SynthAssist[®] Software Version 3.1

User Guide



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Contents

Preface

Chapter 1 Quick Start Checklist

Chapter 2 Introduction

Description of SynthAssist Software Version 3.1	2-2
Hardware and Software Requirements	2-4
Connecting the ABI 433A Peptide Synthesizer to the Computer	2-5
Installing SynthAssist Software Version 3.1	2-6

Chapter 3 Converting Macintosh[®] Files

3-2

Chapter 4 Communications Communications: PC to ABI 433A Peptide Synthesizer 4-2 Sending a Flow Test Chemistry 4-4 Running Flow Tests 4-7

Chapter 5 The Sequence

Specifying the Sequence of Amino Acids	5-2
Undefined Residues and Termini	5-6
Changing the Peptide Sequence	5-8
Deletion Sequences	5-10

Chapter 6 The Run

Setting Up a Peptide Run	6-2
Peptide Resin Calculations	6-5
Sending a Peptide Synthesis	6-10

Chapter 7 Creating a Custom Chemistry File

Overview	7-2
Renaming a Chemistry File	7-4
Changing the Chemistry Information	7-5
Changing the Selected Functions	7-6
Changing the Selected Modules	7-9
Changing Cycles	7-14
Creating a New Default Set	7-21

Chapter 8 Using the Dictionary

Overview	8-2
Opening the Dictionary	8-2
Adding a Compound to the Palette	8-4
Adding Color to a Compound	8-4
Changing the Default Derivative of an Amino Acid	8-4
Adding (or Removing) a Protecting Group	8-6
Changing Resins	8-8
Adding a Resin	8-9
Adding a Terminal	-10
Adding a Protecting Group 8	-12

Appendix A SynthAssist[®] Software Menus

List of Menus A-2
File Menu
Edit Menu A-4
View Menu A-5
Synthesizer Menu A-5
Data Converter Menu A-6
Common Menu A-6
Log Menu A-7
Window Menu A-7
Help Menu A-8

Appendix B SynthAssist[®] Software Screens Overview

Appendix C Software and Hardware Limitations

Appendix D Software Warranty Information

Computer Configuration	D-2
Limited Product Warranty	D-2

Index

Preface

About This Guide

Purpose of This Guide	The Applied Biosystems <i>SynthAssist</i> [®] <i>Software Version 3.1 User Guide</i> is for experienced SynthAssist software users migrating to the personal computer (PC) version or upgrading their SynthAssist software and for novice users. This document begins with a description of the SynthAssist software, the hardware and software requirements for operating the software, instructions for installing the software and for connecting the synthesizer to a PC. The remainder of the guide provides instructions on how to set up peptide synthesis runs, program the synthesizer, and collect data.
Audience	This guide is intended for experienced SynthAssist software users migrating to the personal computer (PC) version of the SynthAssist system or upgrading their SynthAssist software and for novice SynthAssist software users.
Assumptions	This guide uses conventions and terminology that assumes a working knowledge of the Microsoft Windows [®] operating system.
Text Conventions	This guide uses the following conventions:
	• Bold indicates user action. For example:
	Type 0 , then press Enter for each of the remaining fields.
	• <i>Italic</i> text indicates new or important words and is also used for emphasis. For example:
	Before analyzing, <i>always</i> prepare fresh matrix.
	• A right arrow bracket (>) separates successive commands you select from a drop-down or shortcut menu. For example:
	Select File > Open > Spot Set.

Right-click the sample row, then select **View Filter > View All Runs**.

User Attention
WordsTwo user attention words appear in Applied Biosystems user
documentation. Each word implies a particular level of observation
or action as described below:

Note: Provides information that may be of interest or help but is not critical to the use of the product.

IMPORTANT! Provides information that is necessary for proper instrument operation, accurate chemistry kit use, or safe use of a chemical.

Examples of the user attention words appear below:

Note: If you select the C- or N-terminus of the sequence in the Sequence screen, the palette changes to a selection of C- or N-termini.

IMPORTANT! You can copy the amino acids in a sequence but not the termini.

How to Obtain More Information

<i>SynthAssist</i> [®] <i>3.1 Online Help</i> – Describes the SynthAssist version 3.1 software and provides procedures for common tasks.
Note: For additional documentation, see "How to Obtain Services and Support" on page ix.
Applied Biosystems welcomes your comments and suggestions for improving its user documents. You can e-mail your comments to:

techpubs@appliedbiosystems.com

How to Obtain Services and Support

To contact Applied Biosystems Technical Support from North America by telephone, call **1.800.899.5858**.

For the latest services and support information for all locations, go to <u>http://www.appliedbiosystems.com</u>, then click the link for **Services** and **Support**.

At the Services and Support page, you can:

- Search through frequently asked questions (FAQs)
- Submit a question directly to Technical Support
- Order Applied Biosystems user documents, MSDSs, certificates of analysis, and other related documents
- Download PDF documents
- Obtain information about customer training
- Download software updates and patches

In addition, the Services and Support page provides access to worldwide telephone and fax numbers to contact Applied Biosystems Technical Support and Sales facilities. Use this checklist to:

- Install your SynthAssist® Software Version 3.1
- Set up your chemistry
- Set up a peptide run

See the referenced sections for detailed procedures.

Connect the communication cable.
See "Connecting the ABI 433A Peptide Synthesizer to the Computer" on page 2-5.
Install SynthAssist 3.1 software.
 See "Installing SynthAssist Software Version 3.1" on page 2-6
Start SynthAssist 3.1 software.
 See "Starting SynthAssist 3.1" on page 2-14.
Run a flow test.
 See "Running Flow Tests" on page 4-7.
Specify the sequence of amino acids.
See "Specifying the Sequence of Amino Acids" on page 5-2.
Set up a peptide run.
See "Setting Up a Peptide Run" on page 6-2.
Download chemistry and run a peptide synthesis.
See "Sending a Peptide Synthesis" on page 6-10.

This chapter covers:

Description of SynthAssist Software Version 3.1	.2-2
Hardware and Software Requirements	.2-4
Connecting the ABI 433A Peptide Synthesizer to the Computer	.2-5
Installing SynthAssist Software Version 3.1	.2-6

Description of SynthAssist Software Version 3.1

SynthAssist[®] Software Version 3.1 is a peptide synthesis software system that runs on a PC and communicates with the ABI 433A Peptide Synthesizer. With SynthAssist software you can set up peptide synthesis runs, program the synthesizer, and collect data. The software is structured into the following subprograms:

Dictionary – A database of compounds used in peptide synthesis, including amino acids, other derivatives, resins, specified N- and C-terminals, and protecting groups.

Sequence – Allows you to type in or import peptide sequences, modify them, and perform simple calculations (for example, molecular weight and composition).

Chemistry – Allows you to set up the bottle configuration, user functions, cycles, modules, and runs.

Run – Merges sequence and chemistry information to create instructions for making a specified peptide on a specific instrument. It tracks the status of the peptide synthesizer and its current run.

Communications – Allows you to transfer modules, functions, runs, and status information between the PC and the synthesizer.



Figure 2-1 Software Subprogram Relationships

Hardware and Software Requirements

Computer	SynthAssist Software 3.1 has been tested on Intel [®] Pentium III (1 GHz) or Intel [®] Pentium IV (2.4 or 2.8 GHz) processors. No attempt has been made to evaluate other hardware.
RAM	At least 256MB of RAM.
Hard Disk Capacity	At least 1 GB of free hard disk space.
Monitor	A 17-inch flat-panel color monitor with the following display properties:
	 Resolution – 1024 × 768 Fonts – Small Fonts Color – True Color (16 bit)
System Software	SynthAssist 3.1 Software can be installed on a PC running either Microsoft Windows [®] XP Professional (SP1 or higher) or Microsoft Windows [®] 2000 Professional (SP3 or higher).
Peptide Synthesizer	The ABI 433A Peptide Synthesizer.
Communications Cable	DB25 M to DB9 F W/FERRITE 10FT (Part Number 4342732)
Software	The <i>SynthAssist 3.1 Software CD</i> contains the SynthAssist software installation program.

Connecting the ABI 433A Peptide Synthesizer to the Computer

Connect the communications cable from Port A on the ABI 433A Peptide Synthesizer to COM 1 on the computer as shown below in Figure 2-2.



Figure 2-2 Installed Configuration

IMPORTANT! Keep the communications cable away from power cords.

Installing SynthAssist Software Version 3.1

Note: If any problems arise during the installation, cancel the process and remove the Installation CD. Delete the SynthAssist Software 3.1 application files via **Start>Settings>Control Panel>Add/Remove Programs**. Re-insert the Installation CD to start the install process again.

Note: If SynthAssist Software 3.0 is installed but is not found at C:\Program Files\Applied Biosystems\SynthAssist 3.0, then you must delete the SynthAssist Software 3.0 application files via **Start>Settings>Control Panel>Add/Remove Programs**. Note that the user-created files will remain. Re-insert the Installation CD to start the install process again.

IMPORTANT! Under no circumstances should the Version 3.0 and Version 3.1 applications be present simultaneously on the hard drive.

To install SynthAssist Software Version 3.1:

1. Insert the *SynthAssist 3.1 Software CD* into the CD drive of your computer.

If autorun is enabled, the Preparing to Install screen is displayed. If the screen is not displayed, click **setup.exe** in the CD root directory to begin installation or re-start the computer.





2. At the Welcome screen (Figure 2-4), click **Next** to open the Customer Information screen (Figure 2-5).



Figure 2-4 The Welcome Screen

3. Enter your User Name and Organization, then click Next.

SynthAssist™ 3.1-Installation Wizard	×
Customer Information	AB Applied Biosystems
Please enter your information.	SynthAssist 3.1
User Name:	
I	
User Organization:	
	- -
InstallShield	
C	Next > Cancel

Figure 2-5 The Customer Information Screen

- 4. Click to accept the license agreement.
- 5. In the Destination Folder screen (Figure 2-6), click **Next** to accept the default location.



Figure 2-6 The Destination Folder Screen

Note: Always accept the default location, C:\Program Files\.

6. Click **Install** on the Ready to Install the Program screen (Figure 2-7) to begin the installation of SynthAssist Software 3.1.

🐻 SynthAssist™ 3.1 - InstallShield Wizard	
Ready to Install the Program	AB Applied Biosystems
The wizard is ready to begin installation.	SynthAssist 3.]
If you want to review or change any of your installation settings, click Back. C exit the wizard. Current Settings:	lick Cancel to
Setup Type:	
Destination Folder:	
C:\Program Files\	
User Information:	
User Name: 433A Peptide R and D	
User Organization: Applied Biosystems/Foster City	
InstaliShield < Back Install	Cancel

Figure 2-7 The Ready to Install the Program Screen

The Installing SynthAssist Software 3.1 screen (Figure 2-8) tracks the progress of the installation.



Figure 2-8 The Installing SynthAssist Software 3.1 Screen

IMPORTANT! If you are installing SynthAssist Software for the first time, skip directly to step 9. If you are upgrading to SynthAssist Software Version 3.1 from SynthAssist Software Version 3.0, continue to step 7.

7. The Detecting Previous Installation screen appears over the Installing SynthAssist Software 3.1 screen. Click **Ok** to continue.

j🛃 SynthAss	ist™ 3.1 - I	nstallShield Wi	zard		
Installing	SynthAssis	st™ 3.1			AB Applied Biosystems
The prog	ram features	you selected are	being installed.		SynthAssist" 3. 1
1	Please wait may take s	while the Installs everal minutes.	ihield Wizard instal	ls SynthAssist™ 3,1,	This
	Status:				
	SynthAss	i st™ 3.1			X
	٩	SynthAssist 3.1 of SynthAssist previous versio	installer has dete existing on your m on's data files to th	cted a previous versio achine. It will copy th e new installed locati	on te on.
			OK		
InstallShield					
			< <u>B</u> ack	Next >	Cancel

Figure 2-9 The Detecting Previous Installation Screen

The installation now removes SynthAssist Software 3.0, leaving the Chemisty, Run and Sequence folders. It moves each data file to the appropriate folder in SynthAssist 3.1.

8. Click **Ok** on the Files Copied Notification screen.



Figure 2-10 The Files Copied Notification Screen

9. Click **Finish** to complete the installation process.



Figure 2-11 The Wizard Completed Screen

- **Shortcuts** A successful installation creates two shortcuts to SynthAssist Software 3.1:
 - A desktop icon



- A Start menu path: Start > Programs > Applied Biosystems > SynthAssist 3.1
- **Folder Structure** The folder structure of SynthAssist Software 3.1 is displayed in Figure 2-12. (C:\Program Files\Applied Biosystems)



Figure 2-12 SynthAssist Software 3.1 Folders

Folder Contents Bin

Contains the application and the dynamic link library files necessary to run SynthAssist Software 3.1. These are the only files that should be in the Bin folder. Never store other files in Bin.

Chemistry

Contains the standard AB conductivity chemistry files, any new chemistry files created with SynthAssist Software 3.1 or copied from Version 3.0, and any converted Macintosh[®] chemistry files. This folder contains two additional sub-directories:

- the 3 mL Original Chemistry (conductivity, PNA)
- the Series 200 UV Detector Chemistries

Common

Contains the SynthAssist Software Version 3.1 Dictionary, Lab, and Log files. Never store other files in Common.

Documentation

Contains the SynthAssist Software User Guide.

Help

Contains the screen accessible Help files. Press F1 to access Help.

Log

Contains the new Log files created via SynthAssist Software 3.1 or copied from Version 3.0.

Macintosh Files

Contains the Macintosh files, *e.g.*, chemistries, runs, and sequences that you wish to convert to the PC format and use with SynthAssist Software 3.1. This folder must also contain the Macintosh "SynthAssist Directory" used to create the sequences, chemistries, and runs you wish to convert. See Chapter 3, "Converting Macintosh[®] Files," for more information.

Monitor Bmps

Contains the Monitor displays that have been converted to a bmp file. See Chapter 6, "Setting Up a Peptide Run," for directions on saving monitor traces (UV or conductivity) as bmp files.

Run

Contains the run files created by SynthAssist Software 3.1, any run files copied from SynthAssist Software 3.0, and any converted Macintosh run files.

Sequence

Contains the sequence files created by SynthAssist Software 3.1, any sequence files copied from SynthAssist Software 3.0, and any converted Macintosh files.

Starting SynthAssist 3.1

To start SynthAssist 3.1:

1. Double-click the desktop icon



or use the Start menu: Start > Programs > Applied Biosystems > SynthAssist 3.1.

SynthAssist[®] Software User Guide

This chapter covers:

Overview	.3-2
Converting a Macintosh Dictionary File	.3-4
Converting a Macintosh Chemistry File	.3-7
Converting a Macintosh Sequence File	.3-9
Converting a Macintosh Run File	3-11

Overview

Introduction SynthAssist[®] Software Version 3.1 allows you to convert your existing SynthAssist Software Version 2.0 Macintosh[®] files into a Microsoft Windows[®] compatible format. You can convert SynthAssist Software 2.0 Dictionary, Chemistry, Run, and Sequence files. You do not have to manually re-enter any files that have been previously developed or customized.

Before Converting Files

Before converting SynthAssist Software 2.0 files, you must copy the Macintosh files into specific SynthAssist Software 3.1 folders on your Windows platform computer. Use Table 3-1 to select the correct folder.

Copy This Macintosh File Type	Into This SynthAssist 3.1 Folder	
Dictionary	Macintosh Files	
Chemistry	Mac Chemistry	
Run Mac Run		
Sequences	Mac Sequence	

Table 3-1Macintosh Files and Their CorrespondingSynthAssist 3.1Folders

Note: SynthAssist Software 3.1 installs a copy of the standard Macintosh 2.0 dictionary in the Macintosh Files folder. The standard v2.0 dictionary can be used to convert Macintosh files unless new residues or blocking groups were defined for the sequences that are to be converted. In this case the v2.0 dictionary containing the new definitions must be copied to the Macintosh Files folder in SynthAssist Software 3.1. Overwrite the standard v2.0 dictionary to a PC floppy.

Transferring Files	The simplest procedure to transfer files from a Macintosh to a PC is to copy the Macintosh files onto a PC diskette. Macintosh computers running OS 7.0 or higher can R/W directly to a PC floppy via PC Exchange.
Problems Copying Files	Problems can occur when copying SynthAssist Software 2.0 Macintosh files onto a PC diskette on a Macintosh computer running an operating system earlier than OS 8.

To copy the Macintosh files successfully onto a PC diskette, ensure PC Exchange is running on the Macintosh computer.

File Name Changes

The Macintosh file names can change when the diskette is viewed on a PC. The following figures show the names of three files that were copied to a PC diskette on a Macintosh computer running OS 7.5.5. Figure 3-1 displays the file names viewed on the Macintosh computer. Figure 3-2 displays the file names – on the same diskette – viewed on a PC running the Windows[®] 2000 operating system. After the Mac files have been copied to the Macintosh Files folder in SynthAssist 3.1, correct the file names as appropriate. Delete any special Macintosh characters, such as " Ω " symbols.

<u>Name</u>	Size	Kind	Label
🗋 FastMoc 0.10 ΩMonPrevPk	45K	SynthAssist™ docur	n –
FastMoc 0.25CondMonPrevPk	46K	SynthAssist™ docun	n —
🗋 SynthAssist™ Dictionary	18K	SynthAssist™ docun	n —

Figure 3-1 Names of Copied Files as Viewed from a Macintosh Computer

<u>Name</u>	Size Kind Label	Size Kir	abel
FASTMO~1.10M	45K PC Exchange document —	45K PC	
FASTM0~1.25C	46K PC Exchange document —	46K PC	
D SYNTHA~1	18K PC Exchange document —	18K PC	



Converting a Macintosh Dictionary File

It is not necessary to convert a Macintosh dictionary file to the PC format unless the file contains the definition of special residues or blocking groups for v2.0 sequences that are to be carried forward into v3.1. If a v2.0 "SynthAssist[™] Dictionary" is converted into PC format, it will overwrite the standard "AB433Dictionary" file that has been installed in the Common folder of v3.1.

To convert a Macintosh dictionary file:

1. Select Convert Macintosh Files in the Data Converter.

The Data Converter dialog box opens with Dictionary selected by default in the Select File Type group box (Figure 3-3).

Convert Files		×
Data Co	nverter	
Select File Type		
Octionary	O Chemistry O Sequence O	Run
Source File Name:	D:\Program Files\Applied Biosyste	Browse
Target File Name:	D:\Program Files\Applied Biosyste	Browse
	<u>C</u> onvert Cl <u>o</u> se	

Figure 3-3 The Data Converter Dialog Box

Place the Macintosh dictionary to be converted into the Macintosh Files folder. Either overwrite the existing Macintosh dictionary that has been installed or remove the standard Macintosh dictionary to a PC floppy. Never allow more than one v2.0 dictionary file to be present in the Macintosh Files folder.

IMPORTANT! If the Macintosh dictionary file containing the special residue definitions has become corrupted, it will fail the conversion process. Use the standard PC dictionary to re-define the special residues and re-create the sequence.

2. Click **Browse** to locate the "SynthAssist[™] Dictionary" installed in the Macintosh Files folder (Figure 3-4).



Figure 3-4 Open Dialog Box

3. Select SynthAssist[™] Dictionary in the desired directory, then click Open.

IMPORTANT! Do not change the Target File Name default directory ([Installation Directory]\Applied Biosystems\ SynthAssist3.1\Common\AB433Dictionary.dic).

4. Click **Convert**. If the software prompts you to replace any existing dictionary with the same name, click **OK**.

A message showing File Converted Successfully is displayed.

5. Click OK.

Converting a Macintosh Chemistry File

To convert a Macintosh Chemistry file:

- 1. Select **Chemistry** in the Select File Type group box of the Data Converter dialog box.
- Click Browse to search for the Source File Name. A dialog box displays by default the Macintosh Chemistry files in [Installation Directory] \Applied Biosystems\SynthAssist3.1\ Macintosh Files\Mac Chemistry (Figure 3-5).

Open		? ×
Look in: 🔁 Mac Chemistry	- 🔁 🖻 🗢	≣≣ ▼
Boc_HOBt_DCC 0.10 mmol	🖻 FastMoc 0.10CondMonPrevPk	🔊 FastMc
Boc_HOBt_DCC 0.50 mmol	🗃 FastMoc 0.25 mmol	💌 FastMc
FastMoc 0.10 mmol	🗃 FastMoc 0.25 Mon1st-X	🛋 FastMc
FastMoc 0.10 Mon1st-X	🗃 FastMoc 0.25 MonPrevPk	🖻 Flow Tr
FastMoc 0.10 MonPrevPk	FastMoc 0.25CondMon1-X	🖻 Flow Tr
FastMoc 0.10CondMon1-X	🗃 FastMoc 0.25CondMonPrevPk	🖻 Fmoc_l
		•
File <u>n</u> ame: Select Macintosh	Chemistry File	<u>O</u> pen
Files of type:	_	Cancel //

Figure 3-5 Open Mac Chemistry Dialog Box

- 3. Select a Chemistry file, then click **Open**.
- 4. Click **Browse** to search for the Target file name.

A dialog box displays any previously converted chemistry files in [Installation Directory]\Applied Biosystems\SynthAssist3.1\ Chemistry (Figure 3-6).

Save As			? ×
Save in: 🔁	Chemistry 💌 🗲	🗈 💣	III -
FastMoc 0.	10 mmol.kem		
, File <u>n</u> ame:	Boc_HOBt_DCC_0.10 mmol		<u>S</u> ave
Save as <u>t</u> ype:	Chemistry File(*.kem)	-	Cancel

Figure 3-6 Save As Dialog Box

By default the file name in the File name box corresponds to the unconverted (Macintosh) chemistry file. You can change this file name, but do not change the default directory.

- 5. Click Save.
- 6. Click Convert.
- 7. Select **SynthAssist Dictionary** in the desired directory, click **Open**, then click **Yes** to confirm the chemistry file as the default.

IMPORTANT! Saving a chemistry file as default enables the file to be write-protected. Click **No** if the Chemistry file is to be modified. If you need to make changes to a write-protected file, you must save the file with a different file name using Save As.

8. Click **OK** to confirm that the file converted successfully.

Converting a Macintosh Sequence File

To convert a Macintosh Sequence file:

- 1. Select **Sequence** in the Select File Type group box of the Data Converter dialog box.
- 2. Click **Browse** to search for the Source File Name.

A dialog box displays the Macintosh Sequence files in [Installation Directory] Applied Biosystems\SynthAssist3.1\ Macintosh Files\Mac Sequence (Figure 3-7).

Open			<u>?×</u>
Look jn: 🔁	Mac Sequence	💌 🗕 🗈 (* 🎟 -
ACP (60-7 ACP (65-7 Angiotensi Kinstal	4) 4) n		
	P		
File <u>n</u> ame:	ACP (60-74)		<u>O</u> pen
Files of <u>typ</u> e:	All Files(*.*)	•	Cancel

Figure 3-7 Open Mac Sequence Dialog Box

- 3. Select a Sequence file, then click **Open**.
- 4. Click **Browse** to search for the Target File Name.

A file Save As dialog box displays any previously converted sequence files in [Installation Directory]\Applied Biosystems\ SynthAssist3.1\Sequence.

IMPORTANT! By default, the file name in the File name box corresponds to the unconverted (Macintosh) sequence file. If required, you can change this file name, but do not change the default directory.

- 5. Click Save.
- 6. Click Convert.

7. Select **SynthAssist Dictionary** in the desired directory, click **Open**, then click **OK** to confirm successful file conversion.
Converting a Macintosh Run File

To convert a Macintosh Run file:

- 1. Select **Run** in the Select File Type group box of the Data Converter dialog box.
- 2. Click Browse to search for the Source File Name.

A dialog box (Figure 3-8) displays the Macintosh Run files under [Installation Directory]\Applied Biosystems\ SynthAssist3.1\Macintosh Files\Mac Run.

Open			? X
Look jn: 🔁	Mac Run	💌 🕈 🖻 (* 🎟 •
Kinstall 03	-06-02		
File <u>n</u> ame:	Select Macintosh Run File		<u>O</u> pen
Files of <u>type</u> :	All Files(*.*)	•	Cancel
Files of <u>type</u> :	All Files(*.*)	_	Cancel

Figure 3-8 Mac Run Open Dialog Box

- 3. Select a Run file, then click **Open**.
- 4. Click **Browse** to search for the Target File Name.

A dialog box displays any previously converted Run files in [Installation Directory]\Applied Biosystems\SynthAssist3.1\ Run (Figure 3-9).

Save As			? X
Save in: 🔁	Run	- 🗧 🕯	* 🎟 🕇
ACP (65-74	i).run		
File <u>n</u> ame:	Kinstall 03-06-02		<u>S</u> ave
Save as <u>t</u> ype:	Run File(*.run)	•	Cancel

Figure 3-9 Run Save As Dialog Box

5. Click Save.

IMPORTANT! By default the file name in the File name edit box corresponds to the unconverted (Macintosh) Run file. If required, you can change this file name, but do not change the default directory.

- 6. Click Convert.
- 7. Select **SynthAssist Dictionary** in the desired directory, then click **Open**.

The Provide Converted Chemistry and Sequence File Name dialog box opens.

Provide Converted Chemistry An	d Sequence File Name	×
Unconverted Chemistry File		Browse
Converted Chemistry File Name		Browse
Converted Sequence File Name		Browse
ОК	Cancel	

Figure 3-10 Provide Converted Chemistry and Sequence File Name Dialog Box

8. Click Browse to search for the Unconverted Chemistry file.

A dialog box displays the Macintosh Chemistry files under [Installation Directory]Applied Biosystems\SynthAssist3.1\ Macintosh Files\Mac Chemistry.

Open		? ×
Look jn: 🔁 Mac Chemistry	- 🔁 🛨 💌	∷ .
Boc_HOBt_DCC 0.10 mmol	FastMoc 0.10CondMonPrevPk	🔊 FastMc
Boc_HOBt_DCC 0.50 mmol	FastMoc 0.25 mmol	🔊 FastMc
FastMoc 0.10 mmol	🔊 FastMoc 0.25 Mon1st-X	🔊 FastMc
FastMoc 0.10 Mon1st-X	🔊 FastMoc 0.25 MonPrevPk	🖻 Flow Tr
FastMoc 0.10 MonPrevPk	FastMoc 0.25CondMon1-X	🔊 Flow Tr
FastMoc 0.10CondMon1-X	🔊 FastMoc 0.25CondMonPrevPk	🔊 Fmoc_l
•		F
File <u>n</u> ame: Select Macintosh	Chemistry File	<u>O</u> pen
Files of type:	•	Cancel

Figure 3-11 Mac Chemistry Open Dialog Box

9. Select the Chemistry file associated with the Run, then click **Open**.

- 10. Click **Browse** to search for the Converted Chemistry File Name, select the converted Chemistry File associated with the above Run, then click **Open**.
- 11. Click **Browse** to search for the Converted Sequence File Name, select the converted Sequence File associated with the above Run, then click **Open**.
- 12. Click **OK** to confirm successful file conversion.

This chapter covers:

Communications: PC to ABI 433A Peptide Synthesizer4-2
Sending a Flow Test Chemistry4-4
Running Flow Tests

Communications: PC to ABI 433A Peptide Synthesizer

Communications between the PC and 433A Synthesizer must be established before chemistry or run files can be sent to the synthesizer. The steps of the software connection process are outlined below. The hardware connection is a cable from Com1 of the PC to the 433A Synthesizer Port A.

Enabling Communication

Communication between the PC and the 433A Synthesizer is established via Synthesizer/Connect from the Main Menu. A Connect to Synthesizer window opens and requires three selections. Click **Communications Enabled**. Click the Select Port tab to choose Com1. Lastly, click **OK**. A status message at the bottom-right of the screen displays the communication status: Not Connected/Connected.



Figure 4-1 Connect to Synthesizer

Set Clock





From the main menu select **Synthesizer/Set Clock.** Click **Set** to change the 433A Synthesizer date and time if they differ from the PC. If communication has not been enabled previously, the Connect to Synthesizer window will open to enable communication before the Set Clock option can continue.

Auto-Save From the main menu click File/Auto-Save to open the screen below.



Figure 4-3 Auto-Save

The Auto-Save checkbox is pre-selected and set to 5 minutes by default. Clicking **Cancel** closes the AutoSave dialog box, leaving the previous settings in effect. Clicking **OK** closes the AutoSave dialog box and implements the settings displayed.

Sending a Flow Test Chemistry

Twenty-one predefined (conductivity monitoring) Chemistry files are provided with SynthAssist 3.1 under the C:\ Program Files\ Applied Biosystems\ SynthAssist3.1\ Chemistry directory. In addition, two subfolders of special chemistry files are now included:

- the 3 mL Original Chemistry (tBoc/PNA and conductivity)
- the S200 UV Chemistry.

See the SynthAssist Software v3.1 Release Notes for a further explanation of the chemistry files in these two folders.

By default the installed chemistry files are locked or read-only. A pre-defined Chemistry file must be "Saved As" an unlocked Chemistry file before any changes to the chemistry can be made, such as, modifying modules and cycles, or using the Functions page to select valves and define a user function.

Click **File/Open** from the SynthAssist Software main menu to display the screen below.



Figure 4-4 The File/Open Screen

Selecting **Chemistry** will open the Chemistry folder to display the screen below.

Open				<u>? ×</u>	
Look in: 🔂	Chemistry	•	+ 🗈 💣	· · · ·	
3 mL Origin	al Chemistry	FastMoc 0.2	SCondMon1-X	kem	
🗋 5200 UV CI	nemistry	FastMoc 0.2	SCondMonPre	vPk.kem	
Boc_HOBt_	DCC 0.10 mmol.kem	FastMoc 1.0) mmol.kem		
Boc_HOBt_	DCC 0.50 mmol.kem	FastMoc 1.0) MonPrevPeak	.kem	
FastMoc 0.	10 mmol.kem	FastMoc 1.0	CondMonPrev	Peak.kem	
FastMoc 0.	10 Mon1st-X.kem	Kow Tests 1-18.kem			
FastMoc 0.	10 MonPrevPk.kem	Kow Tests 19-23.kem			
FastMoc 0.	10CondMon1-X.kem	Fmoc_HOBt_DCC 0.10 mmol.kem			
FastMoc 0.	10CondMonPrevPk.kem	Fmoc_HOBt	Fmoc_HOBt_DCC 0.25 mmol.kem		
FastMoc 0.	25 mmol.kem	FT 1-18 Alternate.kem			
FastMoc 0.	25 Mon1st-X.kem	👫 FT 19-23 Alt	ernate.kem		
FastMoc 0.	25 MonPrevPk.kem				
1					
File name:	Provide Windows Chemis	try File Name		Open	
Files of type:	Chemistry File(*.kem)		•	Cancel	

Figure 4-5 The Chemistry Folders and Files in SynthAssist 3.1

Double-click on **Flow Tests 1-18.kem** to open the Chemistry file below.

unctions Default Set		433A Fm	oc 0.000 mmol "Flow Test 1-18
95	Mo	dules	
		Code	Name
	1	A	10 Bottle 10 to RV
	2	в	11 Bottle 10 to Cartridge
	3	С	12 Bottle 9 to Cartridge
	4	D	13 Bottle 5 to Cartridge
	5	E	14 Bottle 10 to Cart,Act,RV
	6	F	15 Bottle 9 to Act Top w/Drain
	7	G	16 Bottle 10 to RV Top
	8	н	17 Measure 7 to Cartridge
	9	1	18 Measure 8 to Cartridge
	10	а	1 Bottle 1 to RV
	11	b	2 Bottle 2 to RV
	12	c	3 Barcode Reader
	13	d	4 Bottle 4 to RV
	14	e	5 Bottle 5 to RV
	15	f	6 Bottle 6 to RV
	16	g	7 Bottle 7 to Waste
	17	h	8 Bottle 8 to Waste
	18	i	9 Bottle 9 to RV
Show Cycle			Show Module

Figure 4-6 Flow Tests 1-18

Click **Send** to open the Send Dialog box.

Sen	d				×
			.005 mmol 2.1.0		
		Code	Name		
	1		User Function		
	2		Run		
	3	A	Read Cart & Add 7&8		
	4	в	TFA Deprotection		
	5	С	Capping (1 min.)		
	6	D	NMP Washes		
	7	E	Read Cart & Add 2X(7&8)		
	8	F	Transfer, Clean Cart & Co		
	9	G	DCM Washes		
	10	Н	Piperidine Depro (Prev Pk)		Send
	11	I	Vortex (5 min.)	–	
9	Sen	d'As: Flo	w Test 1-18		Cancel

Figure 4-7 The Send Dialog Box

Click **Send** to start the transmission process. The Send Progress box fills as the files are sent over.

Sending module 'G' - 16 Bottle 10 to RV Top	Stop

Figure 4-8 The Send Progress Box

Note: The synthesizer acknowledges the transmission by chirping each time it receives a module.

Running Flow Tests

Consult the ABI 433A Peptide Synthesizer User Guide for details on the Flow Tests and specifications required to verify the proper operation of the instrument. This chapter covers:

Specifying the Sequence of Amino Acids	.5-2
Undefined Residues and Termini	.5-6
Changing the Peptide Sequence	.5-8
Deletion Sequences	5-10

Specifying the Sequence of Amino Acids

Creating a To create an amino acid sequence: Sequence

1. Select **File** > **New**.



Figure 5-1 File Type Dialog Box

2. In the File Type dialog box (Figure 5-1), click Sequence. The Sequence screen opens along with the AA palette screen (Figure 5-2).



Figure 5-2 Sequence Screen and AA Palette

3. At the sequence screen enter the amino acid by clicking the amino acid keys in the AA palette, or by typing the one-letter codes.

The chemical formula, number of amino acids in the sequence, average molecular weight, and the monoisotopic molecular weight are automatically calculated and displayed on the Sequence screen as you make the entries.

4. Highlight the C- or N-terminus (OH or H) of the Sequence in the Sequence screen. The palette changes to a selection of C- or N-termini.

5. Click Save As, then name the sequence.

The name appears in the title bar of the Sequence screen.

- 6. Select a button on the left above the Sequence to specify the format of the amino acid sequence.
- 7. Select A to display the sequence using the one-letter format (Figure 5-3).

🕂 ACP (65-74)	×
Average MW: 1063.176 Formula: C47 H74 N12 016	SS: O Color Isotopic MW: 1062.535
No. of AA in Sequence: 10	
Comment: Acyl Carrier Protein (65-74)	Save As Close
H-V-Q-A-A-I-D-Y-I-N-G-OH	
<u> </u>	

Figure 5-3 One-Letter Sequence Format

8. Select **Aaa** to display the sequence using the three-letter format (Figure 5-4).



Figure 5-4 Three-Letter Sequence Format

- 9. Select **File > Print Preview** to view the sequence as it will appear in printed form.
- 10. Select File > Print (or press Ctrl+P) to print the sequence screen.
- 11. When you finish, select **File > Save As**, then type in the name of the sequence.
- 12. Click **Save**. By default the new sequence will be saved in the Sequence folder.

Undefined Residues and Termini

g a To access an existing sequence:

Accessing a Sequence

- 1. Select File > Open.
- 2. Click Sequence.
- 3. Locate the sequence file of interest, select it, then click Open.

About Undefined Residues When an existing sequence is opened, SynthAssist[®] Software Version 3.1 checks each residue and each terminus in the sequence for its definition in the current dictionary. If a residue in the sequence is not defined, *e.g.*, the sequence was copied into your SynthAssist software from another site with a different dictionary, the following message appears (Figure 5-5).

Mismatched Sequence	×
One (or more) Amino Acid(s) in the sequence file opened is(are) not in the current Dictionary. The residue (or residues) will be deleted from the sequence.	
lle-lle-Lys-Lys-Ser-Thr-AlaGly-	
OK Cancel	

Figure 5-5 Mismatched Sequence Message Box

The dialog box displays the sequence with a blank space substituted for the undefined residue(s). You can click **OK** to open the deleted sequence or click **Cancel**.

About Undefined Termini

Unidentified N-Terminus

If a terminus in the sequence is not defined, *e.g.*, the sequence was copied into your SynthAssist from another site with a different dictionary, the following message appears (Figure 5-6).



Figure 5-6 N-Terminal Substitution Message Box

When the sequence is opened, the new N-terminus is displayed as "H."

Unidentified C-Terminus

For an undefined C-terminus, the following message appears (Figure 5-7).



Figure 5-7 C-Terminal Substitution Message Box

When the sequence is opened, the new C-terminus is displayed as "OH."

Changing the Peptide Sequence

Deleting an Amino Acid	To delete an amino acid, do one of the following:					
	Method A:					
	1. Place the cursor to the right of the amino acid you want to delete.					
	 Press the backspace key () or the Delete key. The amino acid is deleted from the sequence. 					
	Method B:					
	1. Select the amino acids you want to remove by dragging the cursor through them.					
	 Select Edit > Cut, or press the Delete key. The selected amino acid(s) are deleted from the sequence. 					
	3. Select File > Save As and provide a new name for the sequence.					
Adding an Amino	To add an amino acid:					
Acid	1. Place the cursor in the location where you want to add an amino acid.					
	2. Select the amino acid from the AA palette, or type the one-letter code for the amino acid on the keyboard.					
	3. Select File > Save As and provide a new name for the sequence.					
Changing Amino	To change amino acids:					
Acids	1. Select the amino acids you want to change.					
	2. Delete the amino acids you want to change.					
	3. Enter the new amino acids.					
	4. Select File > Save As and provide a new name for the sequence.					
Changing Termini	To change N-terminus or C-terminus					
	1. Select a terminus in the sequence. The corresponding buttons in the palette are enabled.					
	2. Click a new terminus compound in the Palette.					

- 3. When you finish, select the Sequence.
- 4. Select **File > Save As** and provide a new name for the sequence.

To use copy and paste in a Sequence:

Using Cut/Copy/Paste in an Amino Acid Sequence

- 1. Open the Sequence file from which the sequence is to be copied.
- Select a portion of the amino acid sequence, then select Edit > Cut or Edit > Copy.

IMPORTANT! You can copy only the amino acids in a sequence but not the termini.

- 3. Open or create the sequence where the copied amino acids are to be pasted.
- Place the cursor where you want to insert the sequence, then select Edit > Paste.

IMPORTANT! Do not use Ctrl+C, Ctrl+V to copy/paste in the Comment field. To copy a part of a comment, select, then right-click the part of interest, then select **Copy**. To paste text in the Comment field, place the cursor at the right in the Comment field, right-click, then select **Paste**.

Note: You can use Microsoft Word[®], WordPad[®], or Notepad[®] to cut/copy/paste sequences from the Sequence screen to other text editors, or vice versa. However, copying between sequences of single-letter format (A) to triple-letter format (Aaa) or vice versa is not permitted.

Deletion Sequences

Creating Deletion Sequences

The Sequence page is also useful in the search for deletion peptides that may be produced during a difficult synthesis. Removing one or more residues from the starting sequence gives the mass of a suspected deletion peptide that can be compared with mass spec data.

To create deletion sequences:

- 1. Open the starting sequence and copy/paste it into a new sequence.
- 2. Create deletions in the new sequence while the starting sequence remains displayed on the screen for comparison.

Note: If a set of deletions in the new sequence begins to lose track of the original residues, copy/paste again from the starting sequence into the new sequence.

3. When a particular deletion sequence matches a mass spec peak, use **File>Save As** to name the deletion peptide.

The Run

6

This chapter covers:

Setting Up a Peptide Run	••••	 	 	 6-2
Peptide Resin Calculations		 	 	 6-5
Sending a Peptide Synthesis .		 	 	 6-10

Setting Up a Peptide Run

Starting a New Run

To start a new run:

 Select File > New, or press Ctrl+N. The File Type dialog box opens.



Figure 6-1 File Type Dialog Box

2. Click **Run**. The Run screen opens with the Calculation view (Figure 6-2).

Open Sequence Seque			Seque	nce Se	lect	Selec	t					
Open Chemistry	y	Cher	nistry fil	е	Ch	emistry	Seque	ence				
🕂 Kinstall 03-06-02.run											×	1
Run				2					K.	K	55	No. of Concession, name
		Fas	tMoc 0.10 Mo	nPrevPk.kem	·	SAVE ->	SEND 🔶	MONITOR	CLOSE	→		
AA	3*		Kinstall.	seq		ja						
Amino Acid												1
	Ninhy	drin Volume:	5 mL								Γ	
CRT		Amino Acid	Default derivative	Subst. (mmol/g)	Resin (mmols)	Weight (g)	Sample (mgram)	Absorb. (570 mm)	Amine µmol/g	Percent	Resin Eq. Wt.	
		Preloaded Re		0.9500	0.1000	0.1053	0.0000	0.0000	0.0000	0.0000	1052.6316	l
010		Gly		0.9500	0.1000	0.1053	0.0000	0.0000	0.0000	0.0000	1052.6316	l
UYC	1	Leu		0.8578	0.1000	0.1166	0.0000	0.0000	0.0000	100.0000	1165.7910	l
	2	Leu		0.7819	0.1000	0.1279	0.0000	0.0000	0.0000	100.0000	1278.9504	l
Cycles	3	Ala		0.7407	0.1000	0.1350	0.0000	0.0000	0.0000	100.0000	1350.0293	J.
	4	Thr	tBu	0.6635	0.1000	0.1507	0.0000	0.0000	0.0000	100.0000	1507.2419	
CAL	5	Ser	tBu	0.6059	0.1000	0.1650	0.0000	0.0000	0.0000	100.0000	1650.4277	
GAL	6	Lys	Boc	0.5323	0.1000	0.1879	0.0000	0.0000	0.0000	100.0000	1878.7192	
	7	Lys	Boc	0.4746	0.1000	0.2107	0.0000	0.0000	0.0000	100.0000	2107.0107	
Laiculation	8	lle		0.4504	0.1000	0.2220	0.0000	0.0000	0.0000	100.0000	2220.1702	
	9	lle		0.4286	0.1000	0.2333	0.0000	0.0000	0.0000	100.0000	2333.3296	l
	10	н		0.4737	0.1000	0.2111	0.0000	0.0000	0.0000	100.0000	2111.0864 🔻	l
	•											8

Select the pages of a run

Figure 6-2 Run Screen

Selecting a You can sel the Chemistry

You can select a Chemistry file different from the one displayed in the Chemistry file box.

Note: By default a new run always displays the Chemistry previously sent to the synthesizer.

To select a chemistry file:

1. Click the Chemistry file selection icon.

A File Open dialog box opens, displaying the Chemistry folder (Figure 6-3).

2. Select the Chemistry file of interest, then click **Open**.



Figure 6-3 Selecting a Chemistry File

Selecting the Run Sequence

To select the run sequence:

Note: Creating a new run requires selecting a new sequence.

- 1. Click the **Select Sequence icon** on the Run page to open the Sequence folder.
- 2. Double-click the Sequence file of interest, or highlight the file and click **Open**.
- 3. The residues of the sequence fill-in the Run pages. The sequence name appears in the sequence box of the Run.

Peptide Resin Calculations

Note: You can print any of the four views in a Run file by selecting File > Print for the current screen.

Selecting the Type of Resin, Substitution, and Chemistry Scale

To select the type of resin:

1. Click the resin type cell, then select the desired resin type from the drop-down list (Figure 6-4).

	Amino Acid	Default derivative	Subst. (mmol/g)	Resin (mmols)	
	Arnide Resin	-	0.0000	0.1000	Resin ty
1	HMP Resin	1	7.6220	0.1000	
2	Preloaded Resin	Boc	2.7817	0.1000	
3	Amide Resin	Boc	1.7013	0.1000	
4	lle		1.4267	0.1000	
5	Нур		1.2284	0.1000	
6	Arg	Pmc	0.8087	0.1000	
7	Arg	Pmc	0.6027	0.1000	
8	H		0.6027	0 1000	

Figure 6-4 Selecting Resin Types

For FastMoc or Fmoc chemistries, the resin types are Amide Resin, HMP Resin, and Preloaded Resin, as predefined in the Dictionary file. Additional resins can be defined in the Dictionary.

- 2. Press Tab to refresh the view.
- 3. Click the substitution entry (the first field in the Subst. column).
- 4. Enter the Substitution value.
- 5. Press **Tab** to refresh the calculation.
- 6. Click the **Resin** (mmols) field, then enter the mmol scale if necessary.

Note: The Resin (mmols) field is carried over from the selected Chemistry.

7. Press **Tab** to refresh the calculation.

Note: The amount of resin needed is indicated in the Weight (g) field. If you change the Resin Substitution value, the Scale, or the Resin weight, SynthAssist software calculates new values for the other two parameters.

Changing Protecting Groups

To change protecting groups:

- 1. Click the default derivative cell for the amino acid you want to change (Figure 6-5).
- 2. From the drop-down list, select a protecting group, then press **Tab** to refresh the view.

Note: The list of protecting groups is defined in the Dictionary for each amino acid.

	Amino Acid	Default derivative	
	Preloaded Re		
	Tyr	tBu	
1	Thr	tBu	
2	Arg	Pmc 💌	
3	Glu	Pmc -	Select a
4	Trp	Mtr	
5	Gin	Pbf	[
6	Н		

Figure 6-5 Selecting a Protecting Group

Changing the Run Cycles

To change the run cycles:

1. Click **Cycles** in the Run view selection panel (Figure 6-6) of the Run Window.

Test 06jul04.run						
Run			32			Contraction of the
	 	Fasth	foc 0.10 mmol.kem	SAVE ->	SEND ->	
AA	<u>}</u> *		Test.seq	Be		
Amino Acid						
CRT		1	1			
		AA	Cycle	Modules	Comments	
Cartridges	1	Met	NMP Wash	D		
-	2	Lys	Single Couple	BADEF		
	3	Lys	Single Couple	BADEF		
CYC	4	lle	Single Couple	BADEF		
	5	Нур	Single Couple	BADEF		
Eucles	6	Arg	Single Couple	BADEF		
0,000	7	Arg	Single Couple	BADEF		
	8		Final Deprotection	BIDc		
CAL						



- 2. Click the cycle cell for the cycle you want to change (Figure 6-7).
- 3. In the drop-down list, select the cycle you want to change.

	🕂 Test 06jul04.run						
	Run			C Stor			Stork
	AA	3* 3*	Fa	astMoc 0.10 mmol.kem Test.seq	SAVE →	SEND MONITOR	CLOSE 🔶
	CRT		AA	Orde	Modules	Comments	
			Met	NMP Mash	D		
	Lartridges	2	Lvs	Single Couple	BADEF		
		3	Lys	Single Couple	BADEF		
	CYC	4	lle	Single Couple	BADEF		
Use the non-		5	Нур	Double Couple/Ac2O Capping	BADEIADEFCD		
ose the pop	Cycles	6	Arg	<< None >>	BADEF		
up field to		7	Arg	Loading & Benzoic Anhydride Ca	BADEF		
· 1 · 1	041	8		Single Couple Single Couple with RS	BIDC		
override the	UAL			NMP Wash			
avala calcotad				Single Coupling/Ac2O Capping			
cycle selected	Lalculation			Double Couple			
for an amino				Double Couple/Ac2O Capping DCM Wash			
				Final Deprotection			
acid				Cycle 1, Amide			



Determining Different Amino Acids

To determine the number of different amino acids in the peptide:

1. Click Amino Acid in the Run view selection panel.

A list of the different amino acids and the number of amino acids in the peptide (in numeric and bar-graph format) appear in the screen (Figure 6-8).



Figure 6-8 Amino Acid in the Run View

Cartridges 1. Click **Cartridges** in the Run view selection panel.

An amino acid cartridge template is displayed (Figure 6-9).

Kinstall 03-06-02.run	2	<u> </u>
Run		
AA	Case FeastMod 0.10 MonPrevPk.kem Case Serie Serie MonITOR CLOSE CLOSE MonITOR CLOSE MonITOR CLOSE MonITOR CLOSE MonITOR CLOSE MonITOR MonITOR <tht< td=""><td></td></tht<>	
Amino Acid		
Cartridges		Amino acid
CYC	1 2 3 4 5 6 7 8 9 10 lie lie Lys Lys Ser Thr Ala Leu Leu Needle	template
Calculation		L

Figure 6-9 Amino Acid Cartridge Template

- Select File > Print, or press Ctrl+P to print the template.
- 3. Lay out the amino acid cartridges on the template, then load them onto the synthesizer.

IMPORTANT! Load the amino acid cartridges from the C-terminal end.

IMPORTANT! When viewed in the 433A guideway, the N-terminal cartridge is on the left. The first C-terminal cartridge to be activated is on the right and is adjacent to the Needle cartridge. The Needle cartridge is present as a reminder to place an empty (used) cartridge under the needles at the start of every synthesis run.

Sending a Peptide Synthesis

If you have not saved your files, select **File** > **Save**, or press **Ctrl+S**, or click **Save**.

Sending the Chemistry File to the Synthesizer

To send the chemistry file to the synthesizer:

IMPORTANT! If you have not reset the synthesizer or not changed user functions or modules, or if you are not changing chemistry files, you can skip the following steps.

1. Click the chemistry file icon in the Run screen (Figure 6-2). The Chemistry screen opens (Figure 6-10).

🕂 FastMoc 0.10 mmol.kem	<u>×</u>
Functions Default Set	433A. Fmoc 0.100 mmol "FastMoc 0.10"
Cycle 1, Amide	Code Name
DCM Wash	1 A Activation
Double Couple	2 B Deprotection
Final Deprotection	3 C Capping with Ac2O Solution
Loading & Benzoic Anhydride Capping	4 D NMP Washes
NMP Wash Single Sougle	5 E Transfer
Single Couple with BS	6 F Clean, Couple, Drain & Wash
Single Coupling/Ac20 Capping	7 G Resin Sampling
	8 H Load and Cap
	9 I Wait (10 min)
	10 a Module a
	11 b Module b
	12 c DCM Washes
	13 d Module d
	14 e Module e
	15 f Module f
	16 g Module g
	17 h Module h
	18 Module I
Show Cycle New Cycle Delete Undo Save	Show Module Send Close

Figure 6-10 Chemistry Screen

2. Select Synthesizer > Send.

If you are not already connected to the synthesizer, the Connect to Synthesizer dialog box opens (See Chapter 4, Figure 4-1).

Sending the Peptide Run to the Synthesizer

Before starting a synthesis, you must send the peptide run to the ABI 433A Peptide Synthesizer to tell the SynthAssist software which run on the synthesizer is current. Before you send a run, you must first save it. When you send the run to the synthesizer, the cartridge list is also sent.

To send the peptide run to the synthesizer.

1. Select Synthesizer > Send.

If there is a chemistry mismatch, for example, if FastMoc 0.10 is loaded on the synthesizer, but the PC is using Boc_HOBt_DCC 0.10 mmol chemistry, the message shown in Figure 6-11 is displayed.

d		FT1-18Alternate		×	
	Code	Name	▲		Message
1		User Function			displayed when
2		Run		The Synthesizer	the chemistry sen
3	A	10 Bottle 10 to RV		doesn't have the	does not match
4	в	11 Bottle 10 to Cartridge		same chemistry.	the chemistry
5	С	12 Bottle 9 to Cartridge			loaded on the
6	D	13 Bottle 5 to Cartridge			synthesizer
7	E	14 Bottle 10 to Cart,Act,R			
8	F	15 Bottle 9 to Act Top w/D			
9	G	16 Bottle 10 to RV Top			
10	н	17 Measure 7 to Cartridge		Send	
11	1	18 Measure 8 to Cartridge	•		
Sen	d As: FT	'd' GX270+ xp Test		Cancel	



 To correct the condition, open the Chemistry screen, select Synthesizer > Send, then click Send in the Communications screen. Starting the T Peptide Synthesizer

To start the peptide synthesizer:

- 1. On the keyboard of the peptide synthesizer, press the **cycle monitor** soft key.
 - 2. Respond to the questions on the synthesizer screen, then press **begin**.

Viewing the Lab Screen

To view the current status of the run

1. Select **Common** > **Lab**.

The status of the peptide synthesizer appears in the SynthAssist Lab screen (Figure 6-12).

	Lab	
	Run Number:	Click here to change the Run number
	Run ACP (65-74).run	Comment field
	Idle Low Gas Pressure	
	Synthesizer Name: 433A Send Comment Save Close	
Name field	Status display	



2. Type the name of the peptide synthesizer in the Synthesizer Name field.

Note: The run number increments automatically when a run is sent to the synthesizer.

3. Enter your comment in the Comment field, then click **Send Comment** to send the comment to the Log.

Note: If your comment is very long, break it into multiple sentences, where each sentence starts with a new line. Press the **Enter** key each time you want to create a new line in the comment field. Multiple sentences in the Comment field appear as separate log messages in SynthAssist Log.

Note: If you send a Chemistry file to the synthesizer, its name is displayed in the Lab screen. When a new run is created, it uses the Chemistry file displayed in the Lab screen. If the Chemistry file has been moved to a different folder or deleted, the Chemistry File Name field of the run becomes <<None>>. Unlike earlier versions (for Macintosh), SynthAssist 3.1 software does not use the run number as the run file name.

Viewing the Monitoring Status of the Run

To view the monitoring status of the run:

1. Click Monitor in the Run screen.

The Monitor screen opens, displaying the monitoring values measured during a run. Figure 6-13 shows the conductivity deprotections typically observed for a Kinstal synthesis. The monitor window can display any values saved by Function 132, such as deprotections (conductivity or UV) or solvent conductivites measured via Flow Tests 20 and 22.



Figure 6-13 Monitor Screen

2. Print the Monitor graph by clicking **File > Print**.
3. If you want to save the Monitor graph in bitmap (.bmp) format, maximize the Monitor screen to maximize the area of the graph to save, then select **File > Save As BMP**.

Note: Later you can edit and/or export to other formats.

By default the Monitor Bmp folder is displayed.

4. Name the file, then save it in the Bmp folder.

Viewing the Log

When the SynthAssist software communicates with the peptide synthesizer, the information is added to the log. To view the log, select **Common** > **Log** (Figure 6-14).

🕺 L	og		×
l	og		
	Date	Context	Details
1	01/30/2003 20:55:27	Communication	Set Clock for Synthesizer to 01/30/2003 20:55:24
2	01/30/2003 20:55:30	Communication	Sending chemistry file "FastMoc 0.10" to SYNTHESIZER
3	01/30/2003 20:55:33	Communication	Sending user functions
4	01/30/2003 20:55:36	Communication	Sending module 'A' - Activation
5	01/30/2003 20:55:40	Communication	Sending module 'B' - Deprotection
6	01/30/2003 20:55:43	Communication	Sending module 'C' - Capping with Ac2O Solution
7	01/30/2003 20:55:46	Communication	Sending module 'D' - NMP Washes
8	01/30/2003 20:55:50	Communication	Sending module 'E' - Transfer
9	01/30/2003 20:55:53	Communication	Sending module 'F' - Clean, Couple, Drain & Wash
10	01/30/2003 20:55:57	Communication	Sending module 'G' - Resin Sampling
11	01/30/2003 20:56:02	Communication	Sending module 'H' - Load and Cap
12	01/30/2003 20:56:05	Communication	Sending module " - Wait (10 min)
13	01/30/2003 20:56:08	Communication	Sending module 'a' - Module a
14	01/30/2003 20:56:11	Communication	Sending module 'b' - Module b
15	01/30/2003 20:56:14	Communication	Sending module 'c' - DCM Washes
16	01/30/2003 20:56:17	Communication	Sending module 'd' - Module d
17	01/30/2003 20:56:20	Communication	Sending module 'e' - Module e
18	01/30/2003 20:56:22	Communication	Sending module 'f' - Module f
19	01/30/2003 20:56:25	Communication	Sending module 'g' - Module g
20	01/30/2003 20:56:28	Communication	Sending module 'h' - Module h
21	01/30/2003 20:56:31	Communication	Sending module 17 - Module i
22	01/30/2003 20:57:04	Communication	Sending run file "ACP (65-74)" - Run No: 11 to SYNTHESIZER
23	01/30/2003 20:58:33	Lab	Note=This run is using the FastMoc 0.10 mmol scale Chemistry
1			View Other Log Export Save As Close

Figure 6-14 Log Screen

The log has the following features:

• There is only *one* log stored in AB433Log.log file in Applied Biosystems\SynthAssist3.1\Common in the program installation folder (D:\Program Files). The log records and retains all information (for example, run, event, comments, monitoring data, all send/receive/set clock information and application errors. • You cannot edit the log using the SynthAssist software. To edit the log, click **Export**, then enter the name of the exported file. All log data is exported in tab-delimited text format. You can view and edit the exported log data using another application such as Notepad.

IMPORTANT! Use Save As to name and save the Log that accompanies each Run carried out on the synthesizer. After saving the Log, delete it when prompted. Do not allow Logs to concatenate for multiple Runs.

• You can print the Log file by selecting **File** > **Print**.

Note: If the computer and the synthesizer are connected during a run, the monitor and Log data are automatically updated as the run progresses. If the computer and synthesizer are not connected during a run, the data is accumulated in the memory buffer of the synthesizer and will be displayed after communications are re-established.

Opening an Existing Peptide Run

To open an existing run:

- 1. Select the **File** > **Open**, or press **Ctrl+O**. The File Type dialog box opens.
- 2. Click the **Run** button. The File Open dialog box opens.
- 3. Select a Run file, then click **Open**.

When the Software Cannot Open a File

If SynthAssist Software 3.1 cannot open the associated sequence or chemistry files (for example, if the Run file is from another computer running SynthAssist 3.1 software), the following messages are displayed (Figure 6-15 and Figure 6-16).



Figure 6-15 Associated Sequence File Was Not Found in the Expected Path

SynthAssist™ 3.1 X Image: The associated chemistry file C:\Program Files\Applied Biosystems\SynthAssist3.1\Chemistry\pwb\UV FastMoc 1.0 S200.kem not found..!! Please select chemistry....

Figure 6-16 Associated Chemistry File Was Not Found in the Expected Path

SynthAssist Software 3.1 opens the File Open dialog box for sequence and chemistry files, respectively, allowing you to select the appropriate files. After associating the files with the Run, save the run by overwriting the existing Run file. This ensures that the next time the Run file is opened, it correctly shows the old values saved in the Run file.

Note: If any change is made to the associated Chemistry and/or Run file(s), then the Calculation view is initialized. You need to enter the appropriate values in the Calculation view, then save it.

Sequence Mismatch

If the sequence in a Run file contains residues that are not defined in the current Dictionary, a Mismatched Sequence window opens (see Figure 6-17). Click **OK** to open the Run with a deleted sequence or click **Cancel**.

If the sequence contains a C-terminus or N-terminus that is not defined in the current Dictionary, an error message will open. Click **OK** to open the Run with substituted termini ("H" at the N-terminus or "OH" at the C-terminus) or click **Cancel**.

For example, a sequence with Rhodamine B at the N-terminus is being opened on a PC whose SynthAssist Dictionary does not contain a definition for the dye.

	🕺 Rhodamine 13-mer			×
	Average MW: 1843.694	Formula: C90 H142 N20 019 Cl	SS: 0 Color	Isotopic MW: 1842.045
		No. of AA in Sequence: 13		
	CA © Aaa	Comment: Rhodamine B labelled	Save As Close	
ľ	Rhod-Acp-Pro	-Leu-Ser-Arg-Thr-Leu-	Ser-Val-Ala-Ala-Lys-Lys	s-OH

The following error message appears.



Figure 6-17 Missing N-Terminal Error Message

Creating a Custom Chemistry File

This chapter covers:

Overview	.7-2
Renaming a Chemistry File	.7-4
Changing the Chemistry Information	.7-5
Changing the Selected Functions	.7-6
Changing the Selected Modules	.7-9

Overview

New Predefined Chemistry Files	SynthAssist [®] Software Version 3.1 provides 21 predefined chemistry files in the installation directory: Applied Biosystems\SynthAssist 3.1\Chemistry. Nineteen of the files are the same as those provided with SynthAssist 2.0 software and two files are new. The new files are:
	FT 1–18 Alternate – Contains the same test modules as the standard Flow Tests 1–18, except that the alternate tests sound an alarm and set an interrupt in the modules that require a volume reading at the metering vessel.
	FT 19–23 Alternate – Contains a new test in module "c" that pressurizes the MV/RV and checks solvent flow through the activator.
	By default, the installed chemistry files are locked or read-only. A lock icon is displayed on the chemistry screen. The contents of the file can be viewed but cannot be modified. An unlocked chemistry file can be created via Save As, providing a new name, and selecting "No" to the question "Lock Chemistry File?" In an unlocked chemistry file the cycles, modules, functions, or reagent names can be changed as necessary.
	Note: After creating a custom chemistry, the file can be converted to read-only status via Save As, providing a new name, and selecting "Yes" to the question "Lock Chemistry File?"
Chemistry Software	In SynthAssist software a Chemistry file <i>e.g.</i> , FastMoc0.25 mmol, consists of a series of synthesis cycles. During each cycle, one amino acid is added to the peptide-resin by using a series of modules specified by the user. Each module specifies a series of steps or functions that represent reagent deliveries or various mechanical actions, <i>e.g.</i> , venting, draining, or mixing.
	The organization and hierarchy of the chemistry software is shown in Figure 7-1.



Figure 7-1 Hierarchy of the Chemistry Software

The remainder of this chapter describes how to change reagent names, functions, cycles, modules, and the default set.

Note: You can access and change default sets, cycles, functions, or bottles in any order; you do not need to follow the sequence presented here.

Renaming a Chemistry File

IMPORTANT! Before you can modify a Chemistry file, you must unlock it.

1. Open the Chemistry screen by selecting **File** > **Open**. You can also open the Chemistry screen from the Run screen (click the Chemistry file icon) or from the Lab screen.

Chemistry Information button FastMoc 0.10 mmol.kem X Functions Default Set 433A Fmoc 0.100 mmol "FastMoc 0.10" Modules Cycles Double Couple Code Name Double Couple/Ac20 Capping Activation A 1 Final Deprotection 2 B Deprotection Loading & Benzoic Anhydride Capping С NMP Wash 3 Capping with Ac2O Solution Single Couple 4 D NMP Washes Single Couple with RS 5 Е Transfer Single Coupling/Ac20 Capping F 6 Clean, Couple, Drain & Wash 7 G Resin Sampling н 8 Load and Cap 9 Wait (10 min) 10 la. Module a 11 b Module b 12 С DCM Washes 13 d Module d 14 e Module e 15 f Module f 16 g Module g 17 h Module h 18 Module i Show Cycle Show Module New Cycle Delete Send Close

The Chemistry screen opens (Figure 7-2).

Figure 7-2 Chemistry Screen

Changing the Chemistry Information

To update synthesizer and chemistry parameters:

1. In the Chemistry screen, click the **Chemistry Information** button (Figure 7-2).

The Chemistry Information dialog box opens (Figure 7-3).

Information for Fa	stMoc 0.10	×
Model:	433A 💌	
Туре:	Fmoc	
Scale:	0.100 mmol	
Name:	FastMoc 0.10	
·····	OK Cancel	



- 2. In the Model box, select **433A**.
- 3. In the Type box, select **Fmoc** or **Boc**.
- 4. Type in the scale of the chemistry.
- 5. Type in the name of the chemistry up to 15 characters.
- 6. Click OK.

Changing the Selected Functions

To assess the current functions:

1. In the Chemistry screen, click Functions.

The functions screen opens (Figure 7-4).



Figure 7-4 Functions Screen

- 2. Click the **Functions** list box to view the list of functions (Figure 7-5).
- 3. Use the left and right arrow keys next to the list box to go to a different function.



Figure 7-5 The Function List Box

Accessing a Standard Function

Method A

In the Functions screen, click the Functions list box to access standard functions (Figure 7-5).

Method B

If you know the number of the standard function you want, type the number in the Function Number box in the Functions screen, then press **Tab**.



User-defined function box

Figure 7-6 Function 86: Flow NMP Through Reaction Vessel to Auxiliary Waste. Open Valves 2, 9, 10, 20, 23

Creating a User-Defined Function

SynthAssist software has 142 predefined (standard) functions and 10 functions which can be user-defined.

To create a user-defined function:

- 1. In the Function Number box in the Functions screen, type in a function number from 100 to 109, then click **Tab**, or select **User functions** from the Functions list box (Figure 7-5).
- 2. Edit the valves.
- 3. Select or deselect a valve to enable or disable the valve.
- 4. Select or deselect a bottle or vessel to enable or disable the valve that controls the bottle or vessel.

Note: Six activated valves is the maximum allowed.

5. Type in the name of the new user function in the user-defined Function Name box (Figure 7-6). The user-defined function is created.

Changing the Selected Modules

To change modules:

1. In the Chemistry screen (Figure 7-7), select the module number corresponding to the module you want to change (for example, Activation), then click **Show Module**.

The module screen opens (Figure 7-8)

Modi	ules Code	
1	Code	
1		Name
	А	Activation
2	B	Deprotection UV* 3.5%
3	С	Capping Solution @4
4	D	NMP Washes
5	E	Transfer
6	F	*Clean Cartridge & Couple
7	G	Module G
8	н	Module H
9	I	Vortex (5 min)
10	а	*Cond. Act., Wash & Transfer*
11	b	*Cond. Deprotection* 200
12	с	DCM Washes
13	d	NMP Wash from Activator
14	е	MeOH, NMP to Aux.
15	f	*Cond. Extended Coupling*
16	g	Reset to Channel 2
17	h	*Cond. Capping @4*
18	i	*Eject/Advance Cartridge
		Show Module
		Send Close
	4 5 6 7 8 9 10 11 12 13 14 15 16 17 18	4 D 5 E 6 F 7 G 8 H 9 I 10 a 11 b 12 c 13 d 14 e 15 f 16 g 17 h 18 i

Click here to select the module

Figure 7-7 Chemistry Screen

Note: A total of 18 modules are available (a through i and A through I). You cannot delete them, but you can change their contents. You cannot add more modules.

nou	uie Nam	Activation					
	Functi	Name	Time	Add Ti	Elapsed		
1	1	Wait	1	0	1		
2	98	Begin loop UPPER	2	0	1		
3	13	Flush top valve block with NMP to	1	0	16		
4	14	Flush bottom valve block with NMP	3	0	19		
5	9	Flush top valve block with gas to	5	0	24		
6	10	Flush bottom valve block with gas	5	0	29		
7	99	End loop UPPER	1	0	29		Insert
8	4	Read cartridge	10	0	29		
9	6	Needle up	10	0	39		
10	7	Eject cartridge	10	0	49		Delete
11	8	Advance cartridge	10	0	59		
12	5	Needle down	10	0	69		Save
13	14	Flush bottom valve block with NMP	1	0	70		
14	9	Flush top valve block with gas to	2	0	72		
15	65	Deliver NMP to cartridge	5	0	77		Close
16	60	Mix cartridge	5	0	82		
17	78	Pressurize manifold	10	0	92		
18	18	Flush bottom valve block with HBT	1	0	93		
19	94	Deliver HBTU to cartridge	8	0	101		
20	98	Begin loop UPPER	6	0	101		
21	2	Vortex reaction vessel on	1	0	412		
22	60	Mix cartridge	30	0	442		
23	3	Vortex reaction vessel off	1	0	443		
24	60	Mix cartridge	30	0	473		
25	99	End loop UPPER	1	0	473		
26	13	Flush top valve block with NMP to	2	0	475		
27	14	Flush bottom valve block with NMP	2	0	477		
28	9	Flush top valve block with gas to	3	0	480		

Figure 7-8 Module Screen

There are two ways to change the current function in the Module screen:

Method A:

1. Select the name of the function you want to change.

The Function dialog box opens (Figure 7-9).



Click here to display the Function dialog box

Figure 7-9 Function Dialog Box

2. Select a different function, then click **OK**.

Method B:

Via the Functions screen type the number of the function in the Function number box (Figure 7-4), press **Tab**, then click **OK**.

Changing the	To change the duration of a step:
Duration of a Step	1. In the Time column, enter the time (in seconds) for the step to operate. In the monitoring functions Time may be a value other than seconds.
	Use the arrow and numeric keys to select and change the entries in the screen.
	Note: Time for the loop functions represents the number of loops. Time for the monitoring functions, <i>e.g.</i> , 134 or 145, represents a deprotection value.
	 Select Synthesizer > Send to upload the module to the synthesizer.
	3. Close the Module screen by clicking Close .
Renaming a	To rename a module in the Module screen:
Module	Type a new name in the Module Name field, then press Tab .
Inserting a Step	To insert a step in the Module screen:
	1. Highlight the row above which you wish to insert a step.
	2. Click the Insert button, or select Edit > Insert .
	A blank line is inserted below the row you selected.
	IMPORTANT! A module may contain a maximum of 99 steps.
Deleting a Step	To delete a step in the Module screen:
	1. Highlight the row you want to delete.
	2. Click Delete , or select Edit > Delete .
Using	To use copy and paste in a module in the Module screen:
Copy/Paste in a Module	1. Open the Module screen of the Chemistry file from which you want to copy steps.
	2. Click the number of the cell corresponding to the step to copy (Figure 7-10).
	Use Ctrl-click to select multiple steps or drag the mouse.
	3. Press Ctrl+C to copy the steps.

J¥ Fa:	Moo	oc 0.10 9 Jule Nam	5200.kem - A - Activation e Activation				
		Functi	Name	Time	Add Ti	Elapsed	
	1	1	Wait	1	0	1	
	2	98	Begin loop UPPER	2	0	1	
	3	13	Flush top valve block with NMP to	1	0	16	
	4	14	Flush bottom valve block with NMP	3	0	19	
	5	9	Flush top valve block with gas to	5	0	24	
	6	10	Flush bottom valve block with gas	5	0	29	
	7	99	End loop UPPER	1	0	29	Insert
	8	4	Read cartridge	10	0	29	
	9	6	Needle up	10	0	39	
	10	7	Eject cartridge	10	0	49	Delete
	11	8	Advance cartridge	10	0	59	
	12	5	Needle down	10	0	69	Save
	13	14	Flush bottom valve block with NMP	1	0	70	
	14	9	Flush top valve block with gas to	2	0	72	
	15	65	Deliver NMP to cartridge	5	0	77	Llose
	16	60	Mix cartridge	5	0	82	
	17	78	Pressurize manifold	10	0	92	

Click here to select a step

Figure 7-10 Selecting a Step

Note: To select all steps, select the first row, then Shift-click the number of the last row.

- 4. Open the Module screen of the Chemistry file where you wish to paste the steps.
- 5. Select the step where you want to paste the steps.
- 6. Press Ctrl+V to paste the copied steps.

Changing Cycles

You can change the modules that define a cycle in the Cycle screen.

Selecting a Module

To select a module:

1. In the Chemistry screen, double-click the cycle you want to change.

The Cycle screen opens (Figure 7-11).

			List box to specify procedure
Lis nu	t bo mbe	ox to specify er of cartridge	List box to specify number of resin samples
	UV	FastMoc 0.10	5200.kem - Single Couple/Conditional Cap
	Сус	le Name Single	Couple/Conditional Cap
	1	Cartridge 🔽 💌	Single Couple 💌 No Resin Sampl
		Module Code	Module Name
	1	в	Deprotection UV* 3.5%
	2	b	*Cond. Deprotection* 200
	3	A	Activation
	4	D	NMP Washes
	5	E	Transfer
	6	F	*Clean Cartridge & Couple
	7	f	*Cond. Extended Coupling*
	8	h	*Cond. Capping @4*
	9	d	NMP Wash from Activator
	10		
		Insert	Delete Save Close

Figure 7-11 Cycle Screen

Changing a Choose one of the following two methods: Module

Method A:

- 1. In the **Module Name** column, select the name of the module you want to change.
- 2. In the drop-down box, select the new module.

	Module Code	Module Name
1	в	Deprotection
2	A	Deprotection
3	D	Capping with Ac2O Solution
4	E	NMP Washes
5	F	Transfer
6	1	Clean, Couple, Drain & Wash
		Hesin Sampling Load and Cap Wait (10 min) Module a Module b DCM Washes
Γ	Insert	Delete Save Close

Figure 7-12 Select a Module

Method B:

- 3. If you know the letter of the new module, type it in the Module Code column, then press **Tab**.
- 4. Click **Save** to save your changes.

Deleting a Module from the Cycle

To delete a module from the cycle:

1. In the Cycle screen, select the number of the module you want to delete (Figure 7-13).

N		
	Aodule Code	Module Name
- В	1	Deprotection UV* 3.5%
b		*Cond. Deprotection* 200
A	\	Activation
D	I	NMP Washes
E		Transfer
F		*Clean Cartridge & Couple
f		*Cond. Extended Coupling*
d		NMP Wash from Activator

Click here to select a module

Figure 7-13 Selecting a Module.

2.	Click Delete or press	Ctrl+K to delete the module.
----	-----------------------	------------------------------

Inserting a New To Insert a new module in the cycle: Module in the 1. In the cycle screen, highlight the row above which the new Cvcle module will be inserted. 2. Click **Insert** or press **Ctrl+J** to insert a blank module. 3. Type in the module code for the new module, or select the name of the module in the Module Name column. **IMPORTANT!** A cycle may contain a maximum of 20 modules. Creating a New To create a new cycle: Cycle 1. In the Chemistry screen, click New Cycle or press Ctrl+J. A new cycle screen opens with no cycle name (Figure 7-14). 2. Type in a cycle name in the Cycle Name field.

Cyc	FastMoc 0.10	5200.kem - N	ew Cycle	esin Samplı 💌	×	Specify name - here
	Module Code	I	Module Name			
Γ						
					1	
	Insert	Delete	Save	Close		

Figure 7-14 Specifying a Cycle Name.

3. Click the **Cartridges** drop-down list box, then select the number of cartridges you want (Figure 7-15).

Select the number of cartridges

🕂 UV FastMoc 0.10 9	5200.kem - New Cycle	x
Cycle Name		
No Cartridge	Procedure No Resin Sample	
- 2 Cartridge 13 Cartridge	Module Name	
6 Cartridge		
Insert	Delete Save Close	

Figure 7-15 Specifying Cartridges

4. Click the **Procedure** drop-down list box, then make the appropriate selection, for example, Single Couple (Figure 7-16).

Select Coupling

Figure 7-16 Selecting Coupling

IMPORTANT! The standard combinations of cartridge number and coupling are:

- 1 Cartridge, Single Couple;
- 2 Cartridges, Double Couple.

Other cartridge values selected for single or double coupling do not conform to standard usage. SynthAssist software will display a warning message while saving such a cycle.



Figure 7-17 Non-conforming Number of Cartridges

Any cartridge value is allowed with Procedure. A minimum of two cartridges is required for Double Couple.

Note: Single coupling at the 1.0 mm scale requires three cartridges. Double coupling at the 1.0 mm scale requires 6 cartridges.

5. Click the **Resin** samples drop-down list box, then make the appropriate selection, for example, No Resin Samples (Figure 7-18).

WY FastMoc 0.10 5200.kem - Test	
1 Cartridge Single Couple No Resin Sample	Select Resin sampling
Module Code Module 1 Resin Sample 2 Resin Samples 3 Resin Samples 4 Resin Samples	
Insert Delete Save Close	

Figure 7-18 Selecting Resin Samples

6. Type in the module letter in the Module Code column, for example, Module A, corresponding to Activation (Figure 7-19).



Figure 7-19 Entering a Module

7. Press **Ctrl+S** to save the file.

Deleting a Cycle	To delete a cycle:
	1. In the Chemistry screen, select the cycle you want to delete.
	2. Select Edit > Delete.
	3. If you make a mistake, select Edit > Undo , or press Ctrl+Z .
Renaming a	To rename a cycle:
Cycle	1. In the Chemistry screen, double-click the Cycle you want to rename.
	2. in the Cycle Name field, change the cycle name.
	3. Press Ctrl+S to save the Chemistry.
•	

Creating a New Default Set

A default set consists of a series of preset cycles for each chemistry type (for example, Boc, Fmoc or FastMoc). You can change these preset cycles to create a new default set.

Changing a Default Cycle in a Default Set

1. In the Chemistry screen, click **Default Set** (Figure 7-20).

To change a default cycle in the default set:

Default Set	433A Fmoc 0.100 mmol "UV 0.10/S200"]
	Modules	_
	Default Set	Default Set 433A. Fmoc: 0.100 mmol. "UV 0.10/S200" Modules

Click here to open the default set

Figure 7-20 Opening the Default Set

The Default Set screen opens (Figure 7-21).

ι UV	FastMoc 0.10 520	00.kem - Default Se	et	
	AA	Cycle	Module	Comments
1	Default	Single Couple/Condit	BbADEFf	
2	Preload	Complete Wash	ecD	
3	Load	< <none>></none>		
4	Amide	Cycle 1: Amide	ecDBgAD	
5	Other	< <none>></none>		
6	End	Final Deprotection	BblDcc	
F				
•				Þ

Figure 7-21 The Default Set Screen

2. In the drop-down list of cycles, select the desired cycle (Figure 7-22).

	AA	Cycle	Modules	Comments
1	Default	Single Couple/Conditional Cap	BbADEFfh	
2	Preload	Complete Wash	ecD	
3	Load	< <none>></none>		
4	Amide	Cycle 1: Amide	ecDBgAD	
5	Other	< <none>></none>		
6	End	Final Deprotection	BblDcc	
•	Inser	Double Couple/Cap Double Couple/Conditional Final Deprotection Final Deprotection & Acety Final Deprotection/No Feec Final Frace On NMP Wash Single Couple Single Couple/Cap Single Couple/Conditional C Single Couple/No Feedbact	Save	Close

🔆 UV FastMoc 0.10 5200.kem - Default Set 👘



The cycle you select, in this example Final Fmoc On (Figure 7-23), becomes the default End cycle for this Chemistry file.

1 Default Single Couple/Conditional Cap BbADEFfh 2 Preload Complete Wash ecD 3 Load < <none>> ecDBgAD 4 Amide Cycle 1: Amide ecDBgAD 5 Other <<none>> cc 6 End Final Fmoc On cc</none></none>		AA	Cycle	Modules	Comments
2 Preload Complete Wash ecD 3 Load < <none>> ecDBgAD 4 Amide Cycle 1: Amide ecDBgAD 5 Other <<none>> 6 End Final Fmoc On</none></none>	1	Default	Single Couple/Conditional Cap	BbADEFfh	
3 Load < <none>> 4 Amide Cycle 1: Amide ecDBgAD 5 Other <<none>> 6 End Final Fmoc On</none></none>	2	Preload	Complete Wash	ecD	
4 Arnide ecDBgAD 5 Other < <none>> 6 End Final Fmoc On ✓ CC</none>	3	Load	< <none>></none>		
5 Other < <none>> 6 End Final Fraction CC</none>	4	Arnide	Cycle 1: Amide	ecDBgAD	
6 End Final Fmoc On cc	5	Other	< <none>></none>		
	6	End	Final Fmoc On 💌	cc	

Figure 7-23 A new default cycle for End

IMPORTANT! SynthAssist 3.1 software has two additional AA cells in the default set: Amide and Other.

Inserting Amino Acids in a Default Set

To insert amino acids in a default set:

1. In the Default Set screen, click **End**, then click **Insert**. Repeat, to insert each subsequent amino acid (Figure 7-24).

	AA	Cycle	Modules	Comment
1	Default	Single Couple/Conditional Cap	BbADEFfh	
2	Preload	Complete Wash	ecD	
3	Load	< <none>></none>		
4	Arnide	Cycle 1: Amide	ecDBgAD	
5	Other	< <none>></none>		
e	il mana	Final Danketastian	BhiDoo	
<u>.o</u>	End		BRIDGE	
•			BUDGE	

Click to select the last row

Figure 7-24 Inserting an Amino Acid

2. Click the empty AA field to display the amino acid list (Figure 7-25).

	AA	Cycle	Module	Comment
1	Default	Single Couple/Condit	BbADEFf	
2	Preload	Complete Wash	ecD	
3	Load	< <none>></none>		
4	Amide	Cycle 1: Amide	ecDBgAD	
5	Other	< <none>></none>		
6		Single Couple/Condit	BbADEFf	
-	End	Final Depretaction	BhlDee	
/	jena –	Final Deprotection	DDDCC	
<u>/</u>		Final Deprotection		

Figure 7-25 Displaying an Amino Acid List

3. Select an amino acid from the drop-down list (Figure 7-26).

The Default cycle of the chemistry is associated with the new amino acid.

U¥ FastMoc 0.1	0 5200.kem - Default Set		
AA	Cycle	Module	Commen
1 Default	Single Couple/Conditional Cap	BbADEFf	
2 Preload	Complete Wash	ecD	
3 Load	< <none>></none>		
4 Amide	Cycle 1: Amide	ecDBgAD	
5 Other	< <none>></none>		
6 🔻	Single Couple/Conditional Cap	BbADEFf	
7 Ala 🔺	Final Deprotection	BblDcc	
Arg Asn Asp Cys			
			•
Gly His Ile Leu Lys ▼	Delete Save		Close

Figure 7-26 Selecting an Amino Acid.

4. To associate a different cycle with the newly inserted amino acid (Asn), click the cell in the cycle column to the right of the amino acid (Figure 7-27).

2	UY	FastMoc 0.10) S200.kem - Default Set			
		AA	Cycle	Module	Commen	
	1	Default	Single Couple/Conditional Cap	BbADEFf		
	2	Preload	Complete Wash	ecD		
	3	Load	< <none>></none>			
	4	Amide	Cycle 1: Amide	ecDBgAD		
	5	Other	< <none>></none>			_Click here to
	6	Cys	Single Couple/Conditional Cap	BbADEF		display
	7	End	Final Deprotection	BblDcc		Cvcle list
	•				Þ	
	[Insert	Delete Save		Close	

Figure 7-27 Displaying the Cycle List.

5. Select a cycle from the drop-down list (Figure 7-28), then press **Tab**.

×.	UV FastMoc 0.10 S200.kem - Default Set				
		AA	Cycle	Module	Commen
	1	Default	Single Couple/Conditional Cap	BbADEFf	
	2	Preload	Complete Wash	ecD	
	3	Load	< <none>></none>		
	4	Amide	Cycle 1: Amide	ecDBgAD	
	5	Other	< <none>></none>		
	6	Cys	Single Couple/Conditional 💌	BbADEFf	
	7	End	DCM Wash	BblDcc	
	•	Insert	Double Couple Double Couple/Cap Double Couple/Conditional Final Deprotection Final Deprotection & Acety Final Deprotection/No Fee Final Fmoc On NMP Wash Single Couple Single Couple/Cap		► Close



Creating a Non-Default Cycle for an Amino Acid in a Default Set To create a non-default cycle for an amino acid in the Default Set:

- 1. Insert the amino acid in the Default Set screen (See "Inserting Amino Acids in a Default Set" on page 7-24).
- 2. Select None as the cycle (Figure 7-29).

	AA	Cycle	Module	Commer
1	Default	Single Couple/Conditional Cap	BbADEFf	
2	Preload	Complete Wash	ecD	
3	Load	< <none>></none>		
4	Amide	Cycle 1: Amide	ecDBgAD	
5	Other	< <none>></none>		
6	Cys	< <none>> 🔽</none>		
7	End	Final Deprotection	BblDcc	

Figure 7-29 Select None as a Default Cycle

You can now enter any combination of modules in the Run screen for Cys. You must choose the module(s) for the amino acid **Cys** in the Run file for all subsequent runs.



Specify modules here



Changing a Cycle in the Run Screen

If you change a cycle in the Run screen, the change is associated only with that run, not with the chemistry or with any future runs.

To change a cycle in the Run screen:

1. In the Run screen, click the Cycle cell to the right of Cys.

A list of cycles is displayed (Figure 7-31).

2. Select a cycle, for example, Double Couple/Conditional Cap, then press **Tab**.


Figure 7-31 Changing a Cycle in the Run Screen

Double Couple/Conditional Cap is now the default cycle for the amino acid Cys for this run only.

This chapter covers:

Overview

The Dictionary is a database of all compounds (amino acids, other residues, resins, C-terminals, N-terminals, and protecting groups) that SynthAssist® Software Version 3.1 uses. Applied Biosystems has provided the most commonly used compounds but you can delete or modify these compounds or add new compounds of interest.

Opening the Dictionary

To open the dictionary file:

1. Select **Common > Dictionary** from the main menu.

The Dictionary screen for amino acids opens (Figure 8-1).

The default display shows the parameters for the first amino acid in the list on the left. If you select another amino acid, the display shows the parameters for that amino acid (for example, Arg as shown in Figure 8-1).



Figure 8-1 Dictionary Screen

Adding a Compound to the Palette

In the Dictionary screen, select **In Palette**. A \square indicates the compound is in the palette.

IMPORTANT! If you select a non-alphabetic character (for example, a dash or a space) as the single letter code for an amino acid, then that amino acid is not selectable using the keyboard in the Sequence screen.

Adding Color to a Compound

In the Dictionary screen, select a color in the color drop-down list box. The currently selected compound is displayed in this color in the Sequence screen and in the Run Monitor screen.

Note: Default colors for compounds are color coded:

- Black and orange indicate hydrophobic compounds or unknowns.
- Green and blue indicate basic hydrophilic compounds.
- Red indicates acidic hydrophilic compounds.
- Purple indicates -SH residues.

Changing the Default Derivative of an Amino Acid

To change the default derivative of an amino acid:

- In the Dictionary screen (Figure 8-1), click **Boc** or **Fmoc**. The Add/Remove dialog box opens.
- 2. Select a protecting group (Pmc) in the Fmoc derivatives list (Figure 8-2).

The degree symbol (°) to the left of Pmc indicates that Pmc is now the default protecting group.

🕂 Amino Acid Details				×
Dictionary				
AA		JNDO DELETE	NEW → DELETE →	SAVE 🔶 CLOSE 🌩
Amino Acid	Abu Acp Aib Ala	Name:	In Palette	Color: Blue 💌 Code: R Arg 💌
F	Arg Asn Asp	Description:	arginine	
Fmoc Resin	Cit Cys	Formula: Weight:	C6 H14 N4 O2	
В	DAIa DAIa Dbu GABA	Coupling:	H2 0	
Boc Resin	Gla Gln Glu	Derivatives:	Boc	Fmoc
N	Gly His Hyp Ile		Tos	Mtr Pbf
C				
C Terminal				
Р				
Protecting Group				

Degree (°) indicates Pmc is the current default

Figure 8-2 Changing the Default Protecting Group

Adding (or Removing) a Protecting Group

To add a protecting group to, or to remove a protecting group from an amino acid:

1. In the Dictionary screen (Figure 8-1), click the **Boc** or **Fmoc** button (Fmoc and Arg are used in this example).

The Protecting Group Selection dialog box opens (Figure 8-3).

Dictionary: Protecting Group Selection	
Fmoc Derivatives	Arg Derivatives
OPh OtBu PO3H2 SO3H StBu tBu Tfa Trt Xan ▼	*Pmc Mtr Pbf
ОК	Cancel

Figure 8-3 Select a new Fmoc Protecting Group

2. To add a protecting group, scroll the Fmoc Derivatives list and double-click the group (Figure 8-3). The new group (Tos) will be added to the Arg derivatives list (Figure 8-4).

Dictionary: Protecting Group S	election
Fmoc Derivatives	Arg Derivatives
OtBu PO3H2 SO3H StBu tBu Tfa Trt Xan Z V	°Pmc Mtr Pbf Tos
ОК	Cancel

Figure 8-4 The new Protecting Group (Tos)

- 3. To delete a protecting group, double-click the group in the Arg Derivatives list. Protecting groups can also be dragged between the two lists.
- 4. Click **Ok**. The addition or deletion will appear on the Amino Acid page of the Dictionary.

Changing Resins

To change resins:

1. Select **Fmoc** or **Bmoc** Resin in the vertical tool bar of the Dictionary screen.

The display for resins opens (Figure 8-5). Fmoc Resin is used in this example.

Dictionary	
Anino Acid Anino Acid F Froce Resin B Boc Resin C C Terminal Protecting Group	down Amide, aded, other cular t, if vhen hino s d

Shows the associated protecting group, if any, with the resin

Figure 8-5 Resins Display

2. Type the changes in the appropriate fields, select the appropriate resin field, then press **Tab**.

Adding a Resin

To add a resin:

- 1. Select **Edit** > **Insert**, or click **New** in the toolbar at the top of the Dictionary screen.
- 2. If the first amino acid is attached to the resin, select **Preloaded Resin** in the list box.

Note: SynthAssist 3.1 software has four types of cycles that can be associated with resins.

- Amide cycle
- Preloaded
- Load
- Other
- 3. Type in the name, description, coupling, and protecting group, if applicable.

The Default Protecting group for:

- All Fmoc resins is Fmoc
- For all Boc resins is Boc

Adding a Terminal

To add a terminal:

1. Select **C-Terminal** or **N-Terminal** in the vertical tool bar of the Dictionary screen.

The display for terminals opens (Figure 8-6). C-Terminal is used in this example.

Figure 8-6 C-Terminal Display

2. Select Edit > Insert.

If you want the terminal to appear in the palette, select **In Palette**.

3. Type the name, description, formula, and coupling, if applicable, then press **Tab**, or click another field.

SynthAssist software calculates the molecular weight.

Adding a Protecting Group

To add a protecting group:

1. Select **Protecting Group** in the vertical tool bar of the Dictionary screen.

The display for protecting group opens (Figure 8-7).

Kernet Protecting group Details	×
Dictionary	
AA	
Amino Acid	Acm Boc Bor
F	BrZ Name: Ac Bum Bzl Description: acetul
Fmoc Resin	Dcb Ddm Dnp Dnp
Boc Resin	Dod Weight: 43.045219 Et Fmoc Coupling: H
N Terminal	For Mbh Me MeBzl Mob Mts
C C Terminal	
P Protecting Group	

Figure 8-7 Protecting Group Display

2. Select **Edit** > **Insert**, or click **New** in the top toolbar in the Dictionary screen.

3. Type the name, description, formula and coupling, if applicable, then click **Save** or select **File** > **Save**.

SynthAssist software calculates the molecular weight.

Note: You can specify protecting groups as Boc groups, as Fmoc groups, or as groups common to both Boc and Fmoc chemistry. If a protecting group is specified as Boc, then this group appears only in the Boc list for a particular amino acid or other residue. Similarly, if a protecting group is specified as Fmoc, it appears only in the Fmoc list for a given residue. As a default at installation, all protecting groups are specified as both.

Note: Among the list of protecting groups, only Boc and Fmoc are selected "For Resin." As such, the Fmoc-weight is subtracted in the final line, H, of the calculations page for an Fmoc-chemistry run. A similar subtraction occurs for the Boc group in a Boc-chemistry run.

This appendix covers:

List of Menus

The SynthAssist software menu bar has nine drop-down menus, almost all of which have commands with corresponding tool bar button commands. The menus are:

- File menu
- Edit menu
- View menu
- Synthesizer menu
- Data Converter menu
- Common menu
- Log menu
- Window menu
- Help menu

File Menu



Figure A-1 File Menu Commands

Edit Menu



Figure A-2 Edit Menu Commands

View Menu



Figure A-3 View Menu Commands

Synthesizer Menu

Synthesizer



Figure A-4 Synthesizer Menu Commands

Data Converter Menu

Data Converter



Figure A-5 Data Converter Menu Command

Common Menu

Common



Figure A-6 Common Menu Commands

Log Menu



Figure A-7 Log Menu Commands

Window Menu



Figure A-8 Window Menu Commands

Help Menu





SynthAssist® Software User Guide

SynthAssist[®] Software Screens Overview

The following relationships exist among the various SynthAssist software screens:

- From the SynthAssist software menu bar, you can access:
 - File-related dialog boxes and commands
 - Online Help
 - Synthesizer-related dialog boxes
 - The Data Converter dialog box
 - The Dictionary screen
 - The Lab screen
 - The Log screen
 - The Other Log screen
 - The Auto-Save dialog box
 - The Save As Bmp (only for the monitor screen of a Run)
- From the File New dialog box, you can access the:
 - New Run screen
 - New Sequence screen
- From the File Open dialog box, you can access the:
 - Run screen
 - Sequence screen
 - Chemistry screen
- From the Run screen, you can access the:
 - Associated Chemistry screen
 - Associated Sequence screen
 - Monitor screen
- From the Chemistry screen, you can access the:
 - Module screen
 - Cycle screen
 - Functions screen
 - Default Set screen
 - Chemistry Information screen

- From the Lab screen, you can access the:
 - Run screen (the Run sent most recently to the 433A)
 - Chemistry screen (the chemistry sent most recently to the 433A)
 - Text box to send messages to the Log
- Changes made in the Dictionary screen are automatically displayed in the:
 - Sequence screen
 - Compound palette
 - Chemistry screen
 - Run screen

	This section describes the limitations of the module, cycle, run cycle changes, and sequence that are inherent in the SynthAssist [®] Software Version 3.1 and the ABI 433A Peptide Synthesizer.	
Functions	A function can control a maximum of six valves.	
Modules	A module can contain a maximum of 99 steps.	
Cycles	A cycle can contain a maximum of 20 modules.	
Cycles Changes in a Run	A Run can contain a maximum of 30 distinct cycles changes.	
Bar Code Limit	A maximum of 255 bar codes can be sent to or stored in the 433A instrument.	
	• For Single Coupling (one cartridge per residue) the maximum sequence length in a Run file is 255 residues.	
	• For Double Coupling (two cartridges per residue) the maximum sequence length in a Run file is 127 residues.	
	• For 1.0 mMole runs (three cartridges per residue) the maximum sequence length in a Run file is 85 residues.	
	Note: The three length limits above arise from the bar-code memory capacity in the 433A instrument. The practical limits on the length of a peptide sequence in a synthesis are much lower and they arise from the volume capacity of the existing reaction vessels: 8 mL, 38 mL, or 55 mL. For example, a 1.0-mM synthesis in the large reaction vessel will accommodate a sequence length of approximately 20 residues, at which point the peptide-resin volume is approaching the capacity of the reaction vessel.	

Software Warranty Information

D

 This appendix covers:

 Computer Configuration

 Limited Product Warranty

 D-2

Computer Configuration

Applied Biosystems supplies or recommends certain configurations of computer hardware, software, and peripherals for use with its instrumentation. Applied Biosystems reserves the right to decline support for or impose extra charges for supporting nonstandard computer configurations or components that have not been supplied or authorized by Applied Biosystems. Applied Biosystems also reserves the right to require that computer hardware and software be restored to the standard configuration prior to providing service or technical support.

Limited Product Warranty

Limited Warranty

Applied Biosystems warrants that for a period of ninety (90) days from the date the warranty period begins, its SynthAssist[®] 3.1 software will perform substantially in accordance with the functions and features described in its accompanying documentation when properly installed on the instrument system for which it is designated, and that for a period of ninety (90) days from the date the warranty period begins, the tapes, diskettes, or other media bearing the software product will be free of defects in materials and workmanship under normal use. If buyer believes that it has discovered a failure of the software to satisfy the foregoing warranty, and if buyer notifies Applied Biosystems of such failure in writing during the ninety (90) day warranty period, and if Applied Biosystems is able to reliably reproduce such failure, then Applied Biosystems, at its sole option, will either (i) provide any software corrections or "bug-fixes" of the identified failure, if and when they become commercially available, to buyer free of charge, or (ii) notify buyer that Applied Biosystems will accept a return of the software from the buyer and, upon such return and removal of the software from buyer's systems, terminate the license to use the software and refund the buyer's purchase price for the software. If there is a defect in the media covered by the above warranty and the media is returned to Applied Biosystems within the ninety (90) day warranty period, Applied Biosystems will replace the defective media. Applied Biosystems does not warrant that the software will meet buyer's requirements or conform exactly to its documentation, or that operation of the software will be uninterrupted or error free.

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Warranty Claims	Warranty claims must be made within the applicable warranty period.
Warranty Exceptions	The above warranties do not apply to defects resulting from misuse, neglect, or accident, including without limitation: operation outside of the environmental or use specifications, or not in conformance with the instructions for the instrument system, software, or accessories; improper or inadequate maintenance by the user; installation of software or interfacing, or use in combination with software or products, not supplied or authorized by Applied Biosystems; and modification or repair of the product not authorized by Applied Biosystems.
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Index

Α

Adding amino acid 5-8 color to a compound 8-4 protecting group 8-6 Amino acid adding 5-8 changing 5-8 changing default derivative 8-4 deleting 5-8 determining in resin calculations 6-8 modifying sequence 5-9 protecting group 8-6 Auto-save 4-3

В

Bin folder, description 2-13 Bitmap, monitoring graph saved as 6-15

С

Calculating peptide resin 6-5 Cartridges, order of in resin calculations 6-9 Changing amino acid 5-8 chemistry functions 7-6 default derivative 8-4 N- and C-termini 5-8 resins 8-8 Checklist, quick start 1-1 Chemistry changing duration of a step 7-13 changing functions 7-6 changing information 7-5 changing modules 7-9 creating user-defined functions 7-8 description 2-2

file not found message 6-18 match message 6-11 scale in peptide resin calculations 6-5 selecting for a peptide run 6-3 software hierarchy 7-3 Chemistry file confirming default 3-8 modifying 7-4 sending to the synthesizer 6-10 Chemistry, description 2-13 Clock, setting 4-2 Common menu A-6 Common, description 2-13 Communication enabling 4-2 Communications, description 2-2 Computer configuration requirement D-2 technical support for altered configuration D-2 Configuration, system 2-5 Converting Macintosh chemistry file 3-7 Macintosh Dictionary file 3-4 Macintosh run file 3-11 Creating amino acid sequence 5-2 C-terminus, changing 5-8 Cycles creating 7-17 deleting 7-21 inserting a module 7-17 renaming 7-21

D

Data Converter menu A-6 Deleting amino acid 5-8 cycle 7-21 Dictionary adding a compound 8-4 adding color to compound 8-4 adding protecting group 8-6 changing default derivative 8-4 changing resins 8-8 converting Macintosh 3-4 description 2-2 opening the file 8-2 Documentation folder, description 2-13 Duration module deleting a step 7-13 inserting a step in 7-13

Ε

Edit menu A-4

F

File menu A-3 Flow test running 4-7 sending chemistry 4-4 Folder contents 2-13 structure 2-12 Functions changing 7-6 creating user-defined 7-8

G

Graph of deprotections, save as bitmap 6-15

Η

Hardware requirements2-4Help folder, description2-13Help menuA-7

Κ

Kinstall monitor screen 6-14

L

Lab screen, viewing 6-12 Log folder, description 2-14 Log menu A-7 Log, viewing 6-16

Μ

Macintosh converting chemistry file 3-7 converting dictionary file 3-4 converting run file 3-11 problems copying files 3-3 Macintosh Files folder, description 2-14 Menu Common A-6 Data Converter A-6 Edit A-4 File A-3 Help A-7 Log A-7 Synthesizer A-5 View A-5 Window A-7 Message chemistry file not found 6-18 chemistry match 6-11 sequence file not found 6-17 7-4 Modifying a chemistry file Module available in chemistry 7-10 changing in chemistry 7-9 creating in a cycle 7-17 deleting a step in 7-13 inserting a step in 7-13 inserting in cycles 7-17 renaming in step 7-13 Monitor 2-14 Monitor Bmps folder, description 2-14 Monitoring status saving graph 6-15 viewing 6-14

0

Opening the Dictionary file 8-2

Ρ

Palette, adding a compound 8-4 Peptide resin calculations 6-5 changing protecting groups 6-6 changing run cycles 6-7 chemistry scale in 6-5 determining amino acids in 6-8 order of cartridges in 6-9 selecting type 6-5 substitution 6-5 Peptide run opening 6-17 selecting a chemistry 6-3 selecting run sequence 6-4 sending to synthesizer 6-11 setting up 6-2 Peptide synthesis, running 6-10 Peptide synthesizer, starting 6-12 Protecting groups adding or removing 8-6 changing 6-6

Q

Quick Start, checklist 1-1

R

Renaming cycles 7-21 Requirements, hardware and software 2-4 Residues, undefined 5-6 Resin calculations 6-5 changing 8-8 selecting type 6-5 Run changing cycles 6-7 description 2-2 Run cycles, changing 6-7 Run folder, description 2-14 Run log 6-16 Running peptide synthesis 6-10

S

Screens, overview B-1 Sequence creating for amino acids 5-2 description 2-2 file not found message 6-17 format 5-4 selecting for peptide run 6-4 undefined residues 5-6 undefined termini 5-7 using cut/copy/paste 5-9 Sequence folder, description 2-14 Sequence, amino acid creating 5-2 Setting up a peptide run 6-2 Shortcuts desktop icon 2-12 Start Menu 2-12 Software requirements 2-4 Starting peptide synthesizer 6-12 Step changing duration 7-13 deleting 7-13 inserting in a module 7-13 renaming 7-13 Substitution, in peptide resin calculations 6-5 SynthAssist 3.1 Software description 2-2 installing 2-6 software 2-14 Synthesizer in peptide synthesis run 6-10 sending a peptide run 6-11 starting 6-12 Synthesizer menu A-5 System configuration 2-5

Т

Technical support for computers with altered configuration D-2 telephone number and Web address 1-ix Termini, changing 5-8 Termini, undefined 5-7

U

Undefined residues 5-6 termini 5-7 Undefined residues 5-6 Undefined termini 5-7 User-defined functions, creating 7-8

V

View menu A-5 Viewing lab screen 6-12 run log 6-16 run monitoring status 6-14

W

Warranty coverage period D-2 exceptions D-3 for computers with altered configuration D-2 Window menu A-7