

SETTING UP PROTEIN EXPLORER

Protein Explorer is a web site that will allow students to view, rotate, and manipulate molecules in 3D. It requires a computer lab, preferably with Internet access, and also a Netscape plug-in called *Chime*. Plug-ins are extensions to Netscape that expand its capabilities. To run Chime and Protein Explorer, you must be using Windows 95/98/2000/NT, or a Macintosh PPC computer. You also need to use Netscape; it will not work with Internet Explorer.

NOTE: The teacher should review and follow these instructions before presenting them to the class. If you need additional help installing Chime, go to <http://www.umass.edu/microbio/chime/neccsoft.htm> or <http://molvis.sdsc.edu/protexpl/troubles.htm> for a troubleshooting guide. Being familiar with the setup and interface of Protein Explorer will be very helpful during class to help answer student questions.

If your computer lab does not have Internet access, you will need to follow all the instructions on this sheet, especially the section marked RUNNING PROTEIN EXPLORER OFF-LINE. These steps will need to be completed before class.

COMPUTER REQUIREMENTS

The teacher should review these downloading and installation directions prior to class. If necessary, check your school's computer lab to be sure that the computers meet these requirements:

Windows

Windows 95/98/2000/NT

Pentium processor recommended

64MB RAM recommended

800 x 600 screen resolution recommended

Macintosh

MacOS 8.6/9.0

PowerPC processor

32MB RAM or more recommended

800 x 600 screen resolution recommended

NOTE: A version of Netscape between 4.08 and 4.76 is needed. It won't work with anything lower than 4.08, and it won't work with Netscape 6. To check what version of Netscape you are using in Windows, open Netscape and click on the *Help* menu. Then click on *About Navigator...* or *About Communicator...* near the bottom of the choices. This will open a page with the version number.

On a Macintosh, open Netscape and click on the *Apple menu* (apple icon in the top left-hand corner). The first choice will be *About Navigator*, or *About Communicator*. Click on this and a page will open with the version information.

Netscape can be downloaded by visiting <http://www.netscape.com> and clicking on the **Download** button. If downloading is necessary, make sure to select a version between 4.08 and 4.76. Remember that every computer in the lab must be using the correct version.

DOWNLOADING CHIME

Every computer in the lab must have the Chime plug-in installed on it. Because of this, we recommend going through the downloading process with all of the students, so they can learn what is involved and do the actual downloading and installing. This will involve them registering with a company in order to download software. See the notes in Lesson 10 about this.

1. Go to <http://www.mdlchime.com/chime/> and click on the **Register** button.
2. This will take you to a *Terms of Use agreement* that must be agreed to in order to use the web site. Tell the students that *Terms of Use agreements* are common on the Internet, and should always be read first. Many students tend not to read the fine print, but remind them that not every web site is honest or reputable, so they should always read what they are agreeing to. After reading it, scroll to the bottom of the page and click on **I Agree**.
3. This will bring up a form that must be filled out. Remind students that forms are also common on the Internet and should always be reviewed first. Some of the information is required and some is optional. Tell the students that it is their responsibility to decide how much information they want to give to web sites when filling out forms. Again, not all web sites are reputable, so students must make decisions when using the Internet about who they give their personal information to.



- The fields that are required on the form are email address, password, first name, and last name. Tell the students that picking a password is important and is something they will have to do the more they use the Internet. They should pick a password that they will easily remember, but isn't too obvious. The student's name or simple words are bad choices. Good choices for passwords are words that don't appear in a dictionary, or words that include numbers or uppercase *and* lowercase letters. For example, *happy* or *jason* aren't very good choices for passwords, but *haPp72* and *jAso35n* are great choices, if a little complex. Remind students that they must remember their password, as they will need it later.
- After filling out the form, click on the **Register** button. Read the information on the page that appears and then click on the **Close Window** button. That window will close and the Chime home page should be underneath it.
- In the top left-hand corner of the Chime home page is the Member Login area. Tell the students to enter the email address and the password they just used to register. Then click on **Go**.
- Click on the **Download** link underneath the Download heading on the top left-hand side of the next page.
- This will bring up a *License Agreement* page. Click on the **Single-Use End User Agreement** link in the middle of the page to view the agreement (note: Adobe Acrobat Reader must be installed on the computers to view this page. **When you do this with the students, skip this step, because you already passed out the Chime Licensing Agreement in Lesson 9.**) If the license agreement opened in a new window, close that window to return to the Chime page. If it opened in the same window, click on the browser's **Back** button to return to the previous page.
- Now scroll to the bottom of the page and look at the blue *Preferred Version of Chime* heading. Select the operating system your computers are using, either Windows or Macintosh. Then click the **Next >>** button.
- Read the information on the next page, and click on the **Begin Download** or **Download Chime...** link. A dialog box will pop up asking you where to save the file. Create a folder called Chime on the C: drive to save all the Chime files in. When doing this with students, show them how to do this if necessary or have the more computer-savvy students help the others. The program should begin to download.

INSTALLING CHIME

NOTE: If you are using a Macintosh computer, see <http://molvis.sdsc.edu/protexpl/troubles.htm> for specific instructions. These instructions are for Windows.

- Close all browser windows and any other programs that may be running. It is important that no other programs be running.
- Locate the downloaded file by finding the icon called **Chime26SP1** or **Chime26**. It should be in C:\Chime if you saved it there. Double-click it.
- An installation program will start to run. Follow the directions it provides, clicking on the **Next** button to go through the steps.
- When the window titled *Select method for finding web browsers* appears, select the *Find web browsers via the Windows Registry* option. Then click the **Next** button.
- The next window should say, *Chime 2.6 SP1 will be installed for the following web browsers*. Make sure that *Netscape Communicator* is written beneath and that there is a checkmark in the box to the left. If it also lists *Internet Explorer*, uncheck the box to the left. Then click the **Next** button and skip to step 7.
- If *Netscape Communicator* does not appear, do not click **Next**. Instead, click **Back**, and select the option *Search local drives for web browsers*. Then press the **Next** button. Now Netscape should appear, in which case you can press **Next**. (If Netscape still does not appear, click **Back** and select the option *Specify the location of a web browser*. You will have to find the Netscape program folder manually. Click **Browse**. It is generally C:\Program Files\Netscape\Communicator\Program\ If you are still having trouble finding it, contact the computer lab technician or network administrator.
- Once the files have been installed, uncheck *View release notes* and click **Finish** to return to the Desktop.

DOWNLOADING FOURMOLS

- Whether using the on-line or off-line directions, you must download the Fourmols file. Enter the URL: <http://www.umass.edu/microbio/rasmol/distrib/fourmols.exe> to directly download the file. Create a folder called Fourmols in the Chime folder and save the file in there.
- After it has finished downloading, double click Fourmols.exe to unpack the files.



DOWNLOADING BILAYERS

1. If your computer lab has Internet access, you don't have to download the bilayers file. It can be accessed on-line at <http://molvis.sdsc.edu/bilayers/>. However, if you know your Internet connection is slow or would like to speed up the viewing process for the students, you can also download bilayers and view it off-line. Just go to <http://molvis.sdsc.edu/bilayers/> and click on the *download* link about halfway down the page. Create a folder called bilayers in the Chime folder and save the file in it. In lesson 11 when you are using bilayers, tell students to use Netscape to open index.html in the bilayers folder.

LEARNING HOW TO USE PROTEIN EXPLORER (LESSON 10)

NOTE: It is highly recommended that you familiarize yourself with Protein Explorer before class. If a problem arises during class you'll be able to solve it faster.

1. Begin by viewing molecules in Protein Explorer and learning how to use the various buttons and the mouse to observe them. Double-click on the icon for Netscape. Remember that Protein Explorer files **ONLY** work in Netscape, not Internet Explorer!
2. Once Netscape is open. Click **File**
3. Click **Choose File** – type the information stating where the file is stored. Open first the molecules in C:/Protein Explorer/Chime/Fourmols These molecules are not html files so you will need to click *All Files* in the Open File box to observe them. Start with the file ATP. Click on the icon, then open. Do the following:
 - a. Rotate the molecule by clicking the left mouse button and moving the mouse.
 - b. With the left mouse button, click on an area of the molecule. What do you see on the bottom of the screen? They should see the information on the atom and group number.
 - c. Click the right mouse button to change the aspects of the image. Click *display*, then *sticks*. Observe the molecule again.
 - d. Rotate the molecule with the left mouse as before.
 - e. Click right mouse button, then *display* followed by *ball and stick*. Again observe the molecule and rotate it.
 - f. Click right mouse button, then *display*, followed by *spacefill* and then *Van der Waals radii*. Again observe the molecule. Ask them what a Van der Waal radii is.
 - g. Click the right mouse button, followed by *rotation*. Ask them what happens to the molecule. Can they figure out how to make the molecule stop rotating? Click right mouse, followed by *rotation* again to stop the molecule.
 - h. Click right mouse button, followed by *options*, and *labels*. This will label all the oxygens, nitrogens and phosphates in the molecule.
 - i. Click right mouse button, followed by *options*, *dot surface* and *Van der Waals radii*. What do they see? Can they get rid of the Van der Waals radii?
 - j. Click right mouse button, followed by *select, atom, N* for nitrogen. Then click right mouse button, *display, spacefill*. What happens to the image? Repeat, but click *atom, P* for phosphate.
 - k. Click right mouse button, *file, save molecule as*. They can enter what file type to save the image as and where to save it. Then they can save the molecule to disk, if they like.
 - l. Then they should sketch the molecule and tell what molecule they think it is on their Protein Explorer and Observation sheet. Students should do this with every molecule in the Fourmols folder. Collect their worksheets at the end of class.

RUNNING PROTEIN EXPLORER ON-LINE (LESSON 11)

1. Open Netscape and enter the following URL: <http://molvis.sdsc.edu/bilayers/> for the English version or <http://www2.alcala.es/biomodel/model2/bicapa/> for the Spanish version.
2. Look at the top of the page. If you see rotating molecules in the two boxes at the top left and right of the web page, Chime was installed correctly and everything is ready to run. If you don't see them, try quitting Netscape, (close *all* the windows) and then opening it again. If you still can't see the molecules, refer to the **NOTE** at the beginning of this document.
3. Now you have a choice to make. If you click on the **Start Presentation** button about halfway down the page, a presentation will open showing four different molecules. You move through the presentation by

clicking as it rotates, zooms, and manipulates the molecules for you. This is one option. The other option is to explore the molecules individually in Protein Explorer. Underneath the **Start Presentation** button is a heading that reads, *Explore molecules from the presentation in Protein Explorer*: followed by a list of molecules. If you click on one of the molecules, Protein Explorer will open and you can explore the molecule by yourself. You can zoom and rotate the molecule by clicking and dragging it with the mouse, and manipulate it by right-clicking on it to bring up a menu. You should try both options. It would be advisable to have the students go through the program by the first option as listed in the lesson plan and use the second option if there is extra time in class. You will see three windows. The one above contains information about the molecule and the buttons to click. The window below contains the molecule. The window on the left side gives instructions on how to resize the windows.

4. Read the information and then click the first button to bring the first image of cholesterol onto the screen. You must take notes as you are going through the program so that you understand and can explain what you have seen. You can move or rotate the molecule by clicking the left mouse button and moving the mouse. You should rotate each molecule to get the most information from it as it will provide a clearer 3D image if you move it around. Each atom has a different color in this program. For example, white = hydrogen, red = oxygen, blue = nitrogen, gray = carbon, and orange = phosphorous
5. Continue to read the information given and click the next button to move through the whole series on cholesterol.
6. Click Next page (Phospholipid) to continue with the next series. Continue as before reading, clicking buttons, rotating the molecules and taking notes.
7. After going through the presentation the first time, you can repeat the presentation to pick up on any points you missed. You can also use the right button on your mouse to change the many aspects of the molecule such as display, rotation, color, selection particular molecules, etc. Play with these and see what you can learn.

RUNNING PROTEIN EXPLORER OFF-LINE (LESSON 11)

NOTE: This is useful if your school's access to the Internet is not consistent or rapid, or you have troubles with firewalls. You will need to set aside more time for preparation. It will require downloading all the required files from a computer that does have Internet access, and transferring them to your computer lab. You will need to download the files and then save them on floppy disks or a CD (creating a CD-R of all the files would be ideal, if you have access to a CD writer; some files are too large to fit on a floppy disk), and then installing all the files on each computer that will be used. Get the help of the computer lab tech person, if possible.

1. Follow the above directions for downloading and installing the Chime plug-in. Install the plug-in on every computer that will be used during class.
2. Go to <http://www.umass.edu/microbio/chime/regisfrm/> to download the Protein Explorer files for offline use. Please register first so they can continue to improve and support Protein Explorer! **After registering, print the downloading instructions.** This will make it easy to install once you have downloaded. Once you reach the page of files to download, scroll about halfway down and locate **Protein Explorer** and **Shared Support Package**. Download both these files and save them according to the directions on the downloading instructions page that you printed out. The Shared Support Package file must be saved in the Protein Explorer folder.
3. Make sure you have downloaded and unpacked the fourmols and bilayers files.
 - a. Fourmols – C:\protein explorer\fourmols
(<http://www.umass.edu/microbio/rasmol/distrib/fourmols.exe>)
 - b. Bilayers - C:\protein explorer\bilayers (<http://molvis.sdsc.edu/bilayers/>)**Remember that all the files have to be installed on all the computers.**
4. Start Netscape Communicator. Remember that Protein Explorer files ONLY work in Netscape, not Internet Explorer!
5. Click **File**
6. Click **Open Page**
7. Click **Choose File** –You want to open index.html in the bilayers folder. It should be C:\Protein Explorer\bilayers\index.htm, or just find the bilayers folder and go through it until you find index.html.
8. Once the page has opened and loaded, click **Start Presentation**. You will see three windows. The one above contains information about the molecule and the buttons to click. The window below contains the

- molecule. The window on the left side gives instructions on how to resize the windows.
9. Read the information and then click the first button to bring the first image of cholesterol onto the screen. You must take notes as you are going through the program so that you understand and can explain what you have seen. You can move or rotate the molecule by clicking the left mouse button and moving the mouse. You should rotate each molecule to get the most information from it as it will provide a clearer 3D image if you move it around. Each atom has a different color in this program. For example, white = hydrogen, red = oxygen, blue = nitrogen, gray = carbon, and orange = phosphorous
 10. Continue to read the information given and click the next button to move through the whole series on cholesterol.
 11. Click Next page (Phospholipid) to continue with the next series. Continue as before reading, clicking buttons, rotating the molecules and taking notes.
 12. After going through the presentation the first time, you can repeat the presentation to pick up on any points you missed. You can also use the right button on your mouse to change the many aspects of the molecule such as display, rotation, color, selection particular molecules, etc. Play with these and see what you can learn.