Supported Blocks and Properties
v2000

- Atom
- Bond
- Properties
  - Atom Alias
  - Charge
  - Radical
  - Isotope
  - End of Block

v3000

- CTAB
- COUNTS
- ATOM
  - CHG
  - RAD
  - MASS
  - HCOUNT
- BOND
  - CFG
- BEGIN REACTANT
- END REACTANT
- BEGIN PRODUCT
- END PRODUCT

Notes
- All non-elemental atom labels are converted to Carbon labels in v2000 connection tables, but the Alias property is used for those programs that read it. All labels are retained in v3000 connection tables, with blanks as '*'.
- All bond types are mapped to the closest supported bond type.
- Shapes will not be stored.

- All coordinates are in bond lengths and are centered around the origin.

Molinspiration JME String

About
JME Strings are technically a line notation, but do not compress connection tables. This format is mainly for input and output from Molinspiration's Java Molecular Editor (JME).

Version
Unknown

Extensions
- .jme

Format
Line Notation, plain text

Annotations
No annotations are stored.

Document Settings
No document settings are stored.

Options
Currently, there are no options.

Notes
- All non-elemental atom labels are converted to Carbon labels.
- All bond types are mapped to the closest supported bond type.
- Charges are stored.
- Shapes will not be stored.

RCSB Protein Data Bank Files

About
The Protein Data Bank format is one of the most popular formats for storing 3D chemical data. A large database of Protein Data Bank files is hosted at the RCSB website for public use. The RCSB also hosts a large set of monomer units which describe the topology in PDB files. Since most of the data is based on crystallographic information, bond orders are vague and only single bonds are recognized. PDB files are not recommended for the storage of 2D chemical drawings.

Version
- 3.20
- earlier *(read only)*

Extensions
- .pdb
- .ent

Format
Plain text

Annotations
If provided, the authors, keywords and title will be stored.

Document Settings
No document settings are stored.

Options
Currently, there are no options.

Supported Records
- HEADER
- TITLE
- KEYWDS
- AUTHOR
- REVDAT
- ATOM
- HETATM
- CONECT
- MASTER
- END

Notes
- All non-elemental atom labels are converted to Carbon labels.
- Shapes will not be stored.
- All coordinates are in Ångströms and are centered around the origin.
- When read, the PDB monomer database is contacted to determine topology. If there are no bonds found, then ChemDoodle will attempt to calculate all bonds by covalent radii.

Schrödinger Files

About

MMD Files

The MacroModel format is the primary format for the MacroModel application. It is a modeling format and contains information on atom types.

MAE Files

The Maestro file format is the standard exchange format for Schrödinger products. Technically, it extends the MMD format.

Versions

- **MMD**-7.0
- **MAE**-8.0

Extensions

- .mmd
- .mmod
- .mae

Format

Both MMD and MAE files are plain text

Annotations

No annotations are stored.

Document Settings

No document settings are stored.

Options

Currently, there are no options.

Supported Records

MMD

The Macromodel format is supported fully and in accordance with the official documentation.

MAE

- root
- m_atom
- m_bond
- p_m_ct

Notes

- All non-elemental atom labels are converted to Carbon labels.
- Atom types are mapped as closely as possible.
- All bond types are mapped to the closest supported bond type.
- Shapes will not be stored.
- All coordinates are in Ångströms and are centered around the origin.
- Multiple molecules can be stored as compound files or movies.

Standard Molecular Data

About
Standard Molecular Data is an older ASCII format for storing chemical data. It is mainly dependent on Fortran Format specification. This format is fairly obsolete and most programs will not support it.

Version
- 4.3

Extensions
.smd

Format
ASCII, plain text

Annotations
A title is stored with the STRT block if provided. Otherwise the filename is used. The first comment will be stored in the TEXT block if provided.

Document Settings
No document settings are stored.

Options
Currently, there are no options.

Supported Blocks
- >STRT
- >DTCR
- >DTUP
- >CT
- >CO
- >LB
- >FORM

Notes
- All non-elemental atom labels are converted to Carbon labels.
- All bond types are mapped to the closest supported bond type.
- Shapes will not be stored.
- All coordinates are in pixels.
- Morgan indices are output in the Labels block.

Tripos Mol2

About
A Tripos Mol2 file is a complete, portable representation of a SYBYL molecule. This is a modeling format.

Version
7.1

Extensions
- .mol2
- .ml2
- .sy2

Format
Plain text

Annotations
If provided, annotations are written as comments at the beginning of the file. Title and author annotations are read.

Document Settings
No document settings are stored.

Options
Currently, there are no options.

Supported Records
- @<TRIPOS>ATOM
- @<TRIPOS>BOND
- @<TRIPOS>MOLECULE
- @<TRIPOS>SUBSTRUCTURE

Notes
- All non-elemental atom labels are converted to Carbon labels.
- Atom types are mapped as closely as possible.
- All bond types are mapped to the closest supported bond type.
- Shapes will not be stored.
- All coordinates are in Ångströms and are centered around the origin.
- This format is typically for the storage of a single molecule, but multiple molecules can be saved in a single Mol2 file.

Tripos Sybyl Line Notation

About
SLN is a chemical line notation format. It is derived from SMILES but contains additional explicit information such as Hydrogen counts.

Version
Unknown

Extensions
- .sln

Format
Line Notation, plain text

Annotations
No annotations are stored.

Document Settings
No document settings are stored.

Options
Currently, there are no options.

Notes
- All non-elemental atom labels are converted to Carbon labels.
- All bond types are mapped to the closest supported bond type.
- Line notation formats do not contain coordinates. They will have to be generated by the application that reads the SLN file.
- Shapes will not be stored.
- Macroatoms are read on input.

XYZ

About
The XYZ chemical filetype is a very basic data format for storing atom types and coordinates. There is no official documentation for this format, so other applications may define it differently.

Version
Unknown

Extensions
- .xyz

Format
Plain text

Annotations
If a comment is provided, it will be output in the second line of the file. The second line of the file is also read in as a comment.

Document Settings
No document settings are stored.

Options
- **Atom Identifier**: The element type can be specified with either the element's symbol or its atomic number.
- **Identifier Buffer**: The identifier can be buffered to 3 columns so programs that read it can expect a certain column width.

Notes
- Only atom symbol and coordinate data are stored.
- All non-elemental atom labels are converted to Carbon labels.
- Bonds will not be stored.
- Shapes will not be stored.
- All coordinates are in Ångströms and are centered around the origin.

- Single spaces are used to delimit tokens in the atom table.
- All coordinates are rounded and recorded to the fifth decimal place.

Appendix C: Compatibility with 3rd Party Applications

Overview

ChemDoodle works with many 3rd party applications. The most common applications are discussed in this section. It is not an inclusive list. This section lists:

- Common applications that are used with ChemDoodle.
- Which types of data are transferred to common 3rd party applications.
- Any solutions to issues involved with the 3rd party applications.
- Round trip editing compatibility.

Microsoft Office

Word

On Windows and Mac OS X, text, images and scalable vector graphics can be transferred.

For scalable vector graphics, if using Word on Windows, *Windows Enhanced Metafile* must be selected in the copy settings. For scalable vector graphics, if using Word 2004 on Mac OS X, *Macintosh Vector PICT* must be selected in the copy settings; Word 2008 requires *PDF* to be selected in the copy settings. Make sure all bitmap image types are deselected.

Round trip editing is functional on Windows with Microsoft Office using ChemDoodle's OLE library. Round trip editing is functional on Mac OS X with Microsoft Office 2011 (at update 14.0.1 or more recent).

Powerpoint

Same as Word.

Excel

Same as Word.

Apple iWork

Pages

Text, images and scalable vector graphics can be transferred. For scalable vector graphics, *PDF* must be selected in the copy settings. Round trip editing is supported via the workaround detailed in the **Round Trip Editing** section of **Chapter 10**.

Keynote

Same as Pages. Round trip editing is supported directly supported.

Numbers

Same as Pages. Round trip editing is not supported.

OpenOffice

Writer

On all operating systems, text, images and scalable vector graphics can be transferred. For scalable vector graphics, if using Writer on Windows, *Windows Enhanced Metafile* must be selected in the copy settings. For scalable vector graphics, if using Writer on Mac OS X, *Macintosh Vector PICT* must be selected in the copy settings. For scalable vector graphics, if using Writer on Linux, *OpenDocument Graphics* must be selected in the copy settings.

Round trip editing is supported on Linux by using ChemDoodle UNO plugin.

Calc
On all platforms, text, images and scalable vector graphics can be transferred.

For Mac OS X, first save ChemDoodle content as *Macintosh Vector PICTs* and then insert or drag and drop the file into Calc.

Round trip editing is supported on Linux by using ChemDoodle UNO plugin.

Impress
Same as Calc.

Adobe Products

Photoshop
Images and scalable vector graphics can be transferred. For scalable vector graphics, *PDF* must be selected in the copy settings.

Illustrator
Scalable vector graphics can be transferred. First, save content as *PDF* and then open, insert or drag and drop the file into Illustrator. For direct pasting, make sure all vector graphics are disabled except for *Windows Enhanced Metafile* on Windows or *Macintosh Vector Pict* on Mac OS X.

Browsers

Most browsers will support image and scalable vector graphic output from ChemDoodle for display in web pages. The best scalable vector graphic formats to use are *SVG* and *PDF*.

For information of *ChemDoodle Web Components* browser compatibility, visit the *ChemDoodle Web Components* website: http://web.chemdoodle.com

Other

ChemDoodle is compatible with any application that supports the data ChemDoodle places on the system clipboard. Because ChemDoodle expertly handles *Windows Enhanced Metafiles*, *Macintosh Vector PICT 2*, *PDF and OpenDocument Graphics*, scalable vector graphics can be directly pasted into all native applications.

Round trip editing will be supported with any application that supports OLE on Windows, or that will preserve PDF comments on Mac OS X.

Appendix D: Elemental Data

Overview

ChemDoodle has access to an extensive database of elemental data compiled from published resources. This section introduces the new user to ChemDoodle's chemical data. It covers the following topics:

- The elemental and chemical data provided in ChemDoodle.
- How to view the chemical data.
- Where to find references for the data.
- How to use the interactive periodic table.

Elemental Database

The elemental database allows ChemDoodle to perform many tasks, from filling the dynamic periodic table to deducing covalent bonds to calculating a molecular mass. The data itself can be viewed by opening various data tables in ChemDoodle or by using the dynamic periodic table. The data tables are found in the **View** menu. Currently ChemDoodle provides 3 data tables:

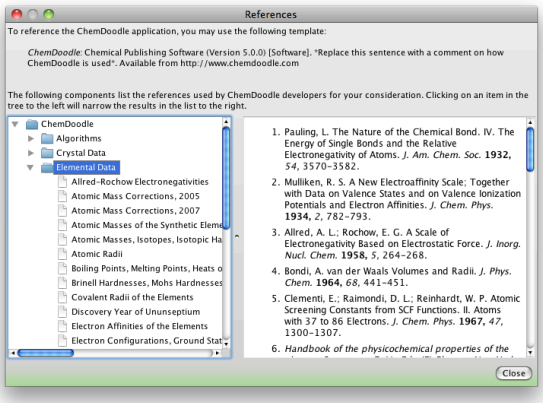
- **Elemental Data** - Displays all data in the elemental database not contained in other tables.
- **Ionization Energies** - Displays all published ionization energies for the elements.
- **Isotopes** - Displays all published isotopes, their masses, natural abundances and half-lives.

Each table is interactive, and you can click on a column header to reorder the content by that column. By clicking again you can reverse the order of that column. By pressing down and dragging, you can reorder the columns to more easily correlate different columns.

References

All data within ChemDoodle's databases are associated with a unit (if not unit-less) and the reference source it originated from so you may assess its quality. The entire set of references can be viewed at any time by selecting the **References** menu item in the **Help** menu as shown in *Figure D.1*. Non-data related references are also displayed in this list, including filetype specifications and algorithms.

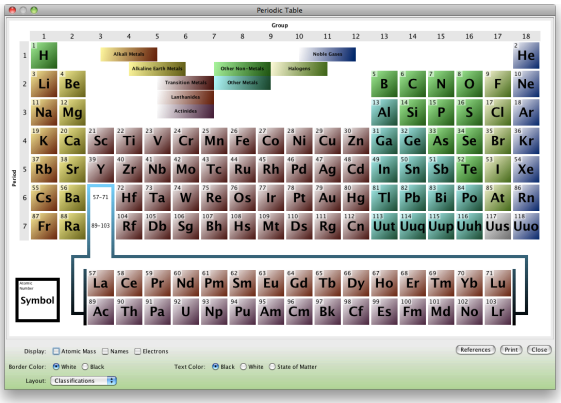
Figure D.1: ChemDoodle's References List



Interactive Periodic Table

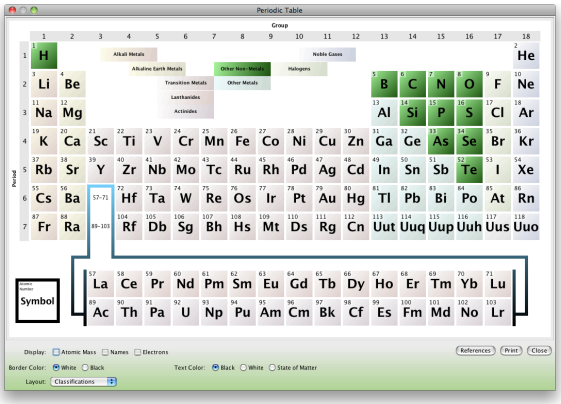
ChemDoodle contains an interactive periodic table of elements for reference, printing and demonstrations. It is viewable by selecting the the **Interactive Periodic Table** menu item in the **View** menu. The window that opens is shown in *Figure D.2*.

Figure D.2: The Interactive Periodic Table



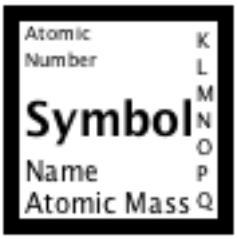
You may hover over elements and click on them for additional information. There may also be groups listed in the top region. Hovering over a group will desaturate all other groups. This is shown in *Figure D.3* when the mouse pointer hovers over the **Other Non-Metals** group.

Figure D.3: Focusing on a group.



The table is customizable and you can choose from several format options, including the display of Atomic Mass, Names and Electron configurations in addition to the element Symbol. The block in the bottom-left corner of the periodic table will display the current format of each element as shown in *Figure D.4*.

Figure D.4: Element Format



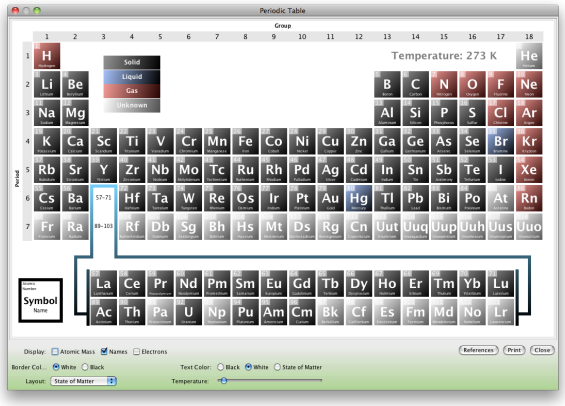
You can also customize graphical options, such as the element border colors and text color.

In addition to the traditional classifications display, you can also choose to display these other features of the elements:

- **CPK Colors** - Displays each element with its CPK (Corey, Pauling, Koltun) color.
- **Jmol Colors** - Displays each element with its Jmol color.
- **PyMOL Colors** - Displays each element with its PyMOL color.
- **State of Matter** - Each element is colored based on its state of matter at the set temperature. Solids are black, liquids are blue and gases are red. Unknown states are grey. A temperature slider will appear in the controls to set the temperature which is displayed on the top right of the figure.
- **Years of Discovery** - Each element is colored if discovered before the set year of discovery. A year slider will appear in the controls to set the year of discovery which is displayed on the top right of the figure.

Each display format shows off interesting properties and makes for great in-class demonstrations, such as the **State of Matter** display shown in *Figure D.5*.

Figure D.5: States of Matter Display



To print the periodic table, click the **Print** button at the bottom-right of the window. The **References** button will display ChemDoodle's references and the **Close** button will close the **Interactive Periodic Table** window.

Appendix E: How NMR is Simulated

Algorithms

The NMR simulation algorithms are a free and experimental feature provided in ChemDoodle. The algorithms are continuously developed and improved.

Shift Prediction

ChemDoodle estimates chemical shifts for all hydrogen or carbon atoms for which incremental constants are available. The algorithm is an empirical approach and begins by identifying key functional groups in a structure. The identified functional groups are used to determine base values for the estimated shifts of the nuclei.

After determining a base shift, a breadth-first algorithm is employed to look at the chemical environment surrounding each nucleus. Based on the functional groups around it, incremental constants are added to the base shift to calculate the estimated shift. Other contributions may be included such as ring strain and other algorithms.

Splitting

Splitting is determined by a table of typical j-constant magnitudes and the spin of the interacting nuclei. Splitting is calculated for all spins. Splitting magnitudes are determined from Pascal's triangle.

Roof Effects

The magnitude for roof effects are determined by the resolution of the spectrum, set by the **Pulse Frequency** parameter, and the relative adjacency of the interacting peaks. The simulated roof effects will show a leaning of the split peak towards the peak that is splitting it. Peaks split by multiple peaks will lean towards all of them.

Solvent Peaks

Solvent peaks are simulated using the same algorithms. Splitting from deuterium occurs. The magnitude ratio for solvent to solute peaks is determined by the **Dilution** parameter.

^{1}H Rapid Exchange

If the temperature is above 273K, rapid exchange will occur for hydrogen bonded protons. These peaks will merge into a single broadened peak with a shift calculated at their weighted average. The shift will then be moved downfield relative to the magnitude of the temperature.

^{1}H Anisotropic Effects

If the solvent or solute contain aromatic or antiaromatic rings, then ^{1}H nuclei will be appropriately shielded or deshielded based on the solvent/solute ratio and the types of rings involved.

^{1}H Diastereotopic Pairs

If a methylene is adjacent to a stereocenter, then the two methylene protons will be separated into individual peaks. The peaks will be separated by .3 ppm centered around the predicted shift for the methylene group. The choice of nucleus to be shifted upfield or downfield is random.

^{13}C Quaternary Carbon Intensity Reductions

To simulate a lack of Overhauser effects, quaternary carbons have their peak intensities reduced by 33%.

Limitations

ChemDoodle can only predict shifts for nuclei where environments are well described

in its database. Functional groups that are not described well will have poorly calculated shifts and may result in values around 0 ppm, which should be ignored.

Since incremental constants do not take into account structure topography, 3D conformations will be poorly analyzed. It is essential that you fully scrutinize all NMR simulation results from ChemDoodle.

To learn more about the algorithms implemented in ChemDoodle and their accuracy, obtain the references listed under the *Algorithms > Spectroscopy > Nuclear Magnetic Resonance* section of ChemDoodle's reference list. The reference list can be viewed by selecting the **References** menu item in the **Help** menu.

Appendix F: ChemDoodle Web Components

Overview

In addition to creating graphics and chemical files, ChemDoodle can also create dynamic web components. This feature utilizes another iChemLabs technology, the ChemDoodle Web Components library. This section lists:

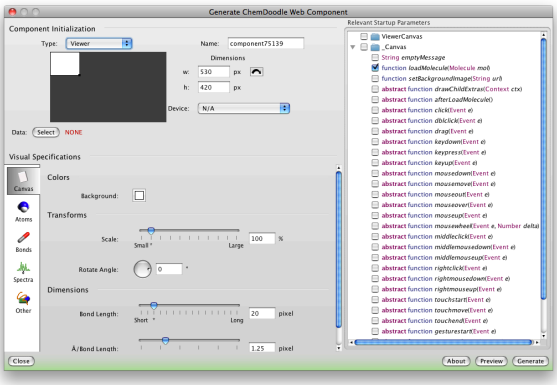
- Creating ChemDoodle Web Components in ChemDoodle.
- ChemDoodle rendering features that are available in the ChemDoodle Web Components library.
- Other functions for working with ChemDoodle Web Components.
- Learn how generated components work for both desktop and mobile browsers.
- Restrictions on using ChemDoodle Web Components in your webpages.

Generating ChemDoodle Web Components

To generate a ChemDoodle Web Component, perform the following steps:

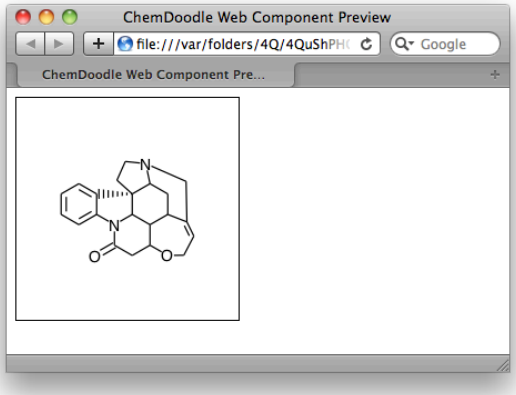
1. In the **File** menu, select the **Generate Web Component...** menu item. Make sure to first have drawn or loaded any content you wish to be displayed on the **Doodle Board**.
2. If you had selected a *Molecule* or *Spectrum* before opening this window, then an appropriate viewer will be selected. Otherwise, choose the **Type** of component you would like to create.
3. If the **Type** of component chosen requires content, then click on the **Select** button and choose the content to be displayed in the component.
4. As is shown in *Figure F.1*, set the size of the component and the component name (a random name is generated for you to avoid name clashes).

Figure F.1: Generate ChemDoodle Web Component Window



5. Define any visual specifications for the component. It will inherit compatible visual specifications from the current document style sheet in ChemDoodle.
6. In the **Relevant Startup Parameters** tree, select any *Javascript* variables or functions you would like to define. Placeholders for them will be generated in the *Javascript* code.
7. Press the **Preview** button to preview your ChemDoodle Web Component in your main browser as shown with Apple Safari in *Figure F.2*.

Figure F.2: Previewing the Web Component (Apple Safari shown)



8. Make any changes, if necessary.
9. Click the **Generate** button to generate the *Javascript* for the component.

Paste the generated *Javascript* directly in your webpage (in the <*body*> tag) in the location you prefer the component to appear. You must first install the **ChemDoodle Web Components** library for your webpage for these components to work. Installation instructions are provided on the official **ChemDoodle Web Components** website at http://web.chemdoodle.com/installation/download.

Generating Javascript Data Files for Use with ChemDoodle Web Components

If you are displaying several Web Components with the same molecule/spectrum or are doing advanced development, it may be more efficient to generate the data first in a *Javascript* data file to be loaded into your webpage. To do this, perform the following steps:

1. Draw all structures and spectra to be used in your webpage on the **Doodle Board**.
2. In the **File** menu, select the **Save as...** menu item.
3. In the file chooser that appears, select the location and the name of the file to be saved.
4. In the drop down selection for the file type, choose **iChemLabs ChemDoodle Javascript Data**.
5. Press the **Save** button.

All structures and spectra on the **Doodle Board** will be saved to the ChemDoodle Web Component JSON format in *Javascript*. To use this file, link it into the *HTML* page as a *Javascript* resource or copy and paste the source of the file into your *Javascript* code. Use the variable names declared in that file to use them.

Molecules begin with 'molecule' and spectra begin with 'spectrum'. You should rename these variables to not clash with other declared *Javascript* variables if necessary. These data structures can be used as is, such as for immediate loading into *Canvases* via load functions.

Optimizing PDB Files

The ChemDoodle Web Components can handle many of the features in PDB files. Unfortunately, reading and processing all of the data in a PDB file can be very time consuming in *Javascript*. ChemDoodle contains a special **Optimize PDB to JSON...** function in the **File** menu to predigest PDB content into the native ChemDoodle Web Components JSON format. To do this, perform the following steps:

1. In the **File** menu, select the **Optimize PDB to JSON...** menu item.

2. A window will appear. Select the **Choose Input** button and locate the PDB file you would like to optimize.
3. The output file path will be automatically generated for the same containing folder and name, but with an extension of *.js*. Click the **Choose Location** button to change the location of the output file. ChemDoodle will automatically change the extension to *.js*.
4. When satisfied with the paths, select the **Optimize** button. Depending on the size of the PDB file, this function may take several seconds to complete.
5. To use the *Javascript* file with the ChemDoodle Web Components, just include it in your web project, and import it as a URI resource on the HTML page it is used. The PDB will be represented as a Molecule data structure with the same name as the input file, prepended by the string "pdb_". For instance, if you optimized the file "1BNA.pdb", then you can load the variable *pdb_1BNA* directly into your component with the *loadMolecule()* function.

Generating Components for Mobile Devices

ChemDoodle Web Components will work in all browsers including those on mobile devices, notably *iPhone OS* (iPhone, iPod Touch, iPad) and *Android* devices. All rendering is supported on the mobile devices and touch events and gestures are recognized by the components.

There is no difference between generating components for desktop browsers versus for mobile browsers. The only consideration would be the size of the component. The ChemDoodle Web Component generator contains a drop down selection to the right of the dimension panel containing preset sizes for mobile devices. Use it to quickly set standard sizes if preferable.

Rendering Compatibility

Even though ChemDoodle and the ChemDoodle Web Components library are in the same family of products, their feature sets are not identical. Many graphical features and visual specifications provided in ChemDoodle are not yet available in ChemDoodle Web Components.

Use the ChemDoodle Web Component window in ChemDoodle to help guide you through the available visual specifications in the ChemDoodle Web Components library. Use the **Preview** button to ensure your graphics will be correctly represented to your satisfaction.

License

The ChemDoodle Web Components library is licensed under version 3 of the GNU GENERAL PUBLIC LICENSE with the following exception:

> *As a special exception to the GPL, any HTML file in a public website or any free web service which merely makes function calls to this code, and for that purpose includes it by reference, shall be deemed a separate work for copyright law purposes. If you modify this code, you may extend this exception to your version of the code, but you are not obligated to do so. If you do not wish to do so, delete this exception statement from your version.*

This means that your websites do NOT need to be released under GPL if you call the ChemDoodle Web Components library,

unless that HTML page is part of a commercial product or service.

Am I allowed to use this?

The license protects the code if one changes it or integrates it with a proprietary product. If you are concerned about how the license will affect you, then you should contact us. If you do not fully understand the GPL license or you answer yes to any of the questions listed next, then you should contact us before using this library.

- Will you be changing this library's source code?
- Will you be integrating this library with another product that you will be distributing to the public in any form?
- Are you part of a commercial organization?
- Will you need access to iChemLabs cloud services (using the ChemDoodle.iChemLabs package)?

Attributions

Attributions on webpages for the use of ChemDoodle and ChemDoodle Web Components are greatly appreciated, but not required.

Several ChemDoodle Web Component badges are provided for this purpose if you choose to use them at http://web.chemdoodle.com/installation/badges.

Further Information

For further information regarding the ChemDoodle Web Components, including webpage installation instructions, the most recent version and updates, advanced programming and use of the API, examples and browser compatibility, visit the official ChemDoodle Web Components website at http://web.chemdoodle.com.

Appendix G: ChemDoodle Mobile

Overview

ChemDoodle Mobile is the mobile companion to ChemDoodle. ChemDoodle Mobile is free for all customers of ChemDoodle. This section lists:

- What ChemDoodle Mobile is.
- How to log into ChemDoodle Mobile.
- The features in ChemDoodle Mobile.
- Transferring structure data between ChemDoodle and ChemDoodle Mobile.

Supported Platforms

ChemDoodle Mobile is supported on both iOS and Android.

iOS

ChemDoodle Mobile can be installed on iPhones, iPod Touches and iPads via the iTunes AppStore. You can find ChemDoodle Mobile for iOS here: ChemDoodle Mobile on the iTunes AppStore

Android

ChemDoodle Mobile can be installed on phones running the Android operating system via the Android Marketplace here: ChemDoodle Mobile on Google Play

Logging in to ChemDoodle Mobile

All ChemDoodle customers receive free accounts to log into ChemDoodle Mobile. This is the same account you use to sync with your online account in ChemDoodle desktop. Your username is the email address your activation code is associated with, and your password is the last 4 characters of your activation code. The password must be either in all uppercase or all lowercase.

ChemDoodle Mobile Features

ChemDoodle Mobile is a calculator for drawn organic structures. There are four main windows: **Draw**, **Calculate**, **Spectra** and **Help**. The **Draw** window shows a typical ChemDoodle sketcher, where you can draw and store your structures. The **Calculate** page calculates properties and the **Spectra** page simulates NMR spectra. All spectra are interactive. The **Help** page contains a thorough help guide.

Calculations

- Molecular Formula
- Molecular Mass
- Monoisotopic Mass
- Degree of Unsaturation
- Hydrogen Bond Acceptors
- Hydrogen Bond Donors
- Average Molecular Polarizability
- Molar Refractivity
- Polar Surface Area
- logP

Spectra

- Mass Parent Peak (Isotopic Distribution)
- 1H NMR
- 13C NMR

Transferring Data between ChemDoodle Desktop and ChemDoodle Mobile

Data saved to your online account can be accessed from any iChemLabs application that uses that account.

To create data in ChemDoodle for use in ChemDoodle Mobile, perform the following steps:

1. Draw the structure to be loaded into ChemDoodle Mobile in a new document in ChemDoodle.
2. Log into your online account by using the **Sync with Online Account...** menu item in the **File** menu.
3. Select the **Save as Online File...** menu item in the **File** menu.
4. Choose a name for your structure and save it.
5. Log into ChemDoodle Mobile.
6. Press the **Load** button in ChemDoodle Mobile and then select **From Account**.
7. Choose the file you just saved from ChemDoodle to load it.

In the reverse manner, structures you saved in ChemDoodle Mobile can be edited in ChemDoodle.

NOTE: ChemDoodle Mobile can only handle one molecule a time. If you load a large document with many molecules and shapes, only the first molecule will be used. If you then save that file in ChemDoodle Mobile, you will override the original file and lose the additional structures and shapes present in that file.

Appendix ICL-1: Technical Support

When to Contact Customer Service

While we do our best to debug and test ChemDoodle, a few bugs will always slip past us. Because of this, you may have encountered an issue with ChemDoodle. We certainly want your experience with iChemLabs software to be as enjoyable and hassle free as possible and we will do our best to address any issues you bring to our attention. In fact, we encourage you to report any bugs that you find to help us perfect ChemDoodle.

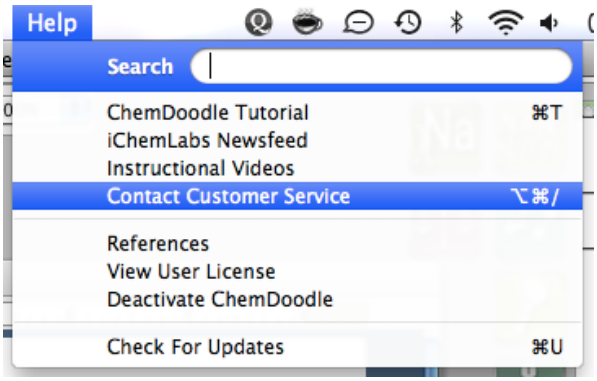
Before contacting us, please do the following:

- Check the system requirements for ChemDoodle at the beginning of this user guide to ensure that your system is supported.
- Search this user guide to see if your issue is addressed here.
- Read the Troubleshooting section of this appendix and follow the possible resolution tactics outlined there.
- Double check that your issue is reproducible and outline the exact steps performed to cause it.
- Take screenshots of any relevant graphical issues or popup errors in their entirety.
- Make note of anything you have tried to correct the problem.

How to Contact Customer Service

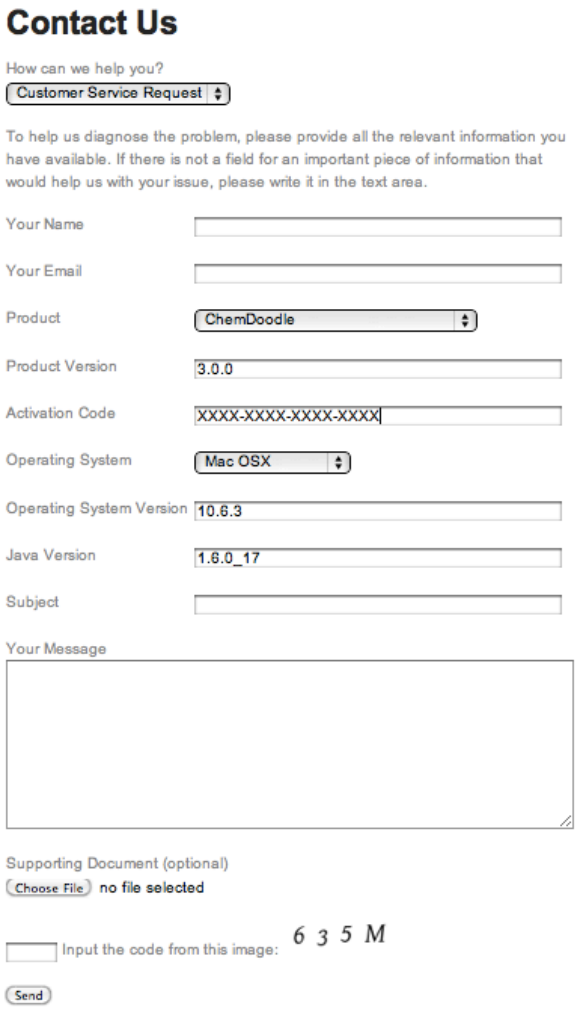
After collecting all relevant information, click on the **Contact Customer Service** menu item in the **Help** menu as shown in *Figure ICL-1.1*. This is the best way to contact iChemLabs customer service and to receive fast support. We always respond to inquiries within one business day, will most likely answer your email within a few hours and very often respond within an hour.

Figure ICL-1.1: Contact Customer Service Menu Item



This function will automatically pre-populate fields in our customer service form as shown in *Figure ICL-1.2*. Just fill in your name, your email, the subject and your message to complete the form. You can also attach a supporting file using the **Choose File** button. If you would like to attach multiple files, archive them all into a ZIP file and attach that (You should also zip any files that the form will not allow you to attach). When finished, input the CAPTCHA code present in the image at the bottom of the form and click the **Send** button. The page will confirm that your message has been sent and you will receive a confirmation email regarding your inquiry.

FIgure ICL-1.2: The iChemLabs Customer Service Request Form



If you do not want to use email to contact us, you can also contact us by the following methods:

NOTE: Requesting support with the following methods will proceed slower than requesting service using our online form. Some methods, such as phone support, require fees.

Phone: 888-505-2436

Mail: iChemLabs
200 Centennnial Ave., Suite 200
Piscataway, NJ, 08854

Feature Requests

We are happy to receive feature requests from all users. You can submit a request using the customer service form as described in the previous section.

Feature requests are made for ChemDoodle every day. Some features are beyond the scope of ChemDoodle and we will try to explain why in a response. For example, a widget to perform *ab initio* calculations is beyond the scope of ChemDoodle as its focus is on chemical graphics and publishing. Otherwise, every requested feature is intended for a future update to ChemDoodle, and we are serious about implementing the features you want. That being said, some may wonder why the feature they requested is taking so long to implement. The following describes how our feature request system works and how we prioritize the features that we work on.

1. All feature requests (from customers and non-customers) are considered and are reported to our development tracking system.
2. Feature requests are associated with a score based on the popularity of the request. Each feature begins with a score of 0. The score is then incremented by 1 for each unique customer that requests that feature (including the initial request if done by a customer). Non-customers that request features do not affect feature scores.
3. Once a month, we reevaluate the scores and plan our development around the features with the highest scores.

4. When a feature is completed, it is removed from our development tracking system.

Therefore, to get the features you want implemented in ChemDoodle as fast as possible, do the following two things: (1) Please let us know about the feature you would like to see implemented by contacting us using the method described in the previous section and (2) get as many unique ChemDoodle customers to request the same feature as possible.

Following ChemDoodle Development

We are very open about our development and you can learn more about what we are doing by visiting the iChemLabs homepage at http://www.ichemlabs.com. We regularly post stories about ChemDoodle, development and compatibility checks with new operating systems. Make sure you subscribe to the iChemLabs newsfeed *RSS* (http://www.ichemlabs.com/feed/rss2/) to be immediately notified of any new posts.

The iChemLabs newsfeed *RSS* can also be viewed by selecting the **iChemLabs Newsfeed** menu item in the **Help** menu.

Troubleshooting

Windows

Occasionally when you open ChemDoodle it will ask about connections, just select "Keep Blocking". ChemDoodle creates a local socket to open files that are double-clicked, generating this warning. ChemDoodle never accesses the internet unless you allow it to.

Sometimes the JRE can corrupt and you may see weird behavior when using ChemDoodle. Just restart your computer to resolve these issues.

Mac OS X

If you updated ChemDoodle and notice that the new filetype associations aren't being recognized in Finder, just restart your computer. The filetypes should now be recognized in Finder.

Performance Improvements

Hardware

If you see a severe lag in responsiveness in ChemDoodle, then there is likely a scarcity of system resources. Try the following solutions.

1. Upgrade to a more powerful CPU.
2. Increase the amount of memory in the computer.

Software Options

Apart from the hardware upgrades, a few features in ChemDoodle can be disabled to improve performance.

1. Disable the application rendering decorations in the **Preferences** window under the **General** tab in the **Decorations** section.
2. Change the rendering parameters to the options that favor speed in the **Preferences** window under the **Advanced** tab in the **Document Rendering** section.

Using Non-official Java Runtime Environments

On Linux distributions, one cause of slow performance we routinely encounter in our tests is the use of non-official **Java** runtime environments. Make sure that you are using the official **Oracle** JRE when running ChemDoodle.