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Preface

About This Guide

Welcome to BioWorks. The BioWorks software performs analyses of mass spectrometry data from samples containing biological molecules such as proteins and peptides.

Related Documentation

In addition to this guide, Thermo Fisher Scientific provides the following documentation for BioWorks:

- A PDF version of the BioWorks User Guide
- Online Help available from within the software

Safety and Special Notices

Make sure you follow the precautionary statements presented in this guide. The safety and other special notices appear in boxes.

Safety and special notices include the following:

- **CAUTION** Highlights hazards to humans, property, or the environment. Each CAUTION notice is accompanied by an appropriate CAUTION symbol.

- **IMPORTANT** Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or may contain information that is critical for optimal performance of the system.

- **Note** Highlights information of general interest.

- **Tip** Helpful information that can make a task easier.
Contacting Us

There are several ways to contact Thermo Scientific.

Assistance

For new product updates, technical support, and ordering information, contact us in one of the following ways:

Visit Thermo Scientific on the Web

www.thermo.com/finnigan

Contact Technical Support

Phone: 1-800-685-9535
Fax: 1-561-688-8736
E-mail: TechSupport.CMS@thermofisher.com
Knowledge base: http://www.thermokb.com

Find software updates and utilities to download at http://mssupport.thermo.com.

Contact Customer Service

For ordering information in the U.S. and Canada:
Phone: 1-800-532-4752
Fax: 1-561-688-8731
Web site: www.thermo.com/finnigan

Changes to the Manual and Online Help

To suggest changes to this guide or to the online Help, use one of the following:

- Fill out a reader survey online at www.thermo.com/lcms-techpubs.
- Send an e-mail message to the Technical Publications Editor at techpubs.finigan-lcms@thermofisher.com.
Installing Software

BioWorks™ is part of Xcalibur®, the Thermo Scientific mass spectrometry data system.

This chapter provides information about how to install the BioWorks Browser software and the protein databases. It also describes all of the necessary system software and hardware requirements for an upgrade and a full installation of BioWorks.

To install this software you need:

- BioWorks 3.3.1 SP1 CD
- Software requirements completed
- Hardware requirements completed

This chapter contains the following sections:

- Software Requirements
- Hardware Requirements
- Upgrading your BioWorks Installation
- Installing BioWorks Browser
- Installing Example Data Files
- Installing FASTA Databases
- Getting a License for BioWorks
Software Requirements

BioWorks requires Microsoft® Windows® XP and Xcalibur. The BioWorks documentation requires Adobe Reader® or Acrobat®.

Microsoft

Install Microsoft Windows XP Professional with Service Pack 2. You can download the Microsoft Windows XP Service Pack 2 from the following URL:

http://www.microsoft.com/windowsxp/sp2/default.mspx

If you have questions about how to install Windows XP, contact your system administrator. Thermo Fisher Scientific recommends a fresh installation of Windows XP rather than an upgrade from Windows 2000 to Windows XP.

Xcalibur

Install Xcalibur 2.0.6.

Adobe

Install a PDF file viewer, such as Adobe Reader or Acrobat. Acrobat Reader is available on the CD-ROM or from the Adobe web site.

Hardware Requirements

This section defines the minimum hardware configuration required to install BioWorks.

• 2 Ghz processor
• 1 GB minimum (2 GB recommended)
• CD-ROM drive
• Video card and monitor capable of 1280 x 1024 resolution and 65,536 colors (SVGA)
• At least a 75 GB hard drive, NTFS formatted
Upgrading your BioWorks Installation

This section describes the prerequisites you need to complete before you can upgrade BioWorks from a previous installation as described in “Installing BioWorks Browser” on page 4.

To install the BioWorks 3.3.1 SP1 upgrade, you must have a licensed version of BioWorks 3.2 or later installed on your computer. If you do not have an installed and licensed version of BioWorks on your computer, the installation process stops and aborts.

You might require additional BioWorks upgrades prior to the BioWorks 3.3.1 SP1 installation. Use Table 1 to determine if you require additional BioWorks upgrades prior to the installation of the upgrade.

**Table 1. BioWorks Upgrade Requirement**

<table>
<thead>
<tr>
<th>If you own</th>
<th>Upgrade BioWorks to version</th>
</tr>
</thead>
<tbody>
<tr>
<td>BioWorks 3.0 or earlier *</td>
<td>3.3</td>
</tr>
<tr>
<td>BioWorks 3.1 *</td>
<td>No additional upgrade required. Install BioWorks 3.3.1 SP1 upgrade.</td>
</tr>
<tr>
<td>BioWorks 3.1 SR1*</td>
<td>No additional upgrade required. Install BioWorks 3.3.1 SP1 upgrade.</td>
</tr>
<tr>
<td>BioWorks 3.2 *</td>
<td>No additional upgrade required. Install BioWorks 3.3.1 SP1 upgrade.</td>
</tr>
<tr>
<td>BioWorks 3.3 *</td>
<td>No additional upgrade required. Install BioWorks 3.3.1 SP1 upgrade.</td>
</tr>
<tr>
<td>BioWorks 3.3.1 *</td>
<td>No additional upgrade required. Install BioWorks 3.3.1 SP1 upgrade.</td>
</tr>
</tbody>
</table>

* To upgrade to BioWorks 3.3.1 SP1 you need to install Xcalibur 2.0.6 software first. Xcalibur 2.0.6 is included with BioWorks 3.3.1 SP1. You also need to have the Windows XP with SP2 operating system installed on your computer.

Use the steps described in “Installing BioWorks Browser” on page 4 to install the BioWorks 3.3.1 SP1 upgrade.
Installing BioWorks Browser

Use the following steps to do an upgrade or a full installation of BioWorks 3.3.1 SP1.

❖ To install BioWorks Browser

1. Insert the BioWorks 3.3.1 SP1 CD into the CD-ROM drive. The BioWorks Setup dialog box appears automatically. See Figure 1.

   **Note** Click **Readme** to display the BioWorks Browser release notes.

2. Click **BioWorks Browser**. The BioWorks Browser Setup wizard appears, as shown in Figure 2.

   **Note** If some of the Setup buttons are unavailable (grayed out), it is because the required versions of software have not been installed. Installation of the required software enables those buttons so that you can continue the installation sequence. You might be requested to reboot after you install certain portions of the software.
3. On the Welcome page, click **Next** to continue the installation.

4. Click **Print** to get a printed copy of the license agreement from the License Agreement page. Review the license agreement.

5. Select **I Accept the Terms of the License Agreement**, and then click **Next**.

6. On the Database Folder page, choose the specific database folder. For example, install the databases in the Xcalibur\database folder. Then, click **Next**.

   Check the amount of disk space available on the default drive location before you continue. The FASTA databases that you will install in “Installing FASTA Databases” on page 7 require nearly 1 GB of free space to install correctly.

   If the folder you want is not listed, click **Browse** to navigate to another folder.

   **Note** The location for the databases is set during the installation of the BioWorks Browser software so that the BioWorks Browser can correctly access the databases.

   **Note** By default, the database installs in the Xcalibur\database directory. Normally, this directory is located on the C:\ drive. On systems with a 2.0 GB C:\ drive, this creates problems because the databases require nearly 1 GB of disk space. Under these circumstances, consider an alternative location for the databases, such as on another drive (D:\database).

7. On the SEQUEST Output Folder page, select the default folder for SEQUEST results. (The default Xcalibur\sequest.) Then, click **Next**.
1 Installing Software

Installing Example Data Files

If your system does not have enough space on its C:\ drive for the databases, then you must also set the SEQUEST results directory to another drive, such as D:\SEQUEST.

8. On the Select Features page, choose the components of the BioWorks Browser that you need. To install a component, ensure the check box to the left of that component is checked. Then, click Next.

9. On the Desktop Shortcuts page, choose whether you would like to have a desktop shortcut created for BioWorks Browser by selecting the appropriate option button. Then, click Next.

10. On the Select Program Folder page, type in the name of the folder for the program files. The default is Xcalibur. Then, click Next.

11. On the Start Copying Files page, click Next to load the software from the CD to your hard drive.

   The installation progress message box appears, and closes when the installation is complete.

12. Click Exit to close the BioWorks Setup dialog box.

Installing Example Data Files

The BioWorks 3.3.1 SP1 CD contains example data files for use with the different modules of BioWorks. Many of these files are used in examples described in the BioWorks User Guide.

To install the example data files

1. Insert the BioWorks 3.3.1 SP1 CD into the CD-ROM drive. The BioWorks 3.3.1 SP1 Setup dialog box appears automatically.

2. Click Example Datafiles. The BioWorks Data Installation wizard appears.

3. On the Welcome page, click Next to continue the installation.

4. On the Select Features page, ensure that the Example Files check box is selected. Click Next.

5. When the example files have been copied to your hard drive, the Installation wizard closes. Click Exit to close the BioWorks Setup dialog box.
Installing FASTA Databases

Thermo Fisher Scientific supplies the following databases, located in the Xcalibur\database folder, with the BioWorks CD installation.

- arabidopsis thalina
- chick
- e-coli
- frog
- horse
- human
- mouse
- rat
- zebrafish
- yeast

You can obtain additional databases in FASTA file format and place them in the default directory before executing a SEQUEST search.

Table 2 lists commonly used sequence databases, along with the locations of FTP sites from which these databases can be downloaded.

<table>
<thead>
<tr>
<th>Database</th>
<th>Location for download</th>
</tr>
</thead>
<tbody>
<tr>
<td>International Protein Index (IPI)</td>
<td>ftp://ftp.ebi.ac.uk/pub/databases/IPI/current/</td>
</tr>
<tr>
<td>UniProt/Swiss-Prot</td>
<td>ftp://ftp.ebi.ac.uk/pub/databases/uniprot/knowledgebase/</td>
</tr>
</tbody>
</table>

When BioWorks is installed, a small database (equine.fasta) is installed automatically. Additional FASTA databases are located on the BioWorks 3.3.1 CD.

To install additional FASTA databases

1. Insert the BioWorks 3.3.1 SP1 CD into your CD-ROM drive. The BioWorks 3.3.1 SP1 Setup dialog box appears automatically.

2. Click FASTA Databases. The FASTA Protein Databases Setup wizard appears. See Figure 3.
3. Click **Next**. The Databases Folder page appears.

   **Note** During installation of the databases, the wizard provides an option of choosing where the databases are stored. The databases can be stored in any directory; however, only the default location is recognized by the BioWorks Browser application.

4. Choose the folder you want to install the FASTA databases into and click **Next**. The Select Features page appears. See Figure 4.
5. Select the databases you want to install by selecting or deselecting the corresponding check boxes. See Figure 4.

6. Click **Next** to start the installation. The installation progress message box appears, and closes when the installation is complete. Then, the InstallShield Wizard Complete page appears.

7. Click **Finish** to complete the installation.

8. Click **Exit** to close the Xcalibur BioWorks Setup dialog box.

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**Getting a License for BioWorks**

Some components of BioWorks are licensed to Thermo Fisher Scientific by third parties. For legal reasons, Thermo Fisher Scientific is required to prove that only the users who have purchased the software are given access to those components. Thermo Fisher Scientific issues a single license number based on which components of BioWorks have been purchased.

The following components of BioWorks require licensing:

- **BIOMASS**
- **SEQUEST**
- **SALSA**
Other components of BioWorks, such as Pepmatch and Pepmap, do not require a license. Peaks and ProMass, which are separate programs from BioWorks, require separate licenses.

This section contains the following topics:

- Obtaining a New License from Thermo Fisher Scientific
- Installing a New License

## Obtaining a New License from Thermo Fisher Scientific

This section describes how to obtain a new license to extend your applications, while you continue to operate your current software. To get a new license, send an e-mail to Thermo Fisher Scientific with the serial number and the temporary license number.

To obtain a new license from Thermo Fisher Scientific

1. Start the BioWorks Browser program by choosing Start > Programs > Xcalibur > BioWorks Browser.

   The first time BioWorks Browser runs or until a valid license number is entered, the BioWorks Browser License dialog box appears. See Figure 5.

2. Click Reset to generate a new license key.

3. Click Yes to reset the license value when you are prompted.

4. Highlight and copy the license number that displays in the License text box. See Figure 5.

   a. Double-click on the text box that contains the temporary license number to highlight the number.

   b. Press CTRL+c to copy the number to the Windows clipboard.

   c. Click Close to close the BioWorks Browser License dialog box.
1 Installing Software

Getting a License for BioWorks

5. Locate and copy the serial number beneath the bar code on the back of the BioWorks 3.3.1 SP1 CD case. See Figure 6. Provide this serial number to Thermo Fisher Scientific in order to get a license.

Figure 6. BioWorks CD label, showing bar code and serial number.

6. To get a new license, send the temporary license number and the serial number to Thermo Fisher Scientific by e-mail as described in the following section. If you need assistance, contact Thermo Fisher Scientific Customer Support.

To obtain a licence key by e-mail

1. Send an e-mail message to licenses.ms@thermo.com. Type “License request” in the Subject line of the e-mail message.

2. Paste the license number from the Windows clipboard into the body of the message.

3. Locate the bar code on the back of the CD case. Type the serial number that appears below the bar code into the body of the e-mail message.

4. In the body of the e-mail message, include your name, company name, and phone number.
If you do not have access to e-mail and you do not have Internet access, call your Thermo Fisher Scientific Customer Support representative.

Continue your normal operations while your license request is processed. Install your new license after Thermo Fisher Scientific Customer Support provides you with a new license. See Installing a New License.

**Installing a New License**

When you receive your new license from Thermo Fisher Scientific, install the new BioWorks license.

udded
to install a new license number

1. Choose **Start > Programs > Xcalibur > BioWorks Browser.**

2. Choose **Help > About BioWorks Browser**, then click **License**. The License dialog box appears.

3. Type the new license number, and then click **Set**. A message box appears.

4. Click **Yes** to accept the change in license.

5. Click **Close** to close the BioWorks Browser License dialog box.

Your new license is installed, and you can continue your operations with BioWorks and extended applications.
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