

Accessing Accelrys DS GCG, SeqLab and SeqWeb at Marshall University

Michael J. McCarthy
Assistant Dean for Information Technology & Medical Informatics
Marshall University Joan C. Edwards School of Medicine
mccarthy@marshall.edu
(304) 691-1765

Revised: 20 December 2005

Table of Contents

	<u>Page</u>
1. Scope and Subject	1
2. Obtaining DS GCG, SeqLab and/or SeqWeb User Account(s)	1
3. Obtaining Access to the Marshall University VPN	2
Downloading and Installing the Marshall University VPN Client	2
Connecting to the Marshall University VPN	2
Disconnecting from the Marshall University VPN	3
4. Downloading and Running PuTTY Terminal Emulator for DS GCG Command Line Access	4
5. Accessing the Accelrys DS GCG Command-Line	5
Changing Your DS GCG Command-Line Password	8
6. Accessing the SeqLab Xwindows Interface	9
Obtaining the XWindows Viewer (VNC Viewer)	9
Starting the SeqLab Session	9
Exiting from the SeqLab Session	12
Alternative VNC Viewer Access via WWW Browser	13
7. Up- and Downloading Files to and From your GCG / SeqLab Account	15
8. Accessing the SeqWeb Interface	17
Appendix A: Summary of Steps for Access from On- and Off-Campus	19

1. Scope and Subject

This document describes how to obtain and access account(s) to use the Accelrys DS GCG application via the command-line interpreter, the SeqLab (Xwindows) interface and the SeqWeb WWW-based interface. These instructions assume that you have a functioning Internet connection and a WWW-browser (Netscape or Internet Explorer).

Actual usage of these software packages is beyond the scope of this document. Users should refer to <http://www.accelrys.com/support/bio/genhelp/> for documentation and information on usage of these applications.

2. Obtaining DS GCG, SeqLab or SeqWeb User Account(s)

To request an account for DS GCG, SeqLab and/or SeqWeb, send an email message to gcg@marshall.edu with the following information:

- Your full name
- Your MUNet username (e.g., smith18)
- Your status (e.g., student, research staff, faculty)
- Your department affiliation (e.g., microbiology, IS&T, etc.)
- Your email address
- The system(s) you want to use (DS GCG, SeqLab and/or SeqWeb)

Your username(s) will be the same as your MUNet username and your password(s) will be set to a default, initial password (which you should change during your first login session. Please note that the passwords for DS GCG, VNCServer (for SeqLab) and SeqWeb are all maintained separately; changing one does not change the other.

3. Obtaining Access to the Marshall University VPN (if accessing DS GCG or SeqLab from outside of a Marshall University campus)

If you wish to access either the DS GCG command-line or the SeqLab Xwindows interfaces from within a Marshall University campus (e.g., the Huntington, South Charleston or Medical School campuses), you can skip this section and go to “Accessing the Accelrys DS GCG Command-Line,” below.

Similarly, if you wish to access only the SeqWeb interface, regardless of your location, you can skip this section and go to “Accessing the SeqWeb Interface,” below.

If, however, you wish to access the DS GCG command-line or the SeqLab Xwindows interface from outside of a Marshall University campus, you will need first to connect to the Marshall University Virtual Private Network (VPN) in order to gain access through the university’s firewall.

Downloading and Installing the Marshall University VPN Client

The Marshall University VPN Client can be downloaded from the following URL:

www.marshall.edu/ucs/networking/vpnintro.asp

You will need an active MUNet username and password in order to download the VPN Client. When prompted for a username and password, provide your MUNet username and password. Note that if you are medical school user, you should enter your username as follows:

Username: `username@som.marshall.edu`

Where *username* is your MUNet username. For example:

Username: `smith18@som.marshall.edu`

Download and run the VPN client installation executable program.

Connecting to the Marshall University VPN

To connect to the Marshall University VPN prior to your DS GCG or SeqLab sessions, launch the Cisco Systems VPN Client that you downloaded and installed, select the profile labeled “Split-VPN” and click on the icon labeled **Connect** (Fig. 3-1).

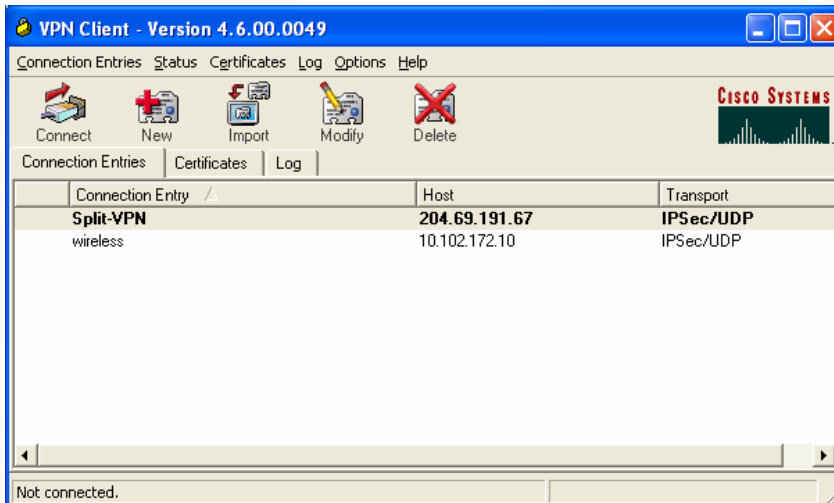


Figure 3-1. Cisco VPN Client for Marshall University. Select "Split-VPN" and click the icon labeled "Connect."

When prompted for a username and password, provide your MUNet username and password. Note that if you are medical school user, you should enter your username as follows:

Username: **username@som.marshall.edu**

Where *username* is your MUNet username. For example:

Username: **smith18@som.marshall.edu**

When you are running the VPN client, you will see a small, yellow padlock icon in your system tray at the bottom right corner of your screen. The padlock's hasp appears closed while you are connected to the VPN. Once you are connected, you can proceed to access the Accelrys DS GCG Command-Line and/or SeqLab.

Disconnecting from the Marshall University VPN

When your Accelrys DS GCG Command-Line and/or SeqLab sessions are complete and you have logged out of the bioinformatics.marshall.edu server, you can disconnect from the Marshall University VPN by double-clicking on the yellow padlock icon in your system tray at the bottom right corner of your screen and then clicking on the button labeled **Disconnect**.

4. Downloading and Running PuTTY Terminal Emulator for DS GCG Command Line Access

IMPORTANT NOTE: Telnet access to bioinformatics is no longer supported. Users will need to use a terminal emulator client that supports “secure shell” (SSH), such as PuTTY, described here.

A version of the PuTTY Terminal Emulator for Windows is available on the WV-INBRE website on the “Accelrys & SeqWeb” page:

www.wv-inbre.net/bioinformatics/accelrys.asp

Click on the link labeled “PuTTY.exe” and save the PuTTY executable file to your PC. PuTTY does not need to be installed – simply double click on the **putty.exe** file on your PC to launch PuTTY. You will see the “PuTTY Configuration” window shown in Fig. 4-1.

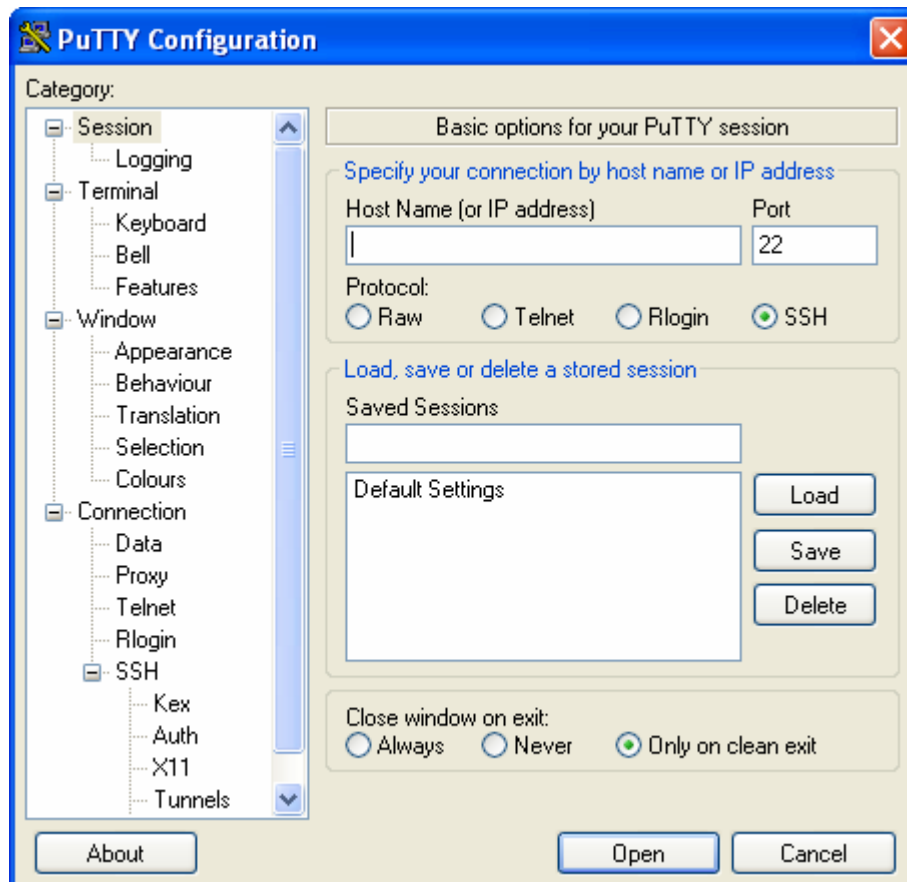


Figure 4-1. PuTTY Configuration Window.

5. Accessing the Accelrys DS GCG Command-Line

NOTE: If you are attempting to access the Accelrys DS GCG Command-Line from outside of outside of a Marshall University campus, you will need first to connect to the Marshall University Virtual Private Network (VPN) in order to gain access through the university's firewall. See "Obtaining Access to the Marshall University VPN," above.

To access the DS GCG suite command-line interpreter, connect via SSH to `bioinformatics.marshall.edu` and login with your username and password (not your SeqWeb password). To connect via SSH, do the following (Windows):

Double click on **putty.exe** to launch the PuTTY Terminal Emulator (see "Downloading and Running the PuTTY Terminal Emulator for DS GCG Command Line Access," above). You will see the "PuTTY Configuration Window" shown in Figure 2, above.

In the "Host Name" field, type:

bioinformatics.marshall.edu

Make sure that the "Port" is set to **22** and that **SSH** is the selected "Protocol."

Click on the button labeled **[Open]**

The first time you connect to `bioinformatics.marshall.edu` via SSH, you will be asked to confirm your trust of the host's RSA2 key fingerprint. This is a unique public key value that assures you that you are connecting to the host that you intend to, and not to a bogus host or via a hijacked session. You will see a "PuTTY Security Alert" window like the one shown in Fig. 5-1:



Figure 5-1. PuTTY Security Alert window asking that you confirm a trust for the server's RSA2 key fingerprint.

As of this version of these instructions (20 December 2005), the RSA2 key fingerprint for bioinformatics.marshall.edu is:

E4:60:8f:8e:44:4e:93:3f:0a:ff:1f:4f:e5:84:24:84

Verify that the key fingerprint shown to you matches the one listed above and click on the button labeled **[Yes]** to confirm your trust of this host and to add this key fingerprint to your PC's registry. You will not be prompted to confirm this key fingerprint on subsequent connections.

You will see a login prompt like the one shown in Fig. 5-2.

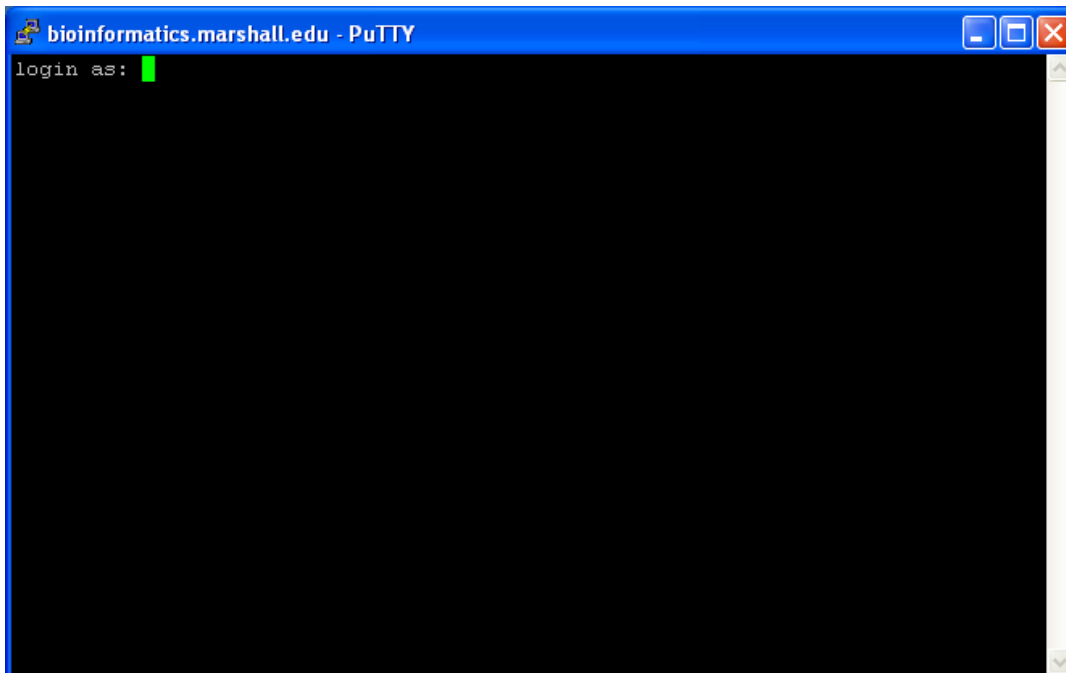
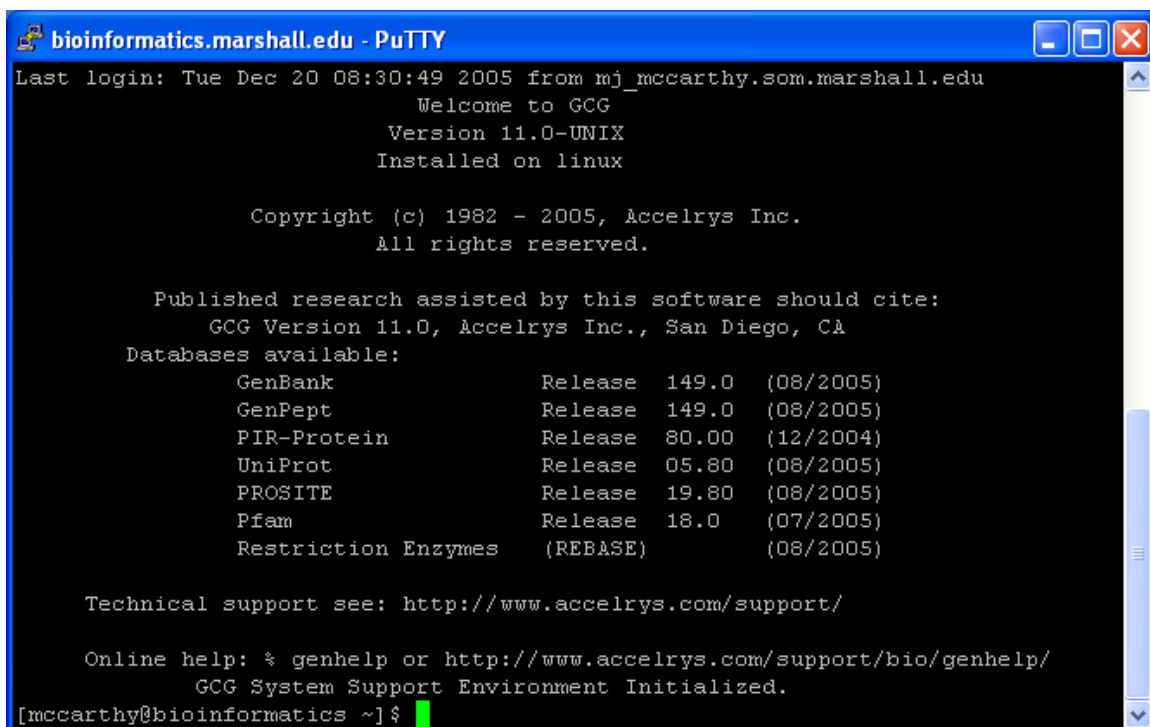


Figure 5-2. PuTTY SSH connection to bioinformatics.marshall.edu with login prompt.

Enter your username and press **[Enter]**. You will see a page displaying a system usage policy statement. When prompted, enter your password and press **[Enter]**. If you login successfully, you will see a welcome screen like the one shown in Fig. 5-2. This screen shows the version of DS GCG installed on the server (Version 11.0-UNIX installed on linux) and lists the databases and release dates that are available (e.g., GenBank Release 147.0 (04/2005)). The command prompt at which you can enter DS GCG commands looks like:

```
[username@bioinformatics ~]$
```

where *username* is your username. You may now begin using the DS GCG package via the command-line interpreter.



```
bioinformatics.marshall.edu - PuTTY
Last login: Tue Dec 20 08:30:49 2005 from mj_mccarthy.som.marshall.edu
Welcome to GCG
Version 11.0-UNIX
Installed on linux

Copyright (c) 1982 - 2005, Accelrys Inc.
All rights reserved.

Published research assisted by this software should cite:
GCG Version 11.0, Accelrys Inc., San Diego, CA
Databases available:
GenBank           Release 149.0 (08/2005)
GenPept          Release 149.0 (08/2005)
PIR-Protein      Release 80.00 (12/2004)
UniProt          Release 05.80 (08/2005)
PROSITE          Release 19.80 (08/2005)
Pfam             Release 18.0 (07/2005)
Restriction Enzymes (REBASE) (08/2005)

Technical support see: http://www.accelrys.com/support/

Online help: % genhelp or http://www.accelrys.com/support/bio/genhelp/
GCG System Support Environment Initialized.
[mccarthy@bioinformatics ~]$
```

Figure 5-2. DS GCG Welcome Screen

When you are finished with the DS GCG session, you can logout of the server by typing **exit** and then pressing **[Enter]** at the command prompt:

```
[smith18@bioinformatics ~]$ exit
```

Changing Your DS GCG Command-Line Password

You should change the default password assigned to you for DS GCG Command-Lin. To change your password, type the command **passwd** and then press **[Enter]** at the command prompt. You will be prompted for your current password and then your new password. You will also be asked to re-type your new password to verify it:

```
[smith18@bioinformatics ~]$ passwd
Changing password for smith18
(current) UNIX password: *****
New password: *****
Retype new password: *****
```

Remember that your passwords for the DS GCG Command-Line, SeqLab and SeqWeb are all maintained separately. Changing one password does not automatically change them all.

6. Accessing the SeqLab Xwindows Interface

Obtaining the Xwindows Viewer (VNC Viewer)

The Accelrys DS GCG suite includes a graphical user interface called SeqLab that is deployed via an Xwindows connection between your workstation and the server. In order to use the SeqLab interface on bioinformatics.marshall.edu, you must first download the VNC Viewer, which is available at the following URL:

www.wv-inbre.org/bioinformatics/accelrys.asp.

Download and install the VNC Viewer executable file to install RealVNC Viewer. You must download and have the VNC Viewer installed on your workstation before you can access SeqLab.

Starting the SeqLab Session

When you are ready to launch SeqLab, you should first establish an SSH connection to the bioinformatics.marshall.edu server (follow the steps in “Accessing the Accelrys DS GCG Command-Line,” above). At the command prompt, type **vncserver** and press **[Enter]**. For example:

```
[mccarthy@bioinformatics ~]$ vncserver
```

The first time you launch vncserver you will be prompted to enter and then verify a password:

```
You will require a password to access your desktops.
```

```
Password:
```

If you ever wish to change your password later, you can do so by entering the command **vncpasswd** at the command prompt. Make sure you remember the password that you provide, and note that this password is stored separately from your DS GCG or SeqWeb password. Changing one does not change any of the others.

When the VNC Server is launched and ready for your connection, you will see a screen like the one shown in Fig. 6-1. Make careful note of the “display” number, which follows the server name and a colon in the VNC Server message that you see on the screen. In Fig. 6-1, the display number is “1” as shown by the line:

```
New 'X' desktop is bioinformatics:1.
```

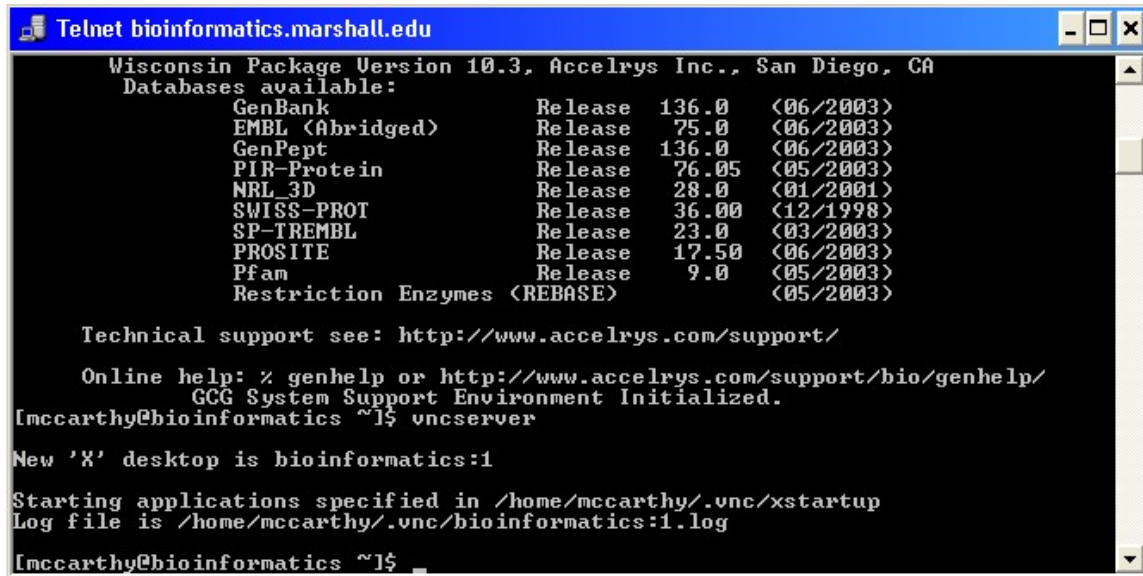


Figure 6-1. VNC Server startup screen. Note "display" number following the server name and a colon (1 in this example).

When you return to the command prompt, launch the VNC Viewer on your workstation to establish the Xwindows connection. You will be prompted for a VNC Server to which to connect (Fig. 6-2). Enter **bioinformatics.marshall.edu:n** and click **[OK]**, where *n* is the "display" number you noted carefully from the VNC Server startup screen.

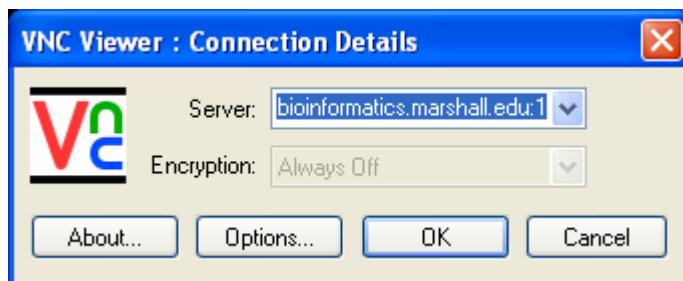


Figure 6-2. VNC Viewer connection window. Note "display" number following the server address and a colon.

You will be prompted for your VNC Server password that you provided the first time you launched VNC Server (or the password that you have changed via the `vncpasswd` command; Fig. 6-3). Enter the password and click **[OK]**.

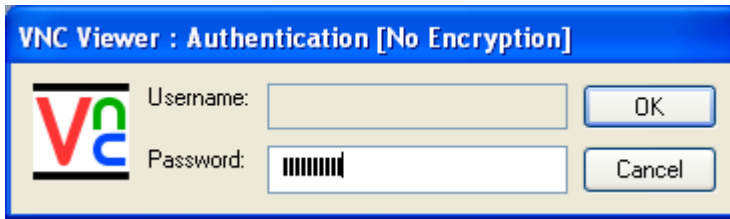


Figure 6-3. VNC Viewer authentication window.

You will see a window open labeled “*username*’s X desktop (bioinformatics:*n*)” where *username* is your username and *n* is the “display” number for your Xwindows connection. This window will contain an xterm terminal window with a command prompt that looks like:

```
[mccarthy@bioinformatics ~]$
```

Type **seqlab** and press **[Enter]** to launch your SeqLab session. A transparent window frame will appear within the X desktop window that will move as you move your mouse. Click once with your left mouse button to define the location at which this window will be placed. You will now see two new windows open with your X desktop session, the front one labeled “About SeqLab” and the one behind it labeled “SeqLab Main Window on bioinformatics” (Fig. 6-4). Click on the **[OK]** button in the “About SeqLab” window to close it and begin working in the SeqLab Main Window.

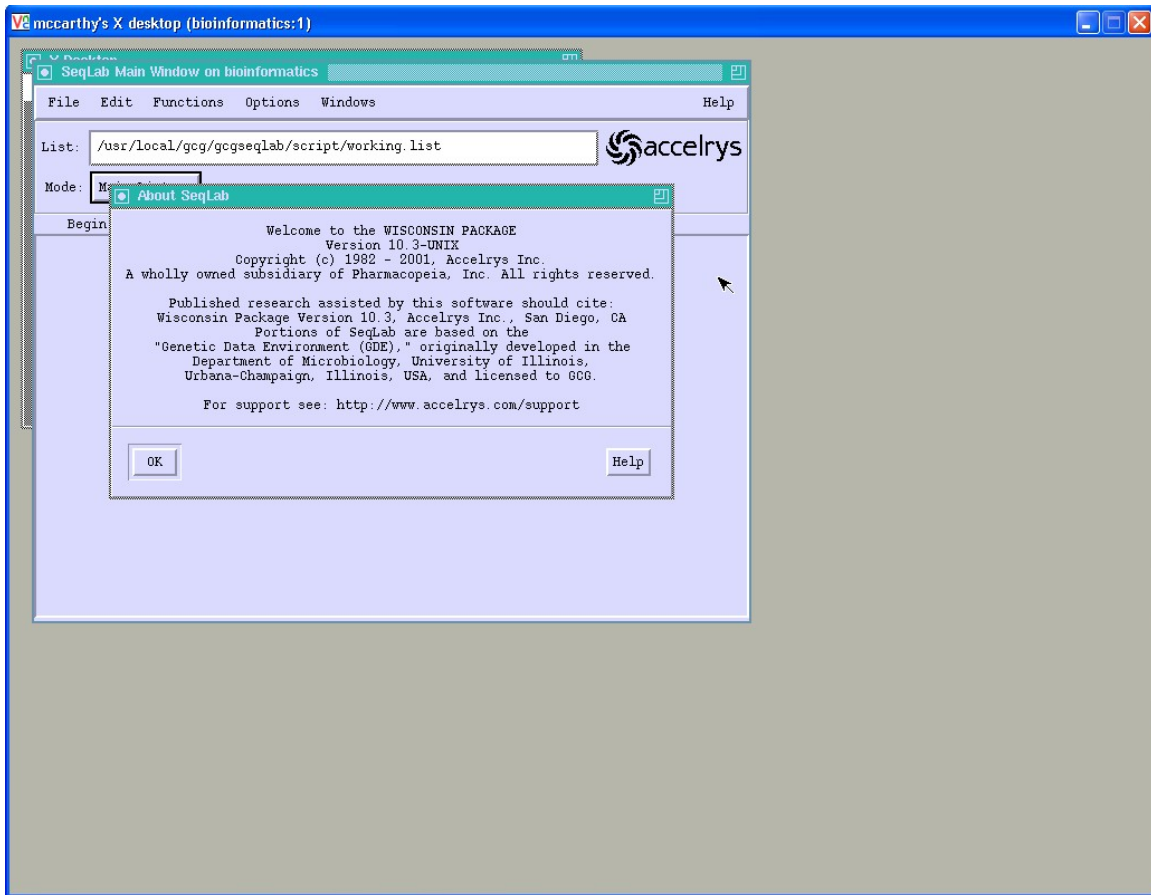


Figure 6-4. X desktop window with SeqLab Main Window.

Exiting From the SeqLab Session

When your SeqLab session is complete, click on **File** in the menu bar of the “SeqLab Main Window” and then click on **Exit** in the pull-down menu that appears. Select the xterm terminal window from your X desktop (or select the window on your workstation from which you established the original telnet connection), type the following command and press **[Enter]**:

```
[mccarthy@bioinformatics ~]$ vncserver -kill :n
```

where *n* is the “display” number that you have used to establish this Xwindows connection. Important note: it is very important that you “kill” this VNC Server session before logging out from the bioinformatics server. Orphaned display sessions will bog down the server and can comprise security vulnerabilities. Orphaned displays discovered by the system’s administrators will be killed with no warning and may result in loss of access privileges to the bioinformatics.marshall.edu server.

After you have terminated (“killed”) your VNC Server session, you can logout from the bioinformatics.marshall.edu server by typing **exit** and pressing **[Enter]** in the workstation window you used to establish your original telnet session to the server.

Alternative VNC Viewer Access via WWW Browser

NOTE: If you are attempting to access the alternative VNC Viewer via the WWW browser from outside of a Marshall University campus, you will need first to connect to the Marshall University Virtual Private Network (VPN) in order to gain access through the university’s firewall. See “Obtaining Access to the Marshall University VPN,” above.

Instead of downloading and running the VNC Viewer, you can create a VNC Viewer session via a Java-enabled browser. Note that performance and responsiveness will be a bit slower than using the actual VNC Viewer.

To establish a browser-based VNC Viewer connection, telnet to bioinformatics.marshall.edu, login and launch **vncserver** as noted, above. Once VNC Server is running and you have noted the “display” number, open your WWW browser and enter the following URL:

<http://bioinformatics.marshall.edu:58nn/>

where *nn* is the “display” number you noted when VNC Server launched. For example, if VNC Server launched with the following message:

```
New 'X' desktop is bioinformatics:1.
```

then you would enter the following URL:

<http://bioinformatics.marshall.edu:5801/>

You will see a VNC Authentication page in your browser. Provide your SeqLab password and click the **[OK]** button. You will then see an X desktop window similar to the one shown in Fig. 6-5.

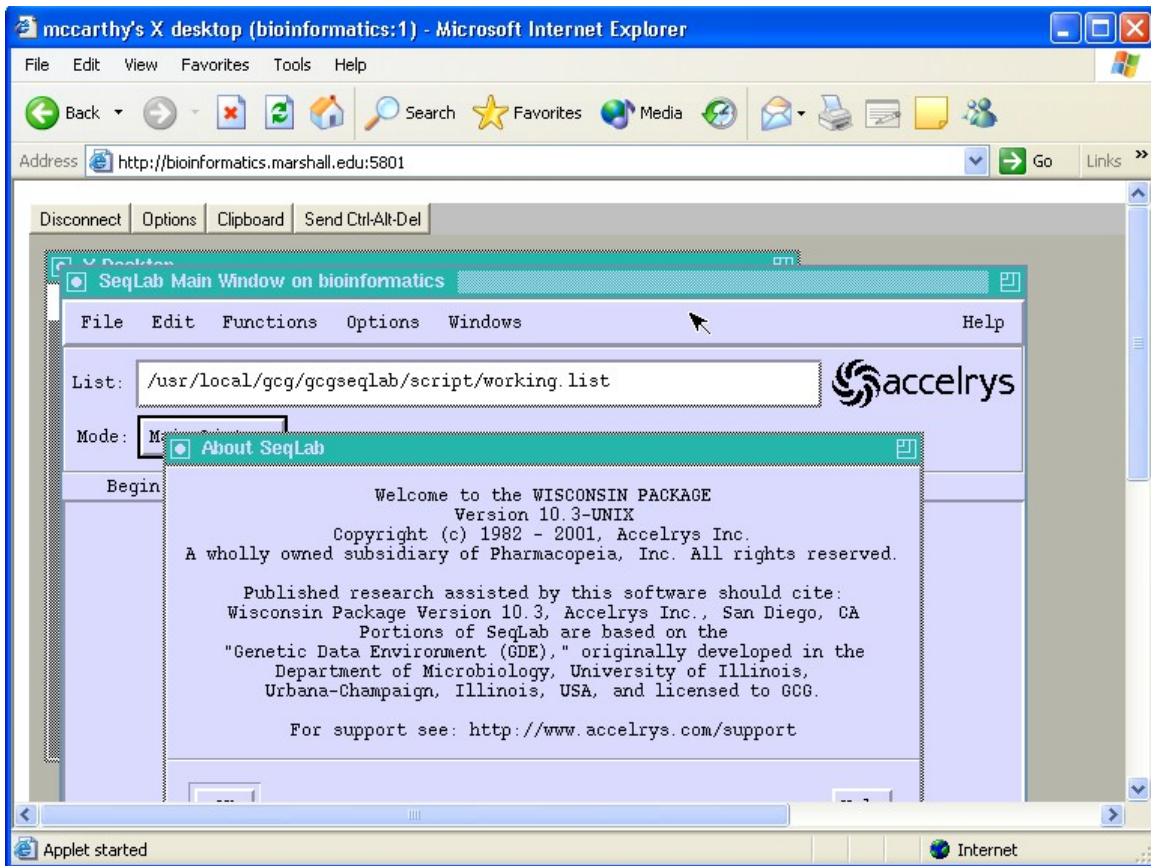


Figure 6-5. SeqLab via VNC Viewer X desktop in WWW browser.

When your SeqLab session is complete, select the “xterm” window and terminate (“kill”) the VNC Server process as you would in a normal VNC Viewer connection with a command such as the following:

```
[mccarthy@bioinformatics ~]$ vncserver -kill :n
```

Important note: it is very important that you “kill” this VNC Server session before closing the WWW browser window. Orphaned display sessions will bog down the server and can comprise security vulnerabilities. Orphaned displays discovered by the system’s administrators will be killed with no warning and may result in loss of access privileges to the bioinformatics.marshall.edu server.

7. Up- and Downloading Files To and From your GCG / SeqLab Account

In order to upload input files from your PC to your GCG Command-Line or SeqLab account, or to download output files from your GCG Command-Line or SeqLab account to your PC, you will use a process known as File Transfer Protocol (FTP).

In order to start an FTP session between your PC and the bioinformatics.marshall.edu server, open **Internet Explorer** on your PC and enter the following URL into the “Address” field near the top of the window (see Fig. 7-1):

```
ftp://bioinformatics.marshall.edu/
```

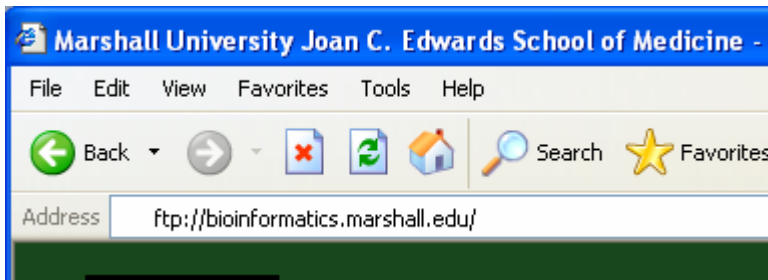


Figure 7-1. Enter the URL ftp://bioinformatics.marshall.edu/ into the Address field of Internet Explorer to start your FTP session.

When prompted for your username and password, supply your GCG Command-Line username and password (the same one you would use when establishing your initial telnet connection to bioinformatics.marshall.edu to use the DS GCG Command-Line or SeqLab) and click on the **[Log On]** button (see Fig. 7-2).

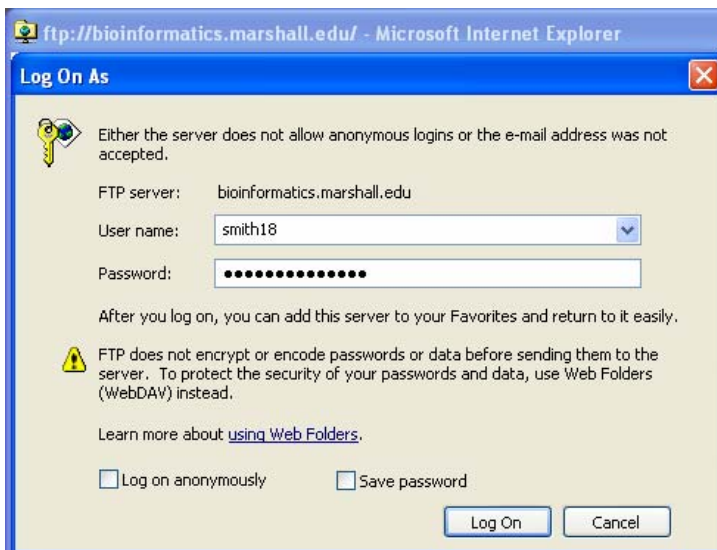


Figure 7-2. User name and Password prompt for FTP access.

After you login, you will see an Internet Explorer window showing you the contents of your home directory on bioinformatics.marshall.edu (Fig. 7-3). You can copy files to this directory from your PC (i.e., upload them from your PC to your GCG Command-Line / SeqLab account on the server) or you can copy files from this directory to your PC (i.e., download them from your GCG Command-Line / SeqLab account on the server to your PC).

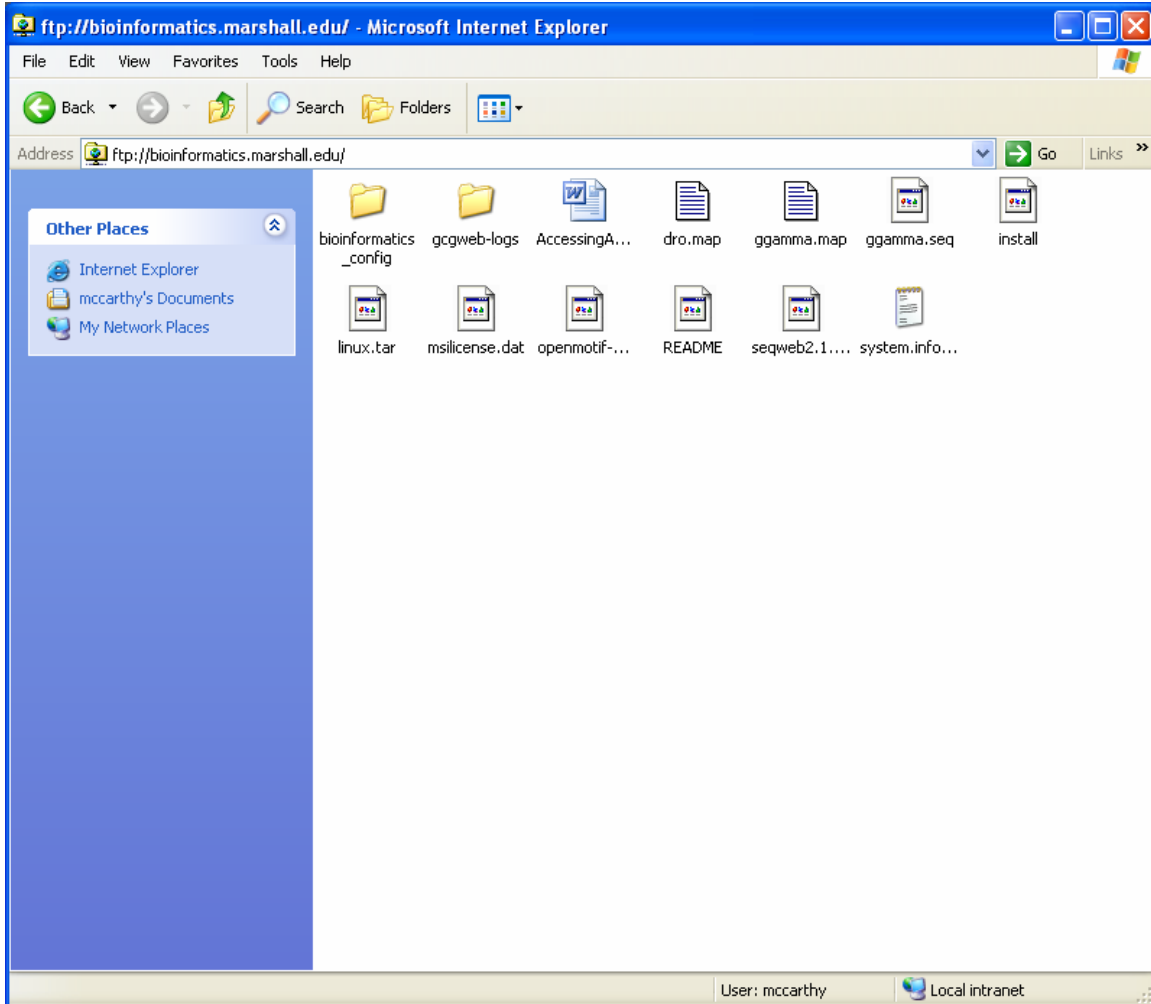


Figure 7-3. Internet Explorer FTP window showing contents of DS GCG Command-Line / SeqWeb account.

When you are finishing up- or downloading files, simply close this Internet Explorer window to terminate your FTP session to bioinformatics.marshall.edu.

8. Accessing the SeqWeb Interface

The Accelrys (GCG) Wisconsin Package provides a WWW-based interface called SeqWeb.

Use of this interface requires one of the following supported browser versions:

Internet Explorer

Windows	5.5	6.0		
Macintosh	5.0	5.1	5.1x	

Netscape Navigator

Windows	4.77	4.78	4.79	6.2	6.2.x
Macintosh	4.77	4.78	4.79	6.2	6.2.x
UNIX	4.77	4.78	4.79	6.2	6.2.x

To access the SeqWeb interface, open the following URL in your WWW browser window:

<http://bioinformatics.marshall.edu>

You will see an authentication window prompting you for your SeqWeb username and password (Fig. 8-1). Provide them at the appropriate prompts and click on the **[OK]** button. Remember, your DS GCG, SeqLab and SeqWeb passwords are all stored separately, so changing one does not automatically change any others.

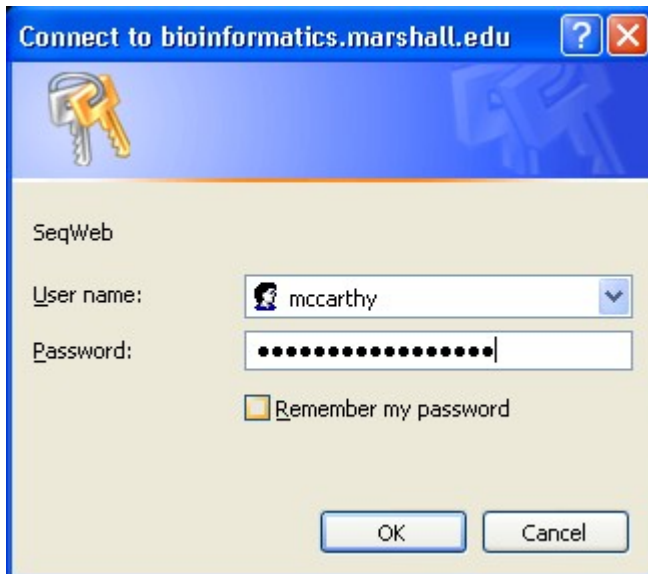


Figure 1. SeqWeb authentication window.

After you login you will see an Accelrys SeqWeb program screen (Fig. 8-2). You are now ready to use SeqWeb.

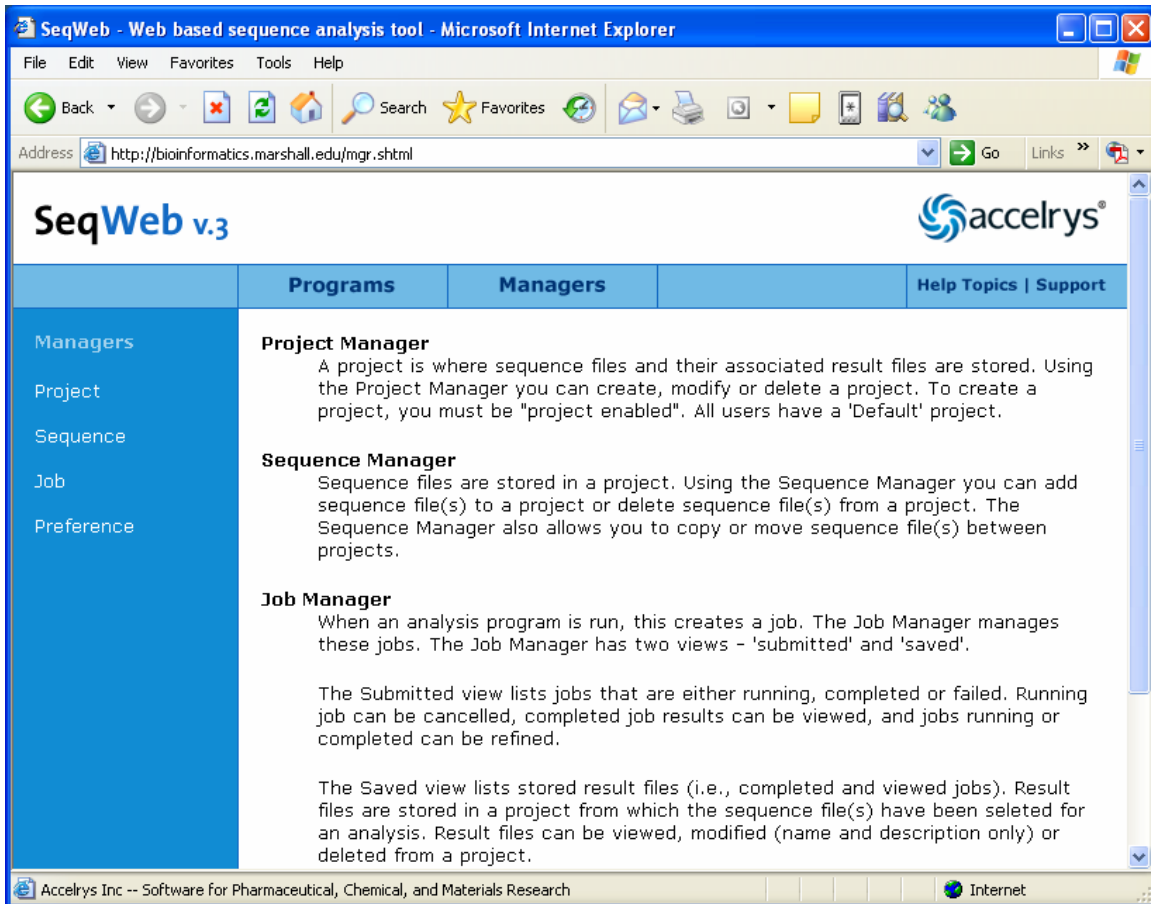


Figure 28-2. SeqWeb main program screen.

Appendix A

Summary of Steps for Access From On- and Off-Campus

	You are <u>ON</u> a Marshall Univ. Campus	You are <u>NOT ON</u> a Marshall Univ. Campus
DS GCG Command- Line	<ol style="list-style-type: none"> 1. T SSH (using PuTTY) to bioinformatics.marshall.edu. 2. Enter DS GCG commands at command prompt. 	<ol style="list-style-type: none"> 1. Connect to Marshall University VPN 2. SSH (using PuTTY) to bioinformatics.marshall.edu. 3. Enter DS GCG commands at command prompt.
SeqLab (with Xwindows viewer)	<ol style="list-style-type: none"> 1. SSH (using PuTTY) to bioinformatics.marshall.edu 2. Type vncserver and press [Enter] at command prompt and note “display number” returned. 3. Launch VNC Viewer from your workstation and connect to bioinformatics.marshall.edu:n, where <i>n</i> is the display number from step #2. 4. Type seqlab and press [Enter] at command prompt of Xwindows session. 5. When done, type vncserver –kill :n and press [Enter] at command prompt, where <i>n</i> is the display number from step #2. 	<ol style="list-style-type: none"> 1. Connect to Marshall University VPN 2. SSH (using PuTTY) to bioinformatics.marshall.edu. 3. Type vncserver and press [Enter] at command prompt and note “display number” returned. 4. Launch VNC Viewer from your workstation and connect to bioinformatics.marshall.edu:n, where <i>n</i> is the display number from step #2. 5. Type seqlab and press [Enter] at command prompt of Xwindows session. 6. When done, type vncserver –kill :n and press [Enter] at command prompt, where <i>n</i> is the display number from step #2.
SeqLab (with alternative, browser-based VNC Viewer)	<ol style="list-style-type: none"> 1. SSH (using PuTTY) to bioinformatics.marshall.edu 2. Type vncserver and press [Enter] at command prompt and note “display number” returned. 3. Open web browser and go to http://bioinformatics.marshall.edu:58nn, where <i>nn</i> is the display number from step#2 (e.g., “5801” if display number was “:1”). 4. Type seqlab and press [Enter] at command prompt of Xwindows session. 5. When done, type vncserver –kill :n and press [Enter] at command prompt, where <i>n</i> is the display number from step #2. 	<ol style="list-style-type: none"> 1. Connect to Marshall University VPN 2. SSH (using PuTTY) to bioinformatics.marshall.edu 3. Type vncserver and press [Enter] at command prompt and note “display number” returned. 4. Open web browser and go to http://bioinformatics.marshall.edu:58nn, where <i>nn</i> is the display number from step#2 (e.g., “5801” if display number was “:1”). 5. Type seqlab and press [Enter] at command prompt of Xwindows session. 6. When done, type vncserver –kill :n and press [Enter] at command prompt, where <i>n</i> is the display number from step #2.
SeqWeb	<ol style="list-style-type: none"> 1. Open web browser and go to http://bioinformatics.marshall.edu 	<ol style="list-style-type: none"> 1. Open web browser and go to http://bioinformatics.marshall.edu