Getting Started in Jmol

Part of the Jmol Training Guide from the MSOE Center for BioMolecular Modeling
Interactive version available at http://cbm.msoe.edu/teachingResources/jmol/jmolTraining/started.html

Introduction

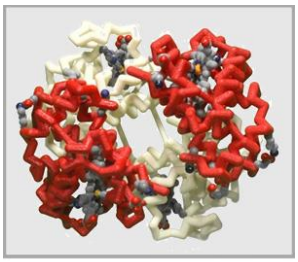
Physical models of proteins are powerful tools that can be used synergistically with computer visualizations to explore protein structure and function. Although it is interesting to explore models and visualizations created by others, **it is much more engaging to create your own**!

At the **MSOE Center for BioMolecular Modeling** we use the molecular visualization program **Jmol** to explore protein and molecular structures in fully interactive 3-dimensional displays. Jmol a free, open source molecular visualization program used by students, educators and researchers internationally.

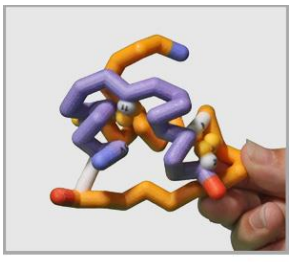
The Jmol Training Guide from the MSOE Center for BioMolecular Modeling will provide the tools needed to create molecular renderings, physical models using 3-D printing technologies, as well as Jmol animations for online tutorials or electronic posters.

Examples of Proteins in Jmol

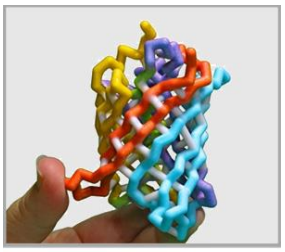
Jmol allows users to rotate proteins and molecular structures in a fully interactive 3-dimensional display. Some sample proteins designed with Jmol are shown to the right.



Hemoglobin Proteins safely carry oxygen in the blood.



Insulin Proteins help regulate sugar in the bloodstream.



Green Fluorescent Proteins create bioluminescence in animals like jellyfish.

Downloading Jmol

Jmol Can be Used in Two Ways:

1. **As an independent program on a desktop -** Jmol can be downloaded to run on your desktop like any other program. It uses a Java platform and therefore functions equally well in a PC or Mac environment.

2. **As a web application -** Jmol has a web-based version (oftern refered to as "JSmol") that runs on a JavaScript platform and therefore functions equally well on all HTML5 compatible browsers such as Firefox, Internet Explorer, Safari and Chrome.

Downloading Jmol

As an open source program, the most current version of Jmol is distributed through the code-sharing website **Source Forge** (https://sourceforge.net/projects/jmol/), along with past versions and other development materials.

However, we suggest that if you plan to design and build physical models with the CBM, you download Jmol directly from the CBM using the links available in the **Teacher Resources** section of our website. This will ensure you are using the same version of Jmol that the CBM staff members are. The CBM will choose the version of Jmol to be used for the coming school year each September.

Note that you will need to have **Java** on your computer to run the desktop version of Jmol. Most computers will already have a Java installed, but if you do not, you can download it for free from https://java.com/en/download/.

Organizing Your Jmol Files

As a desktop Java program, Jmol does not need to be "installed", so once the .jar file has been downloaded, the program will be ready to use. Click on the .jar file to start Jmol on your computer.

We usually suggest keeping your Jmol .jar file in a safe and logical location, like your "Program Files" folder. For each project you work on, you can then create a shortcut to this Jmol .jar file to keep with your other project files.

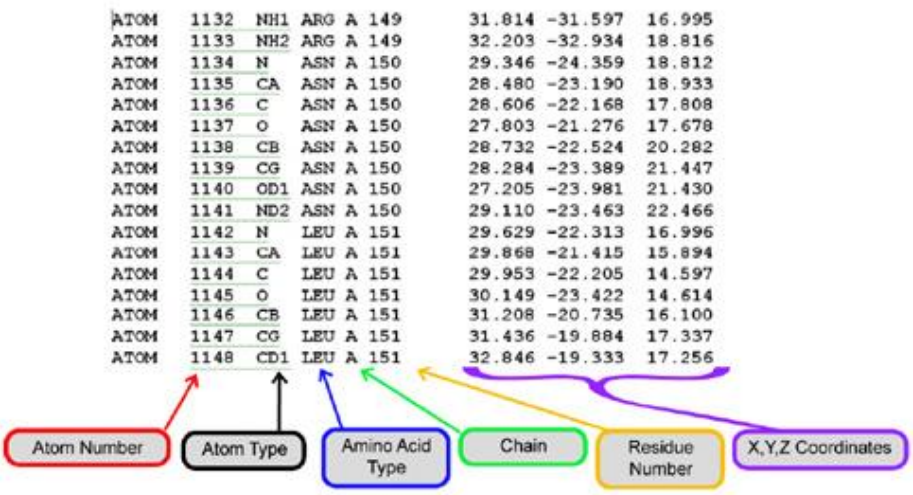
Molecular Structure Files

Molecular structures can be determined through the use of:

- X-ray Crystallography
- Nuclear Magnetic Resonance (NMR)
- computer algorithm-based calculations

Once a structure has been determined, each atom in the structure is assigned an (X, Y, Z) coordinate to mark its location in 3-dimensional space. These coordinates are then stored in a file. The two most common molecular structure files we will be working with in this Jmol Training Guide are **RCSB Protein Databank (.pdb) files** and **MDL Molfile (.mol) files**. Molecular visualization software, such as Jmol, can use the coordinates stored in these file to create an interactive 3-dimensional visualization of a molecular structure.

The image below shows a short bit of code from inside of a structure file.



Structure Files for the Jmol Training Guide

The most common source of free .pdb files of macromolecules is the **RCSB Protein Data Bank** website at http://www.pdb.org, which is discussed in more detail in the **Finding Protein and Molecular Structures** section of the Jmol Training Guide. For these Jmol Training Guide tutorials, we will be using Jmol to primarily view the .pdb file **1qys.pdb** which contains the atomic coordinates for a single molecule of the protein **Top 7**.

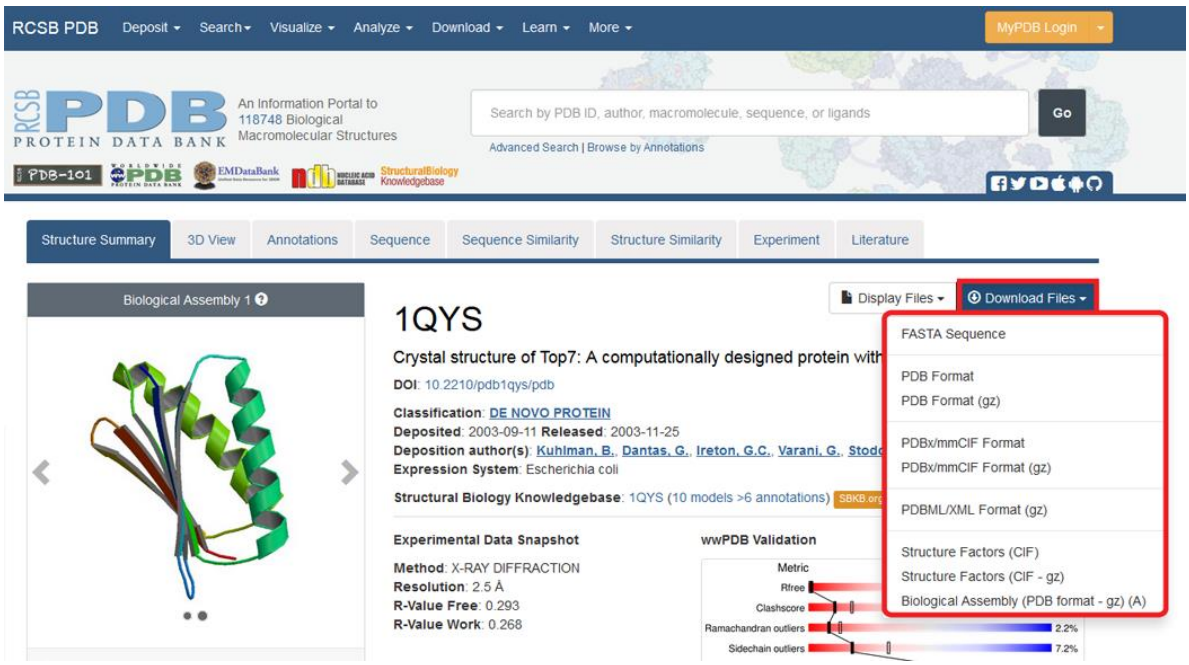
You can download this file (and all other .pdb files) from the Protein Data Bank to use with your own copy of Jmol running on your computer.

To Download the 1qys.pdb Structure File:

1. Go to the website http://www.pdb.org

2. In the top right corner of the website is a search bar similar to the image below. Type in the four number/letter file name, in this case we are looking for "**1qys**", and click the "**Go**" button.

3. This should bring you to the page for "1qys.pdb – Top 7". Just below the search box on the right should be a list of four options. Click "**Download Files**" and you will see an expanded menu similar to the image shown below.



4. Click "**PDB Format**" to begin the download of the .pdb file containing the coordinates for Top 7. This file, named "**1qys.pdb**", can be saved to the location of your choosing on your computer.

Note that is a good idea to create a new folder for each molecule you work on to organize all of your .pdb files, images, and other related work.

Opening Jmol and Loading the 1qys.pdb File

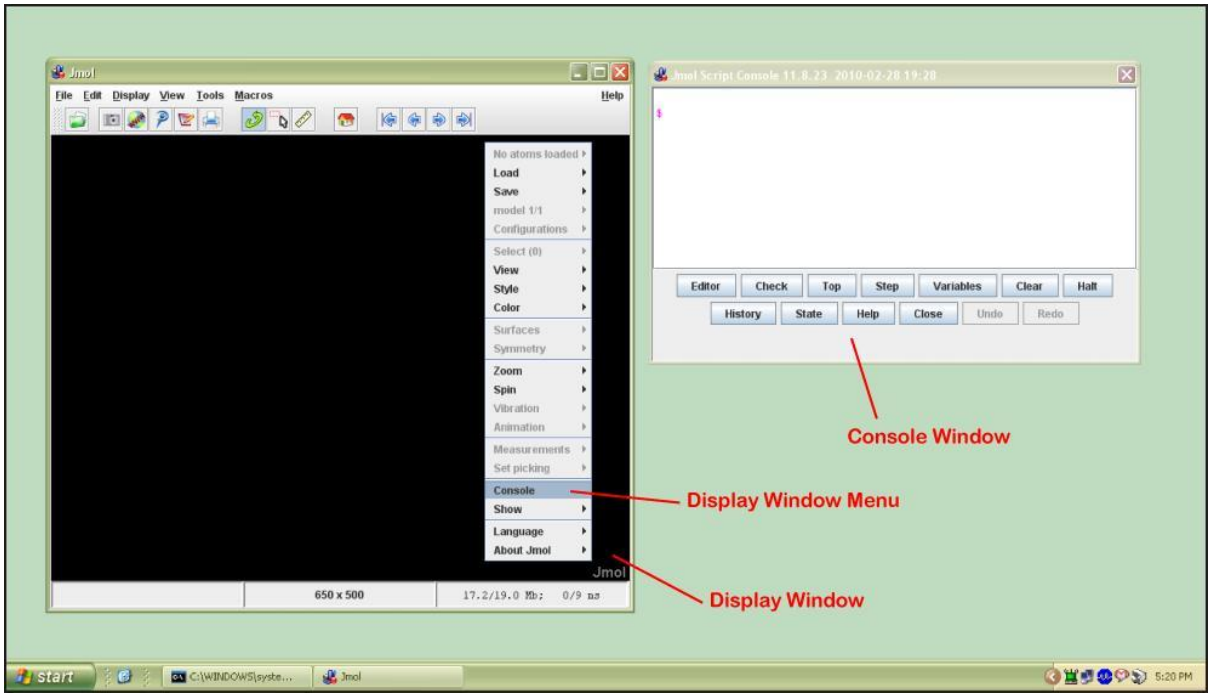
Launching Jmol

To launch Jmol, open the folder containing the Jmol .jar file that you downloaded earlier and double click the .jar file.

Note that for convenience, it is a good idea to create a shortcut to this "Jmol.jar" file on your desktop as well as in each of your working folders so you can easily launch Jmol as you are working.

Jmol Windows

Once launched, Jmol will display two windows. The Jmol **Display Window** (below, left) is used to view your 3-dimensional protein or molecular structure. The Jmol **Console**(below, right) will be used to input commands that can alter your display.



Note that if the Jmol Console does not pop up when you open Jmol, right click anywhere in the Display Window to bring up the **Display Window Menu**. In this menu, click on the button "**Console**" which will open the Jmol Console.

Because the Console and Display Windows will almost always be used in unison, we suggest you arrange the windows so that they do not overlap and both fit comfortably on your screen. Most people prefer a larger Display Window.

Opening a .pdb File

Open the folder that contains your .pdb file and drag your .pdb file into the Display Window. You can also use the "**File > Open**" menu options if you are running Jmol on the desktop. For the remainder of this section in the Jmol Training Guide, we will be using the protein Top 7 based on the .pdb file 1qys.pdb.

The default **Display Format** for a protein opened in Jmol is **Cartoon Format** colored by **Secondary Structures** (alpha helices are magenta and beta sheets are orange). Ligands are displayed in **Ball and Stick Format**, while ions or individual water molecules are displayed in **Spacefill Format**.

These various display formats will be discussed in more detail later on in the Jmol Training Guide.

Moving a Molecule in Jmol

Your Jmol Display Window should now show the molecule "**Top 7**" once you have clicked and dragged your .pdb file into it. You can manipulate this 3-dimensional display using your mouse and keyboard. To the right are two tables, one for PC and one for Mac, that highlight the basic translation, rotation and zooming movements.

For PC:

Rotate on the X-Y axes:	Zoom in and out: Shift
Translate the Molecule: Ctrl Alt	Rotate on the Z axis: Shift

For Mac:

Rotate on the X-Y axes:	Zoom in and out: Shift
Translate the Molecule: Command	Rotate on the Z axis: Shift Command