

Empower 3

Getting Started Guide

General information

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Table of contents

Ge	eneral information	ii
	Copyright notice	ii
	Trademarks	ii
	Customer comments	ii
	Contacting Waters	iii
1	Getting Started using the Empower System	6
	1.1 Software concepts and organization	
	1.1.1 Key concepts	
2	Empower Software Interface Features	12
3	Prerequisites and Starting Up	16
	3.1 Before you begin	
	3.1.1 Preliminary configuration of Empower	
	3.2 Starting up and logging in	17
	3.3 QuickStart Interface tour 3.3.1 Using Empower Online Help	
4	Developing Methods for Data Acquisition and Processing	29
	4.1 Creating an instrument method	
	4.1.1 Setting solvent delivery system parameters	
	4.2 Creating a method set	36
	4.3 Acquiring data	
	4.4 Creating a processing method	
	4.5 Modifying the method set	57

	4.6 Acquiring data using Run and Process	59
5	Creating a Sample Set Method	61
	5.1 Using the New Sample Set Method Wizard	61
	5.2 Entering Component Information	68
6	Creating a Processing Method Interactively	78
	6.1 Creating a processing method in Review Data main window	78
7	Generating and Reviewing Results	94
	7.1 Altering Samples	94
	7.2 Processing the sample set	101
	7.3 Reviewing the result set	105
	7.4 Reporting	109
8	Backing Up and Restoring Projects	111
	8.1 Backing up projects	111
	8.1.1 Performing a backup	112
	8.2 Restoring Projects	
	8.2.1 Restoring a project	114
Α	Creating Projects	118
	A.1 How to create a project	118
В	Creating Systems	124
	B.1 Creating a chromatographic system	124

1 Getting Started using the Empower System

Empower is a software system for single or multi-system computers, linked to a set of chromatographic instruments, that performs acquisition, processing, and management of chromatographic information.

You should be familiar with the various configurations of Waters products that Empower supports. For additional background information, refer to the Waters website and documentation available for the individual products.

Note: This guide refers to and uses the Defaults project you received with your Empower installation. Ensure this project has been restored and is available before using the guide. Refer to Section 8.2 to learn how to restore a project.

1.1 Software concepts and organization

Empower software provides a graphical, icon-based user interface to acquire, process, manage, and report chromatographic data in the Empower database.

Empower software supports Windows operating systems and their multitasking operations, allowing you to have multiple windows open at the same time. Windows multitasking allows you to view a real-time data acquisition run, while simultaneously producing summary results of previously acquired data, or fine-tuning integration parameters for any previous injection.

The base version of Empower software supports LC, GC, and IC data processing, data from photodiode array (PDA), and mass spectrometry (MS) detectors. Empower software options [Dissolution, System Suitability, Gel Permeation Chromatography (GPC), Gel Permeation Chromatography with Viscometry (GPCV), Light Scattering (LS), Chemical Structures, and Toolkit] are available for integrated operation with the base Empower software.

This section describes the key concepts of Empower and how Empower implements those concepts in the software. It also describes the organization of this guide.

1.1.1 Key concepts

This section provides the important concepts you should understand before starting to use Empower.

Project

The basic organizational unit of Empower software is the Project. A project is a user-defined collection of methods, results, peaks, custom fields, and raw data. A project may also include audit trail and sign-off information. Everything except the raw data is stored in a reserved area of tablespace within the Empower database. Project raw data is stored in a separate directory.

Method

The actions you want to perform in your project are known as Methods. In Empower, a method is equivalent to a set of instructions that describes how you want Empower to perform a task for you. There are several types of methods you can use for various purposes. A method can instruct Empower about how you want it to control a chromatographic system, or acquire, process, report, or export data. Empower stores the methods you create as part of your project. Methods exist independently and are added to a method set within a project to provide all the necessary instructions for chromatography runs.

Method, Sample, and Result Sets

You can also group methods together into a method set to perform multiple functions sequentially (such as running samples and then automatically processing, reporting, and exporting data). For multiple samples, you associate a method set with each sample to form a bound set of samples. After processing the sample set, you will have a bound set of results in the result set.

Requirement: At a minimum, for a single injection, you must create a method set that contains an instrument method to enable data acquisition.

Empower Workflow

Figure 1-1 illustrates the relationship between project elements and the flow of information within a project. The HPLC or UPLC instruments connect to an acquisition server or client (PC for personal and LAC/E for enterprise) and are controlled by the instrument method (IM) in the method set. Data is acquired in the Run Samples area of the software.

A sample set method defines which samples will be run, in which order, the number of injections, the injection volume, and the run time. Once the sample set method is run, a sample set is collected. A sample set is a bound collection of raw data consisting of the injections and all channels of data collected.

If the method set has a specified processing method (PM) then you can provide instructions to process the raw data and a produce a result set. A result set is a bound collection of results. If the method set has a report method (RM), then you can provide instructions to format and print the results (hard copy or electronic copy).

Structure of Empower Waters Project HPLC1 **Run Samples** UPLC1 Sample set Method Sample set Method set Raw data UPLC2 IM PM Inj Ch RM HPLC2 Result Sets Print Results Reports ©2010 Waters Corporation | COMPANY CONFIDENTIAL

Figure 1–1: Empower Workflow

Table 1-1: Types of methods

Method	Description
Instrument	Specifies the control parameters for pumps, solvent management systems, detectors, autosamplers, sample management systems, and gas chromatographs.
Processing	Defines how you want Empower to process data from a 2D channel or a 3D extracted channel. It defines the integration parameters, calibration parameters (non-MS), and component identification. For example, you can specify whether to integrate peaks by determining peak start and peak end for each peak (Traditional integration), or by determining the peak apex (ApexTrack integration). You can also define how to calibrate standards and quantitate unknowns, define the range of allowable values for each component, and calculate detector noise and drift parameters.
Sample Set Method	Specifies functions and parameter settings that Empower uses to acquire data from a set of vials or samples.

Table 1-1: Types of methods (continued)

Method	Description
Sample Set Method Template	Serves as a template for a sample set method. It includes the preset sample parameters you define (so you do not have to reenter these values each time you run a sample), and accommodates for variations from one run to another (by prompting you for those parameters you do not define in the template).
	Tip: Creating a template for a sample set simplifies the process of creating new sample sets for frequently run analyses where some variables are expected to change.
Report	Contains the layout that will be used for data when you generate a report. This layout describes how your data (such as the results and calibration curves) will appear on a printed page.
Export	Specifies the data to export and file format to be used when exporting data. Available formats include ASCII, AIA, OpenLynx, PDF, or EMF.
Method Set	Contains a group of methods.

Data Acquisition

You can acquire, process, and analyze chromatographic data collected from both Waters instrumentation and third-party instrumentation using detection techniques, such as mass spectrometry (MS), photo diode array (PDA), and light scattering (LS), and analysis tools, such as Dissolution, System Suitability, and Chemical Structures.

You can inject and collect data for one sample at a time, quickly analyze a sample, or perform a test injection. When acquiring data from more than one sample, you can save time and ensure consistency by using a predefined set of conditions or instructions (defined in a sample set method) that specifies how and when to acquire data from each sample in a set. Samples can include standards for calibration (both internal and external), unknown samples, and control samples.

Tip: When you run samples to acquire data, Empower relies on the method set (which includes an instrument method) to communicate the control and acquisition parameters, such as the flow rate of a pump or the wavelength of a detector, to the instruments in a configured chromatographic system. It also relies on the sample set method to specify the number and order of samples to run, the function to apply to each sample (such as Inject Standards or Inject Samples), the run mode for a sample, when to equilibrate, calibrate, and quantitate, which method set or report method to use, and so on.

Data Processing

After you acquire data, you use a processing method to process the data and to calculate and analyze results. Processing data involves integrating the raw data, and then calibrating your standard samples, or quantitating your unknown samples. Depending on your department procedures, you may want to process data after acquisition, or process data that was imported from other sources or locations.

You can process data interactively or in the background.

When processing data, you can use a method set that contains all the methods, or you can specify individual methods for the various operations to perform, such as processing the data (processing method), printing the results (report method), or exporting the results (export method). If processing 3D data, use a method set that includes the instrument method, processing method, report method, and export method you created, and any derived channels needed to process data.

Tip: One of the best ways to take advantage of Empower's capabilities is to use a single sample set method to automatically run a sample set and calibrate standards, quantitate samples, analyze controls, generate results, evaluate suitability parameters, print and email reports, and export data.

Altering Samples

You may want to change sample identifiers, modify component amounts after data acquisition, or correct errors made while loading samples, defining sample identifiers, entering component amounts, acquiring sample sets, or changing channels.

Reviewing and Reporting

After you acquire and process your data, you can use Empower to review and compare your raw data or results. Then, after you analyze data, you will most likely want to generate and distribute a report to your team. You can generate reports from processed data, raw data, methods, peaks, or curves. To generate a report, use a previously-created report method to design the main body of your report. Before you distribute the report, you can preview its contents and modify the layout, as needed.

1.1.2 Organization of this guide

This guide emulates a basic chromatography run in your own laboratory. Use your own samples as you follow the example in the guide and obtain actual results from your own installation.

Note: Your instruments and nodes must be pre-configured, available, and accessible over your network to start using this guide. You must also have defined a project and system. See Prerequisites and Starting Up.

As you work through the guide, you will perform the following activities in sequence.

Table 1–2: Basic chromatography run using your samples

Activity	Chapter or appendix location
Create a chromatographic system. This is usually performed by the Waters Field Service Engineer.	А

Table 1–2: Basic chromatography run using your samples (continued)

Activity	Chapter or appendix location
Create a project named Training. This is usually performed by the Waters Field Service Engineer.	В
In the "Training" project, create and configure an instrument method.	4.1
Create a method set named Training Method Set.	4.2
Configure plates, as needed.	4.3
Equilibrate the system, and then start a single injection and acquire the data.	4.4
Create a processing method. Configure integration and calibration parameters in the processing method.	4.5
Add the processing method to the method set.	4.6
Acquire more data using the Run and Process feature.	4.7
Create a sample set method, and then add standard brackets or samples.	5.1
Create a multilevel calibration curve by entering component amounts or concentrations, and then run the sample set.	5.2

Table 1–3: Advanced processing features using the Defaults project data

Activity	Chapter or Appendix Location
Change the project to Defaults . Create a processing method interactively, and then integrate, calibrate, and quantitate the data. Add it to the method set.	6.1
Use the Alter Sample Set feature to correct and add information related to the samples. Specify background processing and reporting, and then process the sample set. Review the results set. Generate and print a report.	7.1-4
Back up the project.	8.1
Restore the project.	8.2

2 Empower Software Interface Features

Empower software provides three different user interfaces for you to select at login:

- QuickStart
- Pro
- Walk-Up

Each interface is designed to meet the needs of a particular type of user. Your system administrator selects which interface appears when you log in and grants access to other interfaces. If you have access to multiple interfaces, you can select a different interface by clicking the **Advanced** button in the Empower Login dialog box (see Starting up and logging in).

Empower QuickStart

The Empower QuickStart interface (Figure 2-1) enables you to perform the tasks required to acquire data, analyze results, and create reports. The one-screen design lets you navigate through the software easily. The **Show Me Help** drives the software so you can learn while performing common tasks and procedures. See QuickStart Interface Tour.

Training in Training as System/Administrator - QuickStart - [Find Data] File Edit View Tools Database Manage Tools Help Filter By: Default Sample Sets Injections Channels Methods Result Sets Results Run Samples Method Name Sample Queue Method Type Method Date Control Panel Alliance Instrument 11/10/2016 10:18:31 AM EST Test 11/11/2016 8:38:47 AM EST Instrument Training Instrument 11/11/2016 8:39:41 AM EST Browse Project Default 11/10/2016 10:18:31 AM EST Processing LC PQ Processing 11/10/2016 10:18:31 AM EST Processing LC PQ ApexTrack 11/10/2016 10:18:32 AM EST **View Data** Chromatogram Labels Report Report 11/10/2016 10:18:32 AM EST 11/10/2016 10:18:32 AM EST Component Summary Report 11/10/2016 10:18:33 AM EST Default Individual Report Report View Method Injection Summary Report Report 11/10/2016 10:18:33 AM EST Method Set 11 LC Calibration Report 11/10/2016 10:18:33 AM EST Report Instrument 12 11/10/2016 10:18:34 AM EST Multi Sample Summary Report Processing Overlay Report

Figure 2–1: Empower QuickStart Browse Project window

Empower Pro

The Empower Pro interface is designed for a user who requires total control and full access to all software features, such as a system administrator or advanced user.

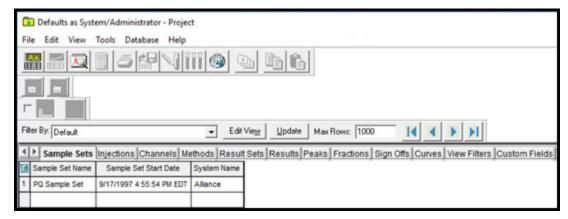
Report

11/10/2016 10:18:34 AM EST

Using the Empower Pro login window, you can access the three key software functions as shown in Figure 2-2. The second figure displays an example of the Pro interface displaying the components of a project contained in Empower.

Figure 2-2: Empower Pro login and interface

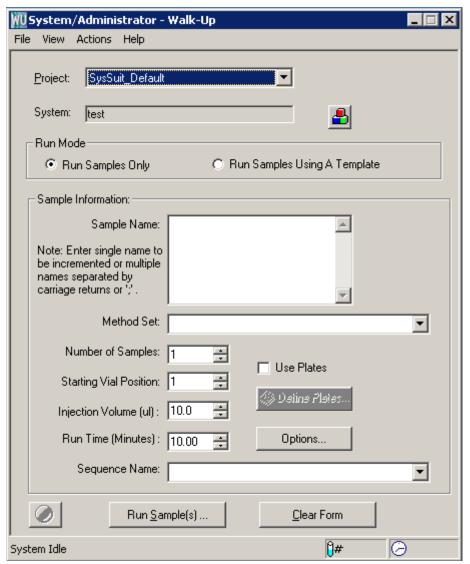




Empower Walk-Up

The Walk-Up interface (Figure 2-3) allows a user to easily submit samples for routine analysis and generate results without extensive chromatography knowledge.





3 Prerequisites and Starting Up

You can work with your own instruments and components while following the example chromatography run and subsequent processing described in this guide. Make sure you have set up your configuration before starting Empower.

3.1 Before you begin

Note: Check the Waters web site for updated information and the latest release notes.

Ensure these conditions are met before using this guide:

- The Empower computer components (monitor, keyboard, and mouse) are installed and powered up with the Empower software as described in the Empower 3 Installation, Configuration, and Upgrade Guide
- You have installed the Empower software as described in the Empower 3 Installation, Configuration, and Upgrade Guide
- Your system includes, at a minimum, the following Waters instrumentation:
 - · Solvent manager
 - · Sample manager
 - Detector
- Your system's chromatographic instruments are connected to the acquisition server, instruments are powered up, any calibration and diagnostic routines are complete, and the instruments appear as a properly configured system in the Systems view of Configuration Manager.
- · Solvents and samples are prepared.
- Optionally, your printer is properly configured in Windows and in Empower.
- · The Defaults project is loaded.

3.1.1 Preliminary configuration of Empower

Before you start using this guide, ensure that either you or the Waters Field Service Engineer have created a system with the appropriate instruments for your chromatography run. The system should be connected to your acquisition system and have a name of your choosing.

The example we use in this guide has a project name of Training. The system includes an ACQUITY H-Class Separations Module and an ACQUITY PDA Detector with the name Hclass with PDA.

Note: The example in this guide is a general description of how to use Empower. Specific instructions will differ according to your individual configuration.

3.1.2 Configuring your printer

Before printing reports from Empower, verify that your printer is configured:

- Select Start > Programs > Empower > Register Acquisition Server Printers (Windows 7 systems). In Windows 10, from Start > click the down arrow to display the Apps page > point to Empower > select Register Empower Node.
- 2. Verify that the list of printers is correct.

3.2 Starting up and logging in

This section describes how to start up the system and log in to your Empower software.

- 1. Power-on the system instrumentation as follows:
 - a. Chromatographic instruments (wait until all internal calibration and diagnostic routines are complete before powering-on the next instrument).
 - b. Peripheral devices connected to the Empower system, such as a printer.
 - c. Acquisition server.
- 2. To start Empower software, double-click the Empower icon on your desktop.

Figure 3–1: Login dialog box



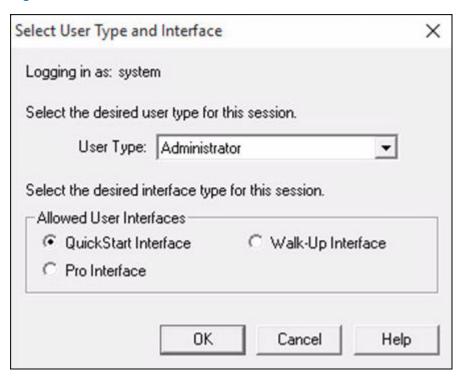
3. In the Login dialog box, enter your user name and password. You must enter your user name and password each time you log in.

Note: For a new installation, the default user name is system and the password is manager.

- 4. If you are using an Empower Workgroup or Enterprise system, select a database from the **Database** list. This list appears only when connected to a client/server system.
- Click Advanced, then select QuickStart Interface from the Allowed User Interfaces list (Figure 3-2). The system administrator determines which interfaces appear in the list and which one is your default interface. Click OK.

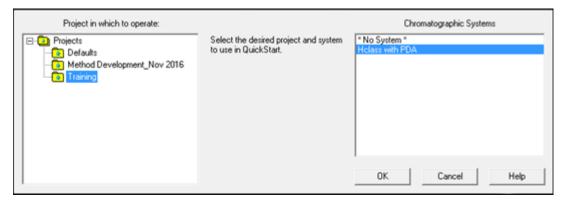
Note: This guide uses the QuickStart interface. If the QuickStart interface does not appear in the Allowed User Interfaces list, it must be enabled by a system administrator.

Figure 3-2: Allowed user interfaces selection



6. In the Select Project and System dialog box (Figure 3-3), select a project.

Figure 3–3: Select Project and System dialog box



- 7. Select the Training project and the H-Class system you created. Click **OK** to start the QuickStart interface.
- 8. The QuickStart interface (Figure 3-4) appears with **Browse Project** selected. Be sure to expand the screen for optimum viewing.

Training in Training as System/Administrator - QuickStart - [Find Data] Tools Database Manage Tools View Filter By: Default Run Samples Sample Sets Injections Channels Methods Result Sets Results Method Name Method Type Method Date Sample Queue Control Panel 1 Alliance Instrument 11/10/2016 10:18:31 AM EST 2 Test 11/11/2016 8:38:47 AM EST Instrument 3 Training Instrument 11/11/2016 8:39:41 AM EST Browse Project 4 Default 11/10/2016 10:18:31 AM EST **Processing** 5 LC PQ 11/10/2016 10:18:31 AM EST Processing 6 Processing LC PQ ApexTrack 11/10/2016 10:18:32 AM EST **View Data** 7 Chromatogram Labels Report 11/10/2016 10:18:32 AM EST Report 8 11/10/2016 10:18:32 AM EST Report Component Summary 9 Default Individual Report Report 11/10/2016 10:18:33 AM EST View Method 10 Injection Summary Report Report 11/10/2016 10:18:33 AM EST Method Set 11 11/10/2016 10:18:33 AM EST LC Calibration Report Report Instrument 12 11/10/2016 10:18:34 AM EST Multi Sample Summary Report Processing 13 Overlay Report 11/10/2016 10:18:34 AM EST Report

Figure 3-4: QuickStart Browse Project window

3.3 QuickStart Interface tour

Though the functionality available from the various interfaces may vary, the procedures to execute tasks in the QuickStart and Pro interfaces are similar. The Walk-Up interface implements a subset of the Empower functionality. In this guide, procedures are performed using the Empower QuickStart interface.

When you open Empower using the QuickStart interface, one of the buttons in the Navigation Bar, such as the Browse Project button, is selected, and the Project window is displayed on the right side with tabs for various project-related activities, as shown below.

When you click a function in the navigation bar, the selected window opens in the work area. A highlighter in the navigation bar indicates which function is active in the work area. You use the **View Acquisition** check box in the navigation bar to choose whether to display or hide the system status, which displays information about the chromatographic system area and real-time plot, which displays your chromatogram or spectra as it is acquired.

Tip: When you point to an icon in the interface, the name of the icon appears in a Tool Tip window.

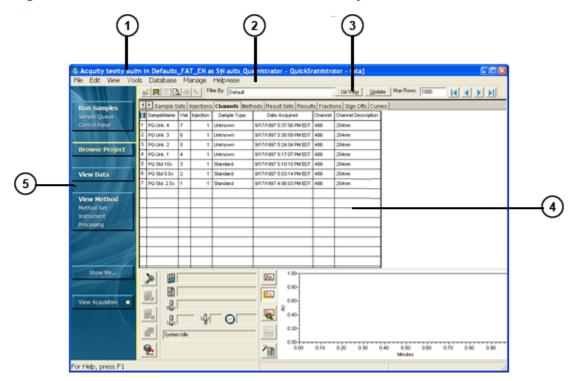


Figure 3-5: QuickStart Main Window with Browse Project selected

The main Empower QuickStart interface is separated into five areas.

- 1 Title Bar displays the current system name, project, user type, and interface.
- 2 Menu Bar options along the top of the Empower window vary based on which button is selected in the Navigation Bar. These menu options are for typical actions performed within the active window in the work area.
- Tool Bar tool icons provide quick access to primary functions. They also vary based on which button you have selected in the Navigation Bar. When you pause the cursor over a toolbar button, ToolTip text is displayed in a ToolTip box and in the status bar at the bottom of the window.
- Work Area this area on the right side of the Empower window changes based on the buttons you select in the Navigation Bar. This area is where you view, process, and report raw data and processed results. It is also where you define data acquisition and instrument control parameters and run samples for display in the real-time plot. For example, if you are developing a method, the work area contains the Method Editor window.

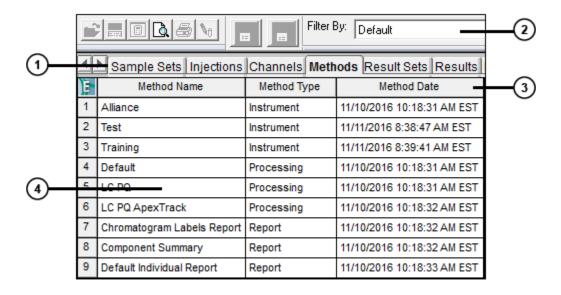
Navigation Bar - the buttons in the left-hand Navigation Bar open windows on the right side of your working environment for specific tasks, such as running samples. Toggle the View Acquisition button in the Navigation Bar to show or hide the work area used for data acquisition.

The Empower interface windows and dialog boxes map to the job-related tasks you perform. Because the order in which you perform these tasks may vary, you will have access to the various windows and dialog boxes when and where you need them.

The interface components you will commonly encounter as you use Empower are listed below. You will learn more about each of these components as you progress through this guide.

Click **Browse Project** in the left pane to access project information at any time.

Figure 3-6: Sections of the Browse Project window work area

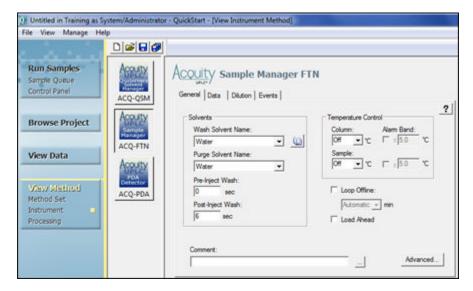


- 1 Project tabs
- 2 Filtering options
- 3 Data column heads
- 4 Project data displayed by component

Click **View Method** in the navigation bar to open the Method Editor, where you define methods for acquiring data, processing data, exporting data, and creating reports. When you click the

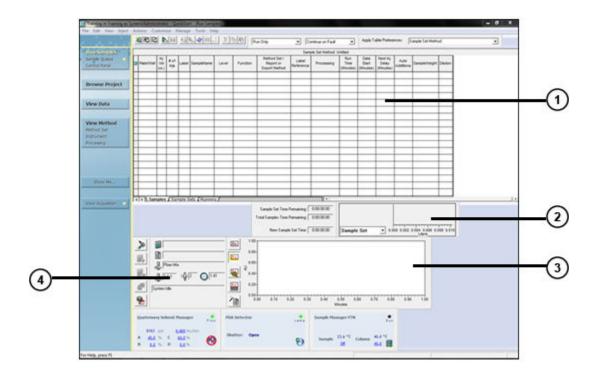
icons to the left of the work area, the system displays editable information about specific instruments in your chromatography system.

Figure 3-7: Method Editor window



Click **Run Samples** in the navigation bar to acquire data, monitor the acquisition, and control instruments.

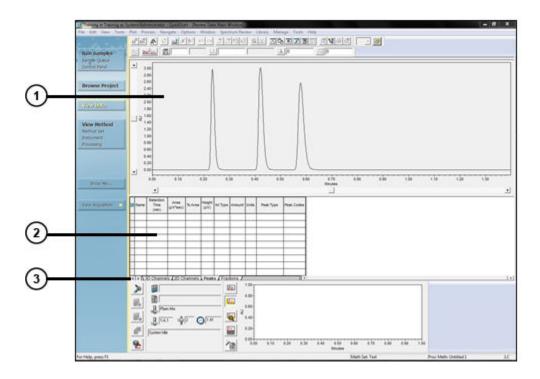
Figure 3-8: Run Samples window sections



- 1 Sample set method
- 2 Real-time run data
- 3 Real-time plot area
- Run samples information, status, and controls

While in the Browse Project window, select **Channels**, select a channel of data, and then click **View Data** in the Navigation Bar to view data that has been collected.





- 1 Data graphical plot area
- 2 Data in table format
- 3 Tabs to change view to 2D and 3D channels, peaks, or fractions

While in the Browse Project window, select the **Results** or **Result Sets** tab, select a result, and then click **View Data** in the Navigation Bar to open the data in report format.

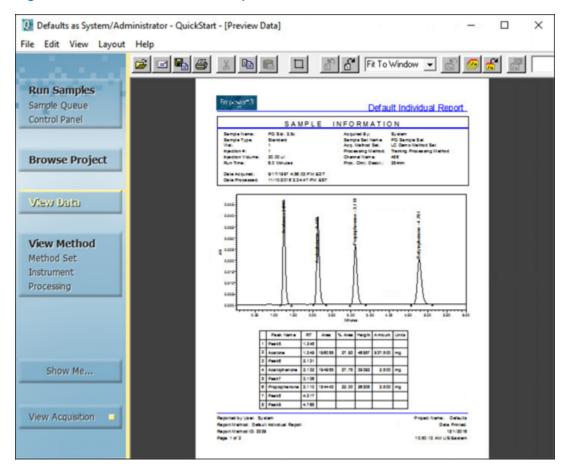


Figure 3-10: View Data window - report view

Click **Browse Project** in the navigation bar. Click **Manage** > **Configuration** to open the Configuration Manager window. Use the Configuration Manager to perform administrative tasks, such as project creation, user permissions, and audit trail specifications.

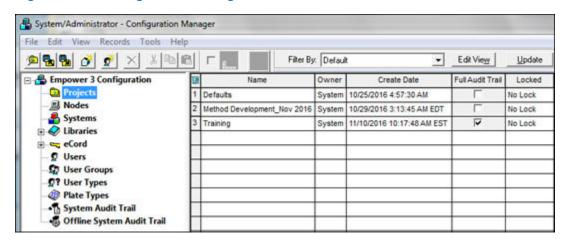


Figure 3–11: Configuration Manager window section

3.3.1 Using Empower Online Help

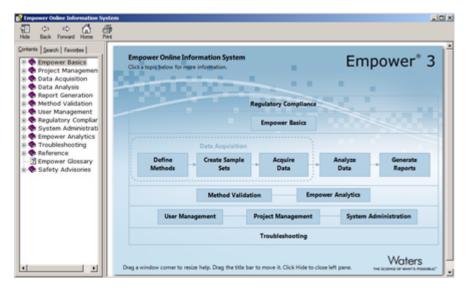
Depending on the complexity of your application, you can perform procedures for data acquisition, processing, and report generation other than those outlined in this guide. See the Empower Help for more detailed information about individual topics.

Notes: If you are using an Empower software option (for example, GPC), refer to the appropriate topics in the Empower Help or to the associated option's Getting Started Guide. In addition to the traditional Empower Help, the "Show Me" Help, available in the QuickStart interface, guides you through many standard tasks.

To access Empower reference information:

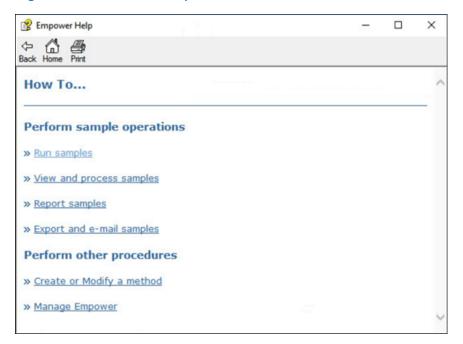
1. With the Empower main page open, click **Help** in the menu bar of an application window. The Help main page appears.

Figure 3-12: Help main page



- 2. To open a topic, click one of the topics in the main pane or click the **Contents** tab and browse the navigation tree.
- 3. Click the **Search** tab to search for a text string. Remember to enclose the text string with quotation marks.
- 4. Click the Favorites tab to add frequently viewed topics to a custom list.
- 5. To access Show Me Help from the QuickStart interface, click **Show Me...** in the navigation bar.

Figure 3-13: Show Me Help



4 Developing Methods for Data Acquisition and Processing

This chapter guides you through the process of acquiring and processing data from a single injection using the Run Samples and View Method features of Empower software.

You will learn how to:

- Create and save an instrument method for your chromatographic system
- · Create a method set that includes your instrument method
- Equilibrate the system, make a single injection, and acquire data
- · Create and save a processing method
- Make a single injection to acquire and process data automatically

Methods

To perform a run, you must first create a method set using the **View Method** feature of Empower. A method set contains all the instructions the software requires to acquire, process, and report data. It consists of several components:

- Instrument Method Tells Empower software how to acquire data and control instrumentation included in your chromatographic system. The Instrument Method must be inside the Method Set to acquire data; the other methods are optional.
- Processing Method Defines integration parameters, calibration parameters, and component identification.
- Report Method Defines how the results are formatted before printing a hard copy or saving an electronic copy.
- Export Method Defines how the results are exported to a specified location.

4.1 Creating an instrument method

The instrument method tells the Empower software how to control your chromatographic instrumentation. In this method, you specify solvent delivery system parameters, such as flow rate and solvent composition, and detector settings, such as wavelength and data rate. Using the Instrument Method Editor, you create the method and specify parameter settings for the selected instrument using the options provided in the editor.

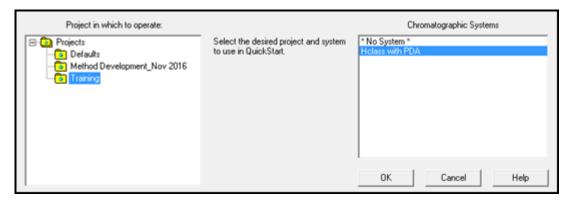
Note: The following procedure uses as an example a chromatographic system that includes an ACQUITY H-Class Separations Module and an ACQUITY PDA Detector. If you are using different instruments, the tabs that appear in the interface will differ from those shown and you must specify the parameter values appropriate for your instrumentation.

To create an instrument method:

Note: If you have logged in already, go to Step 4 in this procedure.

- 1. Log in to Empower software (see Starting up and logging in).
- 2. In the Select Project and System dialog box, do the following:
 - a. From the Project in which to operate list, choose your project. In this case, use the Training project. See Creating Projects, to create the project if it does not appear in the list.
 - From the Chromatographic Systems list, select the Hclass with PDA system.

Figure 4–1: Select Project and System dialog box



- 3. Click OK.
- 4. In the Run Samples window on the navigation bar, under View Method, click **Instrument**.

Result: The View Instrument Method window displays an icon for each component in your selected chromatographic system (solvent delivery system, photodiode array detector, and autosampler). The **General** tab contains information for the first component.

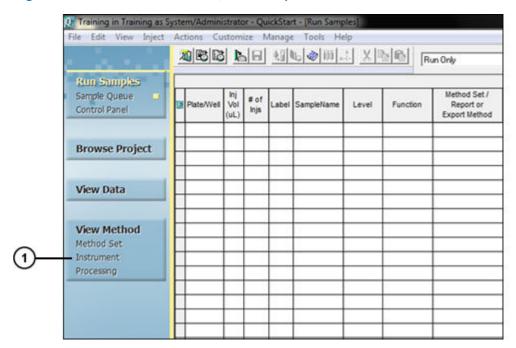


Figure 4-2: QuickStart Interface, Run Samples window

- 1 View Method, Instrument Method
- 5. Click the icon for your solvent delivery system, in this case **ACQ-QSM** (Quaternary Solvent Manager).

Figure 4-3: View Instrument Method, ACQ-QSM, General tab

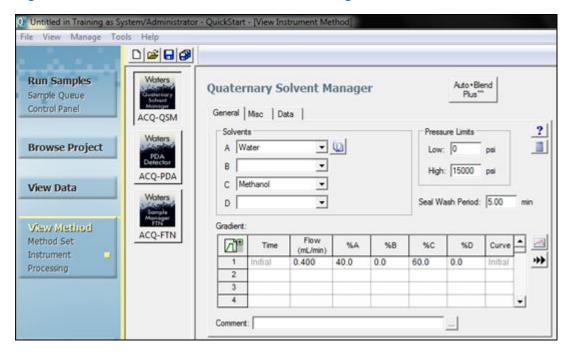


4.1.1 Setting solvent delivery system parameters

- 1. In the **General** tab, specify the following settings and accept the other default settings.
 - From the Solvents list, select Water for A and Methanol for C.
 - Set the **Flow** rate to 0.4.
 - Enter 40 for %A and 60 for %C.

Note: You can assign the solvents to any of the available reservoirs in your instrument.

Figure 4-4: View Instrument Method - solvents assigned



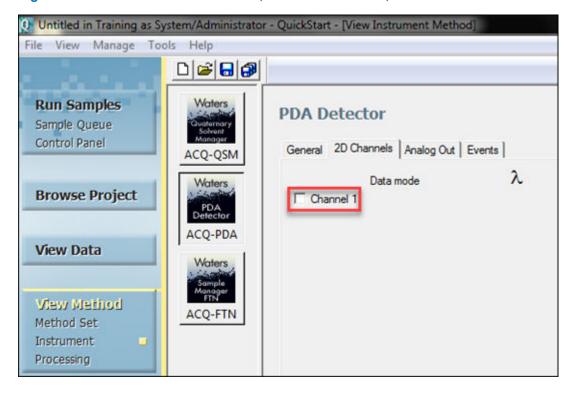
- 2. Click ACQ-PDA.
- 3. Clear the **Enable 3D Data** check box, do not change the other default settings, and then click the **2D Channels** tab.

Figure 4–5: Instrument Method Editor, ACQ-PDA detector, General tab



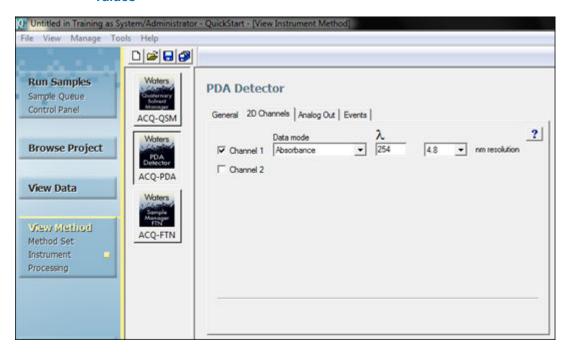
4. Select Channel 1.

Figure 4-6: Instrument Method Editor, ACQ-PDA detector, 2D Channels tab



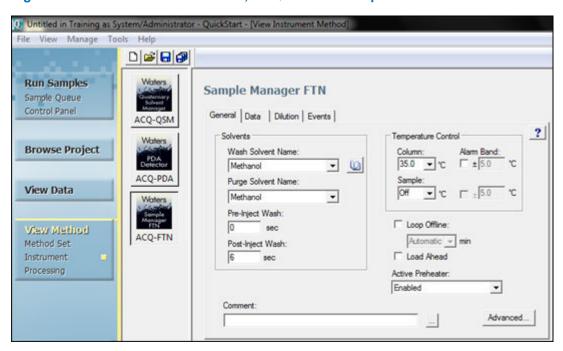
5. Ensure that the Data Mode is set to **Absorbance** and enter 254 for the wavelength.

Figure 4–7: Instrument Method Editor, ACQ-PDA detector, 2D Channels tab - with values



6. Click **ACQ-FTN** to display the parameters for the autosampler.

Figure 4–8: View Instrument Method, ACQ-FTN autosampler



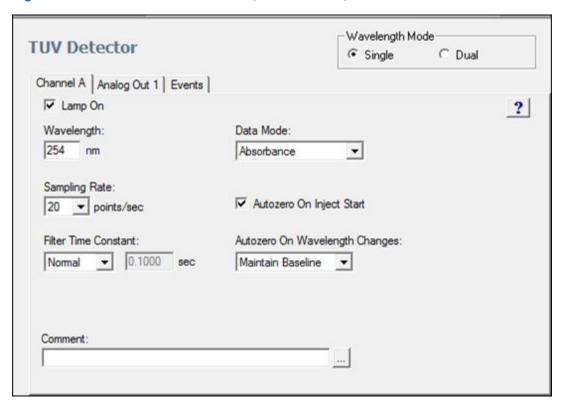
7. Select the **Wash** and **Purge** solvents and the **Temperature Control** appropriate for your selected system.

- In this example, select Methanol for both.
- In the Temperature Control pane, set a temperature of 35 in the Column field.

4.1.1.1 Instrument method settings for TUV detector

The figure below illustrates the settings that you specify if you are using a TUV detector as part of your system.

Figure 4–9: Instrument Method Editor, TUV detector, 2D Channels tab - with values



4.1.2 Saving the instrument method

Select File > Save As.

Save current Instrument Method

Names:
Alliance
Test
Training

Name: Training Instrument Method

Method Comments: For Training

Save Cancel Help

Figure 4-10: Save Current Instrument Method dialog box

2. In the Save current Instrument Method dialog box, enter Training Instrument Method for the instrument method name, add any necessary comments, and then click Save.

Note: If a message indicating that an instrument method with the same name exists, click **Yes** to overwrite the method.

Result: The View Instrument Method window reappears and the name of the method appears in the status bar.

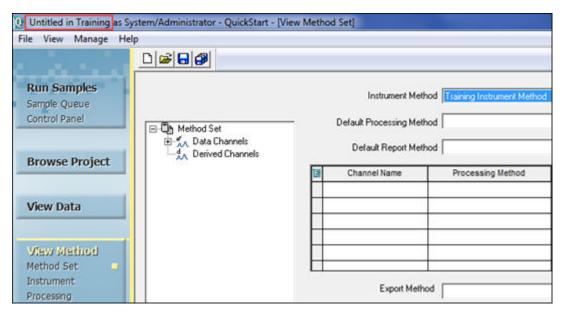
4.2 Creating a method set

After you create an instrument method, you use the **View Method** feature to add it to a method set. You can then save the method set and select the plate configuration.

To create a method set:

 Under View Method, click Method Set. Notice that the method set name is Untitled in the Title Bar.

Figure 4–11: Creating a new method set



2. From the Instrument Method list, select Training Instrument Method.

Note: Leave the Default Processing Method blank.

- 3. Select File > Save As.
- 4. In the Save Current Method Set dialog box (Figure 4-12), enter the name Training Method Set, add any comments describing the method set, and then click **Save**.

Result: The method set name appears in the Status Bar.

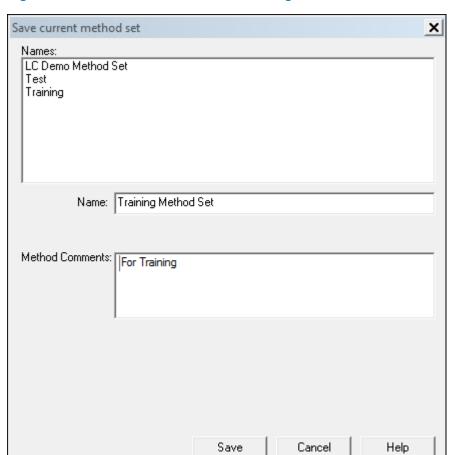


Figure 4–12: Save current method set dialog box

- 5. Click **Run Samples** in the navigation bar.
- 6. To define the plate configuration for the ACQ_FTN autosampler, click **Edit Plates** in the Run Samples toolbar.
- 7. If necessary, click the Plate Type Name field, select the plate type for your instrument, and then click **OK**.

Define Plates For Sample Set Method X ☐ 2790 Layout Create New Plate Type Clear Plates Plate Type Name Plate Layout Position 1 ANSI-48Vial2mLHolder * 2 ANSI-96well1mL ANSI-96well1mLGlassinsert ANSI-96well2mL ANSI-96well350uL ANSI-96well700uLGlassInsert 24 uCfuge tube, 1.5mL 24 vial (open access), 2mL 384 well, 80uL 48 uCfuge tube, 0.5mL Cancel Help Inject Standards

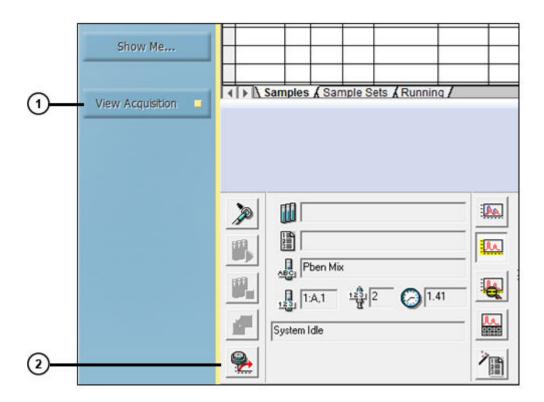
Figure 4–13: Plate Type Name field

4.3 Acquiring data

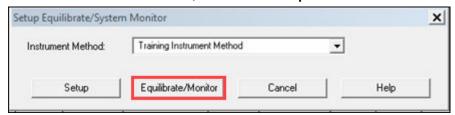
After you create a method set, your goal is to inject a sample and acquire data for processing. First, you equilibrate the system. Then, you inject the sample and acquire raw data. You can then use the acquired data to create your processing method.

1. Click **Run Samples** on the navigation bar.

Figure 4-14: Run Samples-Samples tab

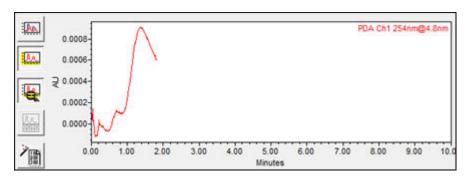


- 1 View Acquisition button
- 2 Equilibrate System/Monitor Baseline icon
- 2. To equilibrate the system, ensure that **View Acquisition** is selected on the navigation bar.
- 3. In the Acquisition bar, click Equilibrate System/Monitor Baseline.
- 4. In the Setup Equilibrate/System Monitor dialog box, select **Training Instrument Method** from the Instrument Method list, and then click **Equilibrate/Monitor**.



5. A baseline appears in the real-time plot area of the window. The baseline appearance differs for each system.

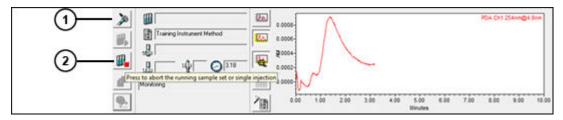
Figure 4–15: Monitoring baseline



6. After the baseline stabilizes (becomes relatively flat), click **Abort** to stop the monitoring process (Figure 4-16).

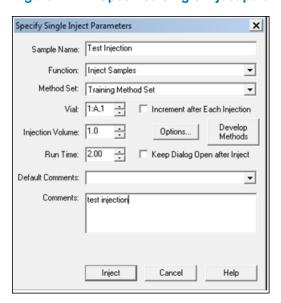
Note: Because the software auto-scales the Real-Time plot, the baseline can appear noisy. Check the scale of your y-axis to adjust the minimum and maximum values for the appropriate range.

Figure 4–16: Stopping the Monitoring Process



- 1 Inject
- (2) Abort
- 7. Place the sample vial in the autosampler in position 1:A,1.
- 8. Click Inject
- 9. In the Specify Single Inject Parameters dialog box, specify Test Injection as the sample name, select **Training Method Set** from the Method Set list, and then enter the appropriate vial, injection volume, and run time.

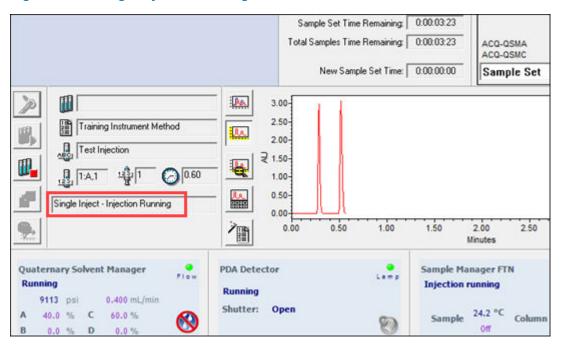
Figure 4-17: Specified single inject parameters



10. Click **Inject** to begin data acquisition.

Result: The status bar indicates when the injection is made and is running. The chromatographic data is acquired and displayed in the real-time plot.

Figure 4-18: Single injection running



11. After the single injection is complete (as indicated in the status bar), the system is ready for the next injection(s).

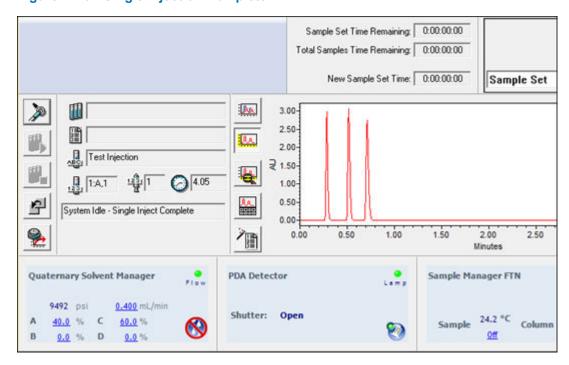


Figure 4-19: Single Injection Complete

4.4 Creating a processing method

A processing method defines how Empower software processes raw data. The processing method is included in a method set to instruct the software how to:

- · Integrate data
- Calibrate standards
- · Quantitate unknowns

When you create your processing method, you define the region for peak detection and integration. You modify the region by specifying peak width and threshold, and then performing a process of peak rejection. In the calibration phase, you specify names, retention times, and default amounts.

Note: You must acquire data before defining the processing and reporting methods. See Acquiring data.

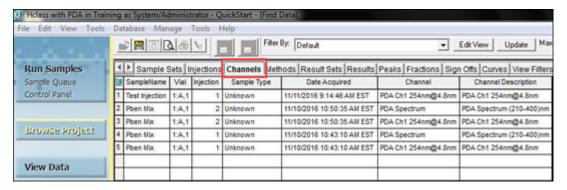
Note: In addition to using the Processing Method Wizard, you can build a processing method interactively (see Chapter 6, Creating a Processing Method Interactively). Interactive processing method development offers more options than using the wizard.

See Also: Empower 3 Data Acquisition and Processing Theory Guide

To create a processing method:

- 1. On the navigation bar, click **Browse Project**.
- 2. Click **View Acquisition** to hide the Acquisition pane.

Figure 4-20: Browse Project window



3. Click the **Channels** tab, select the **Test Injection** row, and then click **View Data** in the navigation bar.

Result: The Review Data main window appears with the data loaded from the test injection (Figure 4-21).

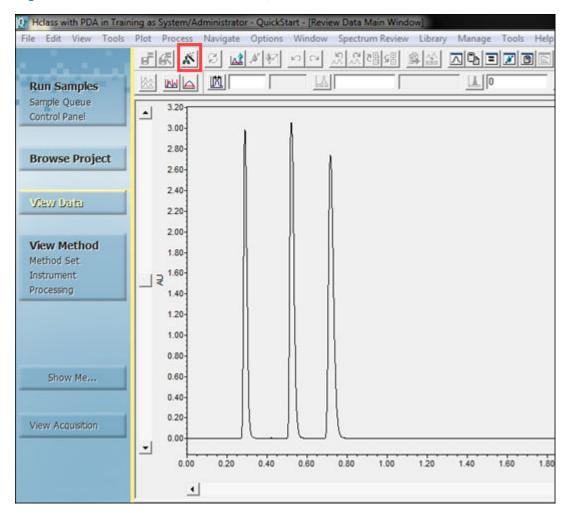


Figure 4-21: Review Data Main window, Peaks tab

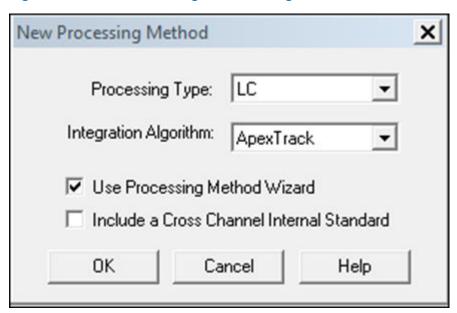
- 4. If you do not see your chromatogram, select **View > 2D Layout**. If you use data acquired with a PDA detector, you must extract a 2D chromatogram from the 3D data to successfully complete this section of the guide. For more information, see the "Extracting Chromatograms from PDA Data" topic in the Empower Help.
- 5. On the Empower toolbar, click **Processing Parameters Wizard**.

Figure 4–22: Processing Method Wizard dialog box



6. Select Create a New Processing Method, and then click OK.

Figure 4–23: New Processing Method dialog box



7. Select the settings as shown above, and then click **OK**.

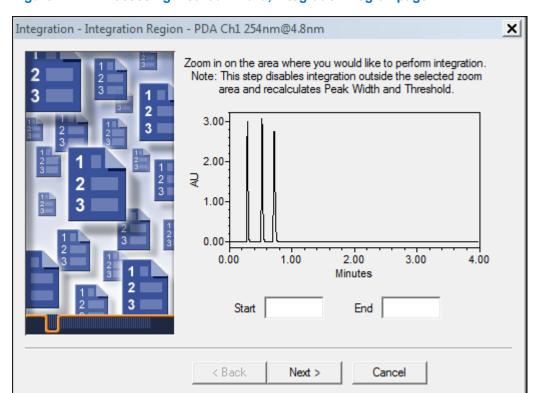


Figure 4-24: Processing method wizard, Integration Region page

8. You use the Integration Region page to set the region for peak detection and integration. Follow the wizard instructions and use the mouse to zoom in on the area of interest (zoom in by clicking a spot in the chart and dragging the mouse over an area).

Note: Right-click the plot to access the Full View/Unzoom shortcut menu selections.

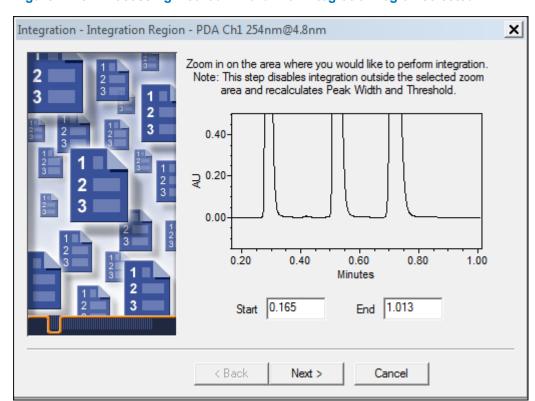
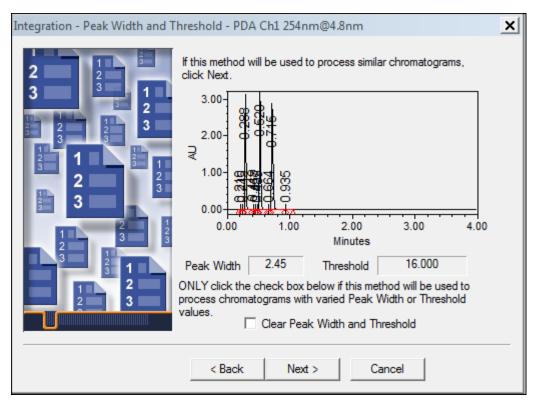


Figure 4–25: Processing Method Wizard with integration region selected

9. Click Next.

 Empower has determined the optimum peak width and threshold values for the region and these values are now displayed. To accept the peak width and detection threshold, click Next.

Figure 4–26: Processing Method Wizard, Integration – Peak Width and Threshold page



11. Specify the criteria for rejecting peaks below a defined area or height.

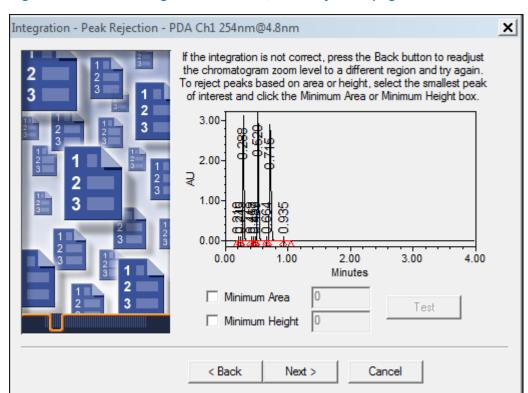


Figure 4-27: Processing Method Wizard, Peak Rejection page

For this example, use the shortest peak to set the Minimum Height. Select the peak by clicking the middle of the peak (the peak turns red). Then click the Minimum Height check box (Figure 4-28). Empower calculates 95% of the selected peak's height (the value appears in the Minimum Height field), and then reintegrates the chromatogram. Note that only three peaks appear (Figure 4-28), because peaks with a height less than 2606491 are not integrated.

Note: If you manually enter values in these fields, you can click **Test** to view how the values you entered affect the integration. If the software enters the values, it automatically tests them, and the **Test** button remains disabled.

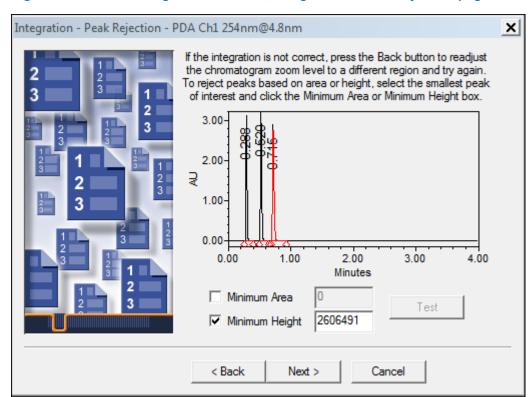


Figure 4–28: Processing Method Wizard, Integration – Peak Rejection page

- 12. When you are satisfied with the integration, click **Next**.
- 13. In the Calibration General page, do not change the default settings, and then click **Next**.
- 14. A message appears asking if you want to add channel names to the new components. Click **No**.

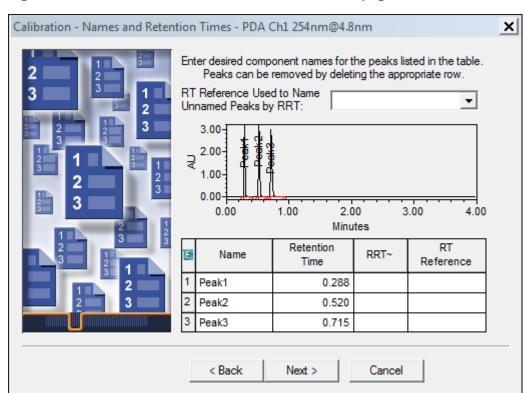


Figure 4–29: Calibration – Names and Retention Times page

- 15. In the Calibration Names and Retention Times page, rename the peaks as follows (Figure 4-30):
 - Peak 1: Uracil
 - Peak 2: Ethyl Paraben
 - Peak 3: Propyl Paraben

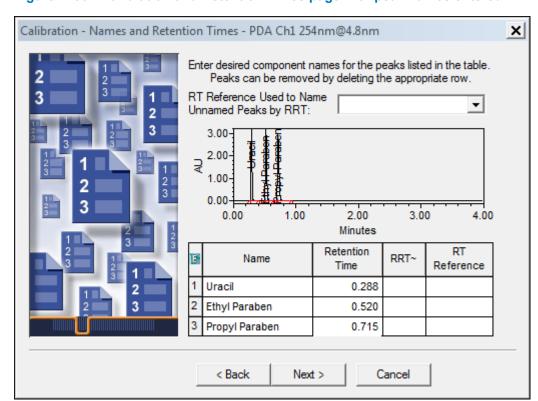


Figure 4–30: Calibration and Retention Times page with peak names entered

Note: Enter the appropriate peak names for your standard.

16. Click Next.

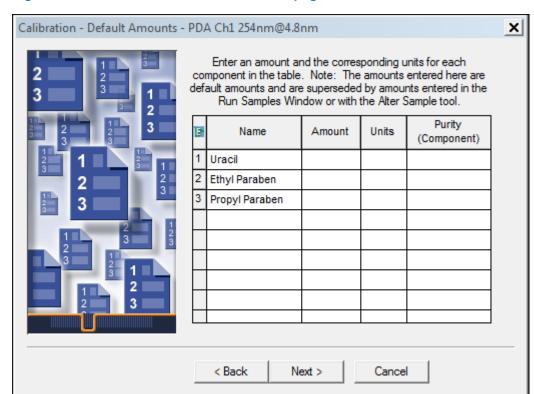


Figure 4-31: Calibration - Default Amounts page

The Calibration – Default Amounts page appears with the new component names in the table. The table has a row for each integrated peak displayed in the chromatogram.

- 17. The Processing Method Wizard only allows you to specify a single-point calibration curve. Multi-point calibration curves will be described in a later section of this guide. Click **Next**.
- 18. In the Calibration Internal Standards page, do not change the default selection of **External Standard Calibration**, and then click **Next**.

Processing Method Name - PDA Ch1 254nm@4.8nm

Method Name: Training Processing Method

Method Comments: For Training

Click Finish to save the modified processing method and return to Review where the saved processing method will be used to process the current chromatogram.

Figure 4–32: Processing Method Name page

19. Specify Training Processing Method as the method name, and any necessary comments, and then click Finish.

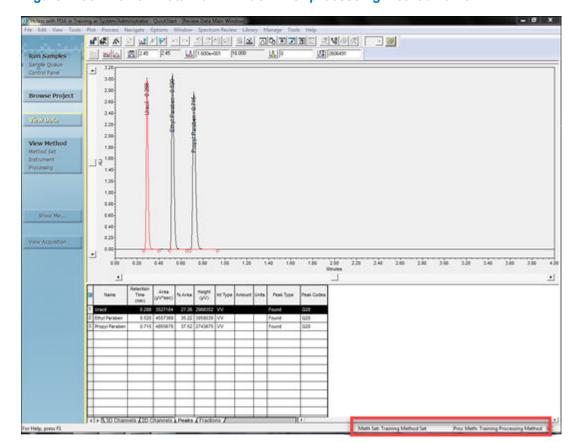


Figure 4–33: Review Data Main Window with processing method name

Empower software integrates the chromatogram using the established parameters. The name of the newly created processing method appears in the lower right corner of the window.

20. All of the Training methods are listed in the project. To view them, click **Browse Project** > **Methods.**

Defaults as System/Administrator - QuickStart - [Find Data] File Edit View Tools Database Manage Help Filter By Run Samples Injections Channels Methods Result Set Sample Queue Method Name Method Type Control Panel 3 Training Instrument Method Method Set 4 Training Instrument Method Instrument 5 Training Processing Method Processing Browse Project

Figure 4–34: Training methods displayed in Methods tab

4.5 Modifying the method set

After you create the processing method, add it to the method set.

To modify the method set:

- 1. In the navigation bar under **View Method**, click **Method Set**.
- 2. Select File > Open.

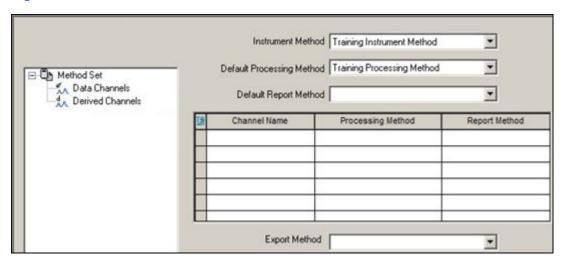


Figure 4–35: Open an existing method set dialog box

- 3. In the Open an existing method set dialog box, select **Training Method Set**, and then click **Open**.
- 4. In the Method Set window, select **Training Processing Method** from the Default Processing Method list.

Note: You may have to scroll down in the list.

Figure 4–36: Method set window



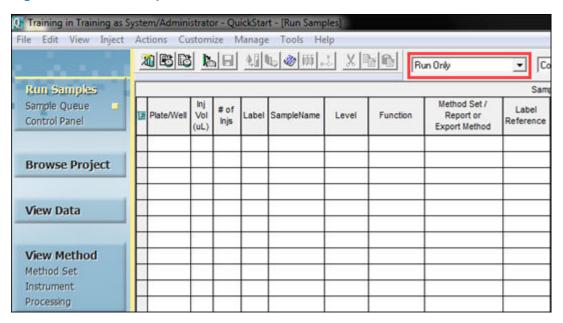
- 5. Verify that Training Instrument Method displays in the Instrument Method list.
- 6. Click Save.

4.6 Acquiring data using Run and Process

By adding the instrument and processing methods to the method set, you have enabled Empower to make an injection and process the acquired data using the Run and Process mode. The processing executes according to the parameters in the processing method you created in the previous section.

- 1. In the navigation bar, select **View Acquisition**.
- 2. Click Run Samples.

Figure 4-37: Run Samples



3. In the Run Samples window, select **Run and Process** from the Run Mode list (Figure 4-38).

Figure 4–38: Run Mode List



- 4. Click **Inject** , located next to the status bar in the lower left pane of the window.
- 5. In the Specify Single Inject Parameters dialog box, specify the same parameters as in Figure 4-17. Then, click **Inject** to begin data acquisition.

Note: Status information appears in the Status Bar during data acquisition. After the acquisition is complete, Empower software automatically processes the injections and stores the processed data as results.

5 Creating a Sample Set Method

When you are ready to acquire data from more than one sample at a time, use Empower's Sample Set Method feature. A sample set method defines instructions about acquiring data for a number of samples. In the sample set method, you can specify the number of samples and the run sequence, as well as sample-specific parameters, such as vial position, injection volume, and run time.

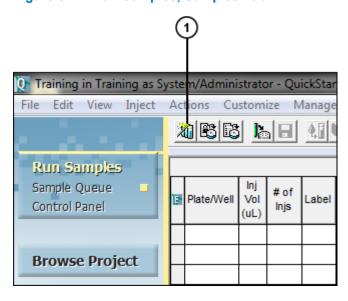
5.1 Using the New Sample Set Method Wizard

The New Sample Set Method Wizard automates the process of defining the injection information for a group of vials.

To create a sample set method using the New Sample Set Method Wizard:

1. In the Run Samples window, click the **Samples** tab.

Figure 5-1: Run Samples, Samples Tab



- 1 Sample Set Wizard Tool
- 2. Click the Sample Set Wizard tool.

Select Sample Set Method Type - Untitled X Select the type of sample set method to create. ← LC or PDA/MS C. GPC or GPC/V F RF Internal Standards C GC GC Syringe Info Define the plates to be used with this sample set method. Define Plates Select a dissolution type. € No Dissolution C Dissolution (Bath A) C Dissolution (Bath B) C Dissolution (Baths A and B) c Back Next > Cancel Help

Figure 5-2: New Sample Set Method Wizard, Select Sample Set Method Type page

If you have not defined the plate configuration previously for the ACQUITY UPLC
 Autosampler, click **Define Plates** and follow the procedure in Creating a Method Set. Do
 not change the default settings (**LC or PDA** and **No Dissolution**), and then click **Next**.

Note: See the following guides for step-by-step tutorials about specific software options.

- Empower Dissolution System Software Quick Start Guide
- · Empower GPC Software Getting Started Guide
- Empower GPCV Software Getting Started Guide
- Empower Gas Chromatography Getting Started Guide

X Select Location of Standards - Untitled First, select where standard injections should occur: ○ No standards At start of sample set At start and end of sample set Throughout sample set (average all) Before each sample group Around each sample group (without overlap) C Around each sample group (with overlap) Start loading vials in tray position: 1A1 -Cancel Help < Back Next >

Figure 5-3: New Sample Set Method Wizard, Select Location of Standards page

In the Select Location of Standards page, click At start of sample set, ensure that the
correct position is indicated in the Start loading vials in tray position, and then click
Next.

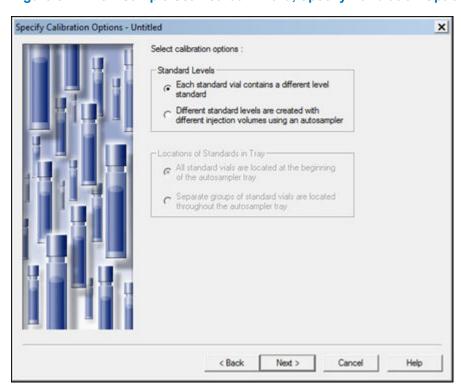


Figure 5–4: New Sample Set Method Wizard, Specify Calibration Options page

5. In the Specify Calibration Options page, select **Each standard vial contains a different level standard**, and then click **Next**.

X Describe Standard Bracket - Untitled Next, describe your standard bracket. Standard Information Number of standard vials in each group: 1 Number of levels in each standard group: ÷ Number of injections per vial: 3 ÷ Injection volume: 1.0 Run time : 2.00 Method Set Select : Training Method Create New Options < Back Next > Cancel Help

Figure 5-5: New Sample Set Method Wizard, Describe Standard Bracket page

- 6. In the Describe Standard Bracket page, specify the following parameter settings:
 - Number of standard vials in each group: 1
 - Number of injections per vial: 3
 - Injection volume: 1.0
 - Run time: 2:00
 - Method Set: Select **Training Method Set** from the list.
- 7. Click Next

Describe Samples - Untitled X Next, describe your samples Sample Information Number of samples: 1 ÷ Number of injections per vial: 1 ÷ Injection volume: 1.0 ÷ Run time: 2.00 Select: Training Method Set • Create New Options < Back Next > Cancel Help

Figure 5-6: New Sample Set Method Wizard, Describe Samples page

- 8. In the Describe Samples page, enter the following parameters:
 - Number of samples: 1
 - Number of injections per vial: 1
 - Injection volume: 1.0
 - Run time: 2:00
- 9. Click Next.

Result: The first of four identification pages appears.

- If desired, in the New Sample Set Method Wizard, Identification page 1, identify your standards and samples by selecting a column name from the corresponding column name list, and then click Next.
- 11. If desired, in the New Sample Set Method Wizard, Identification page 2, identify your standards and samples by selecting a column serial number from the corresponding column serial number list, and then click **Next**.
- 12. If desired, in the New Sample Set Method Wizard, Identification page 3, identify your standards and samples by selecting a sample matrix from the corresponding list, and then click **Next**.

Identification - Untitled

How should your standards be identified?

SampleName:

Stid

Incrementing Prefix:
Incrementing Suffix: 1

How should your samples be identified?

SampleName:

Unk

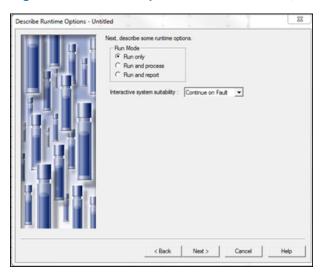
Incrementing Prefix:
Incrementing Suffix: 1

A least and a least a

Figure 5-7: New Sample Set Method Wizard, Identification page 4

- 13. Enter a root name for your standards and samples. Root names can be automatically incremented with either a prefix, a suffix, or both. For this exercise, enter Std for the **Sample Name** and 1 in the **Incrementing Suffix** field, and then click **Next**.
- 14. Choose a runtime option.

Figure 5-8: New Sample Set Method Wizard, Describe Runtime Options page

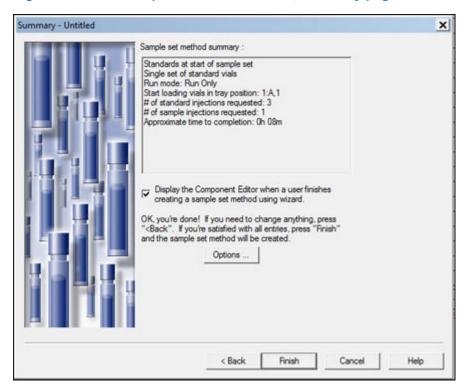


The choices are:

- Run only collect raw data only
- · Run and process collect data and then process it
- Run and report collect data, process data, and create report after results are generated

Select Run Only, ensure that Interactive system suitability is set to Continue on Fault, and then click Next.

Figure 5-9: New Sample Set Method Wizard, Summary page



- 15. On the Summary page, verify that all options chosen in the preceding pages are correct, and note that the check box enabling the Component Editor to automatically open is selected.
- 16. Click **Finish** to exit the wizard.

Result: This opens the Component Editor (Figure 5-10).

5.2 Entering Component Information

To create a multilevel calibration curve, you must first specify component amounts or concentrations using the Component Editor. Figure 5-10 shows the location of Component Editor fields.

_ 🗆 x Component Editor File Edit View SampleSet Type: STANDARDS ONLY • Current Vial Row: 2 Vial: 1:A,1 Level: Sample Name: Std1 Type Standard Vial ID: 0 Components **4** ▶ Value Purity Value Component Units (Vial) (Standard) ∢ I ➤ Current \ All Samples / 1 OK Cancel For Help, press F1 NUM

Figure 5-10: Component Editor fields

- 1 Copy from Processing Method tool
- 2 Sample Set Type list
- 3 All Samples tab
- 4 Component loading table

To enter component information:

- 1. Click the All Samples tab, and then select Standards Only from the Sample Set Type list.
- 2. Click **Copy from Processing Method** . This allows you to copy data from the Training Processing Method.



Figure 5–11: Open an existing Processing Method dialog box

3. In the Open an existing Processing Method dialog box, select **Training Processing Method**, and then click **Open**.

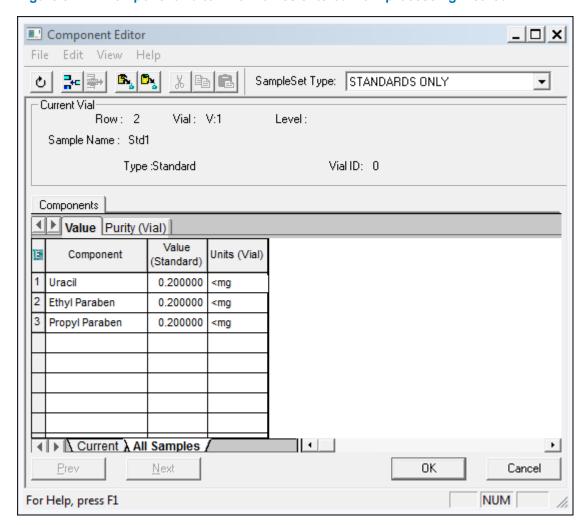


Figure 5–12: Component Editor with names entered from processing method

The software loads the names of the standard components from the Training Processing Method into the Component Loading table.

4. Enter the amounts as shown in Figure 5-12.

Note: Enter the amounts associated with your standards. To specify units (in this case, mg) type the "<" symbol, followed by the unit, in the Units (Vial) column. The < symbol will not appear in the results.

- 5. Click OK.
- 6. Select File > Save Sample Set Method As.

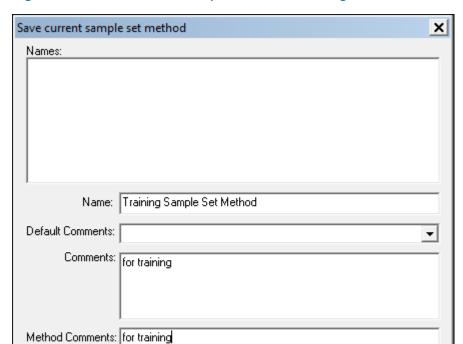


Figure 5-13: Save current sample set method dialog box

7. In the Save current sample set method dialog box, specify Training Sample Set Method for the name, any pertinent comments, and then click **Save**.

Save

Note: You can configure Empower to display Method Comments, as well as, general Comments. Refer to the Empower Online Help for more information.

Cancel

Help

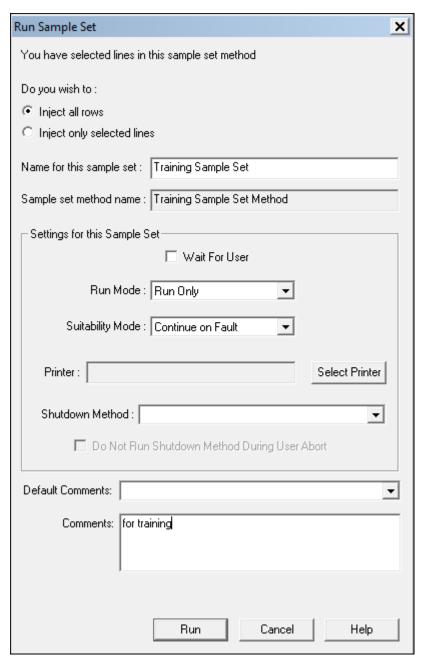
8. Click **Run current sample set method** (Figure 5-14).

Hclass with PDA in Training as System/Administrator - QuickStart - [Run Samples] File Edit View Inject Actions Customize Diagnostics Manage Tools Help Run Only Run Samples Apply Table Preferences Sample Set Method Sample Queue Control Panel Sample Set Method: Training Sample Set Method Method Set / # of Plate/Well Vol Label SampleName Function Report or Injs (uL) Export Method **Browse Project** Clear Calibration Training Method Set 3 S0101 Std 1 1:A,1 1.0 Inject Standards Training Method Set 1:A,2 1.0 1 U0101 Unk 1 Training Method Set Inject Samples View Data Training Sample Set Method Do System Idle - Sample Set Complete

Figure 5-14: Run Current Sample Set Method tool

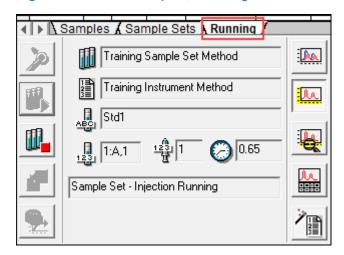
Note: If you selected a row or rows in the Run Samples window, you can specify whether to inject all rows or selected rows. If you did not select rows, this option does not appear in the Run Sample Set dialog box.





- 9. In the Run Sample Set dialog box, do the following:
 - Specify Training Sample Set as the sample set name.
 - If you have highlighted a row in the Run Samples window, ensure that the Inject all rows option is selected.
 - · Click Run to begin.

Figure 5–16: Run Samples, Running Tab



When acquisition starts, the software switches to the **Running** tab to allow you to view the current status of your acquisition (Figure 5-16).

Important: Make sure to let the sample set complete its run (Figure 5-17).

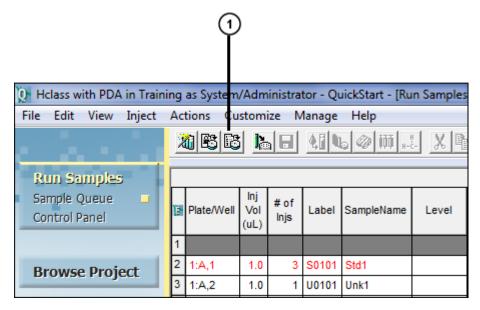
Figure 5-17: Completed run notice

System Idle - Sample Set Complete

Tip: You can return to the **Samples** tab and create a new sample set method while the current one is running.

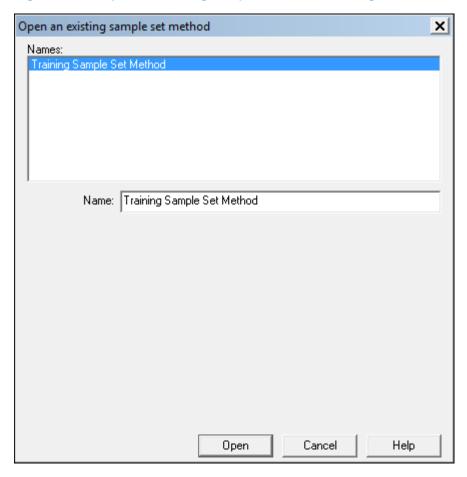
- 10. After you save the sample set method with a name, you can reuse the method.
- 11. Click the Open Sample Set Method tool (Figure 5-18).

Figure 5-18: Open Sample Set Method tool



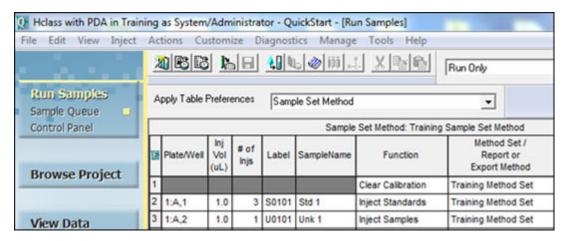
- Open Sample Set Method tool
- 12. In the Open an existing sample set method dialog box, highlight the method of interest and click **Open**.

Figure 5–19: Open an existing sample set method dialog box



Result: The sample set method is loaded into the table and is ready to run (Figure 5-20).

Figure 5–20: Sample Set Method Loaded into the Samples Table



13. With the sample set method loaded into the table, you can run the method by clicking **Run** the current sample set method .

6 Creating a Processing Method Interactively

In a previous chapter, you created a processing method using the Processing Method Wizard (Creating a Processing Method). Now, you will create a processing method interactively without using the wizard.

By interactively creating a processing method, you can access more integration, calibration, and quantitation parameters than is possible using the Processing Method Wizard.

This chapter shows you how to use the Review Data Main window and the Processing Method window to:

- · Optimize peak detection and integration parameters using the Apex Track Algorithm
- Assign peak names

Note: This chapter uses the Defaults project instead of the Training project.

To change projects

- 1. From the Manage menu, select Change Project/System.
- 2. Highlight the Defaults project.
- 3. Select Open in this window or Open in new window.
- 4. Click OK

6.1 Creating a processing method in Review Data main window

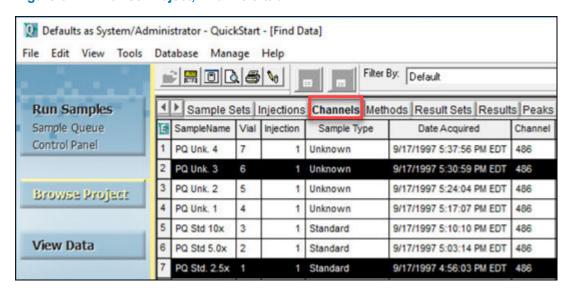
To interactively create a processing method:

- Click Browse Project, and then click Channels to access the unprocessed channels of data (Figure 6-1).
- 2. Select **PQ Std 2.5x**, hold down the Ctrl key, and then click one of the unknown (PQ Unk) samples.

Result: The channels you selected are highlighted in the Channels table.

Note: To ensure that Empower detects all your peaks of interest, base your processing method on the lowest concentration standard that produces a good signal-to-noise ratio.

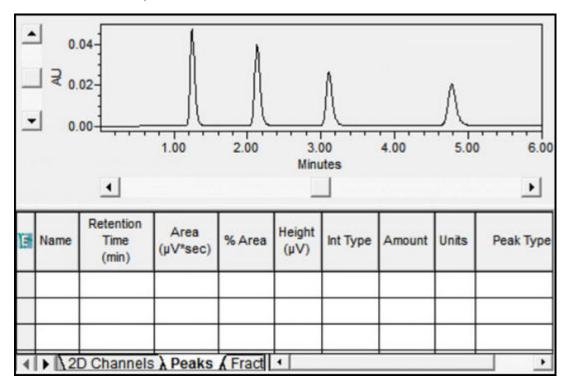
Figure 6-1: Browse Project, Channels tab



3. Click View Data.

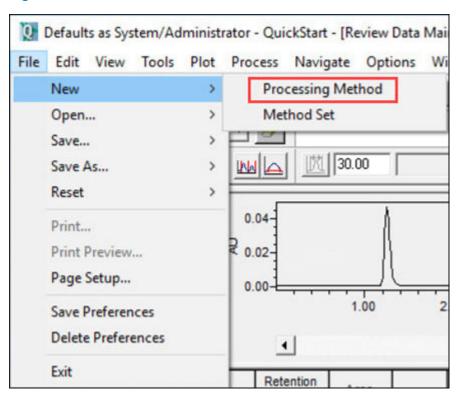
Result: The Review Data main window displays the chromatogram of the first chosen channel (the standard) in the upper plot pane (Figure 6-2).

Figure 6–2: Review Data Main Window with chromatogram of standard (first channel)



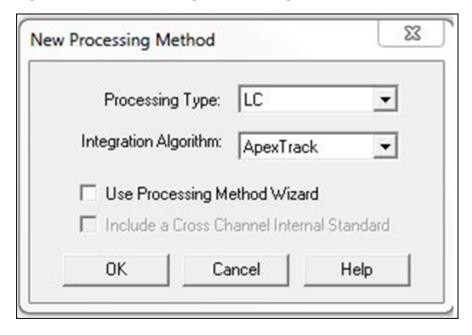
4. Select File > New > Processing Method (Figure 6-3).

Figure 6-3: File menu



5. In the New Processing Method dialog box (Figure 6-4), ensure that Processing Type is set to **LC** and Integration Algorithm is set to **Apex Track**, then click **OK**.

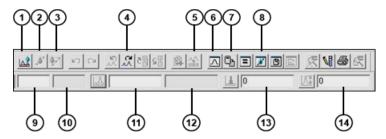
Figure 6-4: New Processing Method dialog box



6. Before proceeding, review the tools for creating and optimizing processing methods (Figure 6-5).

Tip: When you point to an icon in the interface, the name of the icon appears in a Tool Tip window.

Figure 6-5: Tool Bar



- 1 Integrate
- 2 Calibrate
- (3) Quantitate
- 4 Next 2D Channel
- 5 Fill from Result
- 6 Review Main Window
- Processing Parameters
- 8 Calibration Curve
- 9 Processing Method Peak Width
- (10) Result Peak Width
- 11) Processing Method Threshold
- 12 Result Threshold
- 13 Processing Method Minimum Area
- 14 Processing Method Minimum Height
- 7. Click **Processing Parameters** (see Figure 6-5).

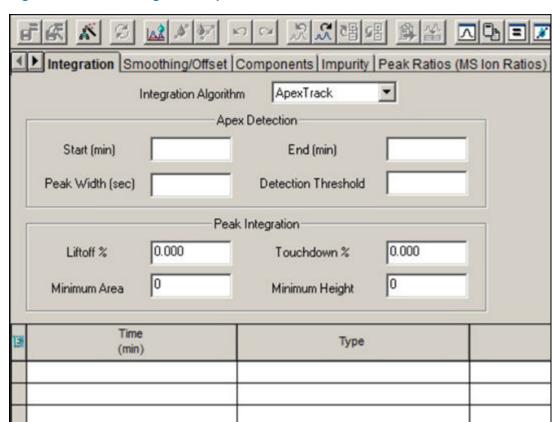
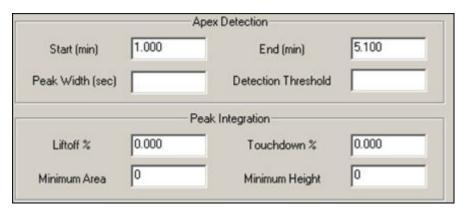


Figure 6–6: Processing method parameters

- 8. Click **Integration** to set the peak detection and integration parameters. Peak detection parameters consist of the following:
 - Start (min) and End (min) Region of the chromatogram for peak detection. For this exercise, enter a start time of 1 and an end time of 5.1 (Figure 6-7).
 - **Peak Width (sec)** Sets a digital filter for smoothing. Leave this blank so that Empower determines the optimum value.
 - **Detection Threshold** Based on peak-to-peak noise. Leave this blank so that Empower determines the optimum value.

Figure 6–7: Processing method parameters with start and end times



9. Click **Review Main Window** to return to the chromatogram, then click **Integrate**

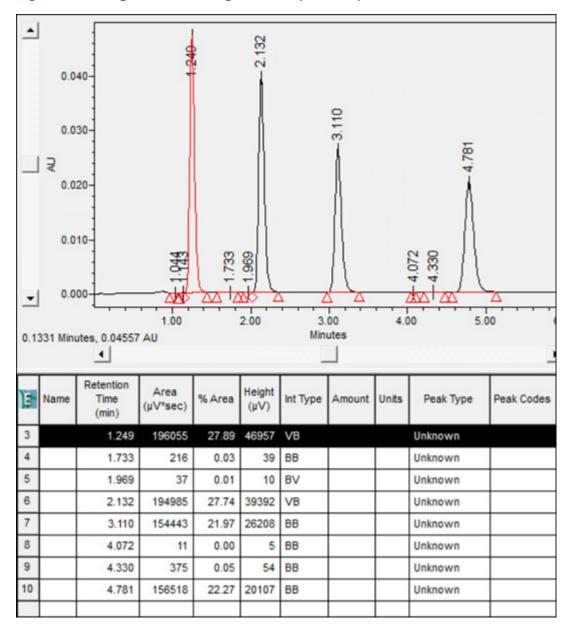


Figure 6-8: Integrated chromatogram with optimized peak width and threshold

Empower determines the auto peak width and auto threshold, and calculates the optimum values for these parameters (Figure 6-8).

10. Now you can fine-tune the method for the four large peaks of interest. To prompt Empower to ignore the remaining peaks, use either the Minimum Area or Minimum Height to reject them. Because the peak areas for the small peaks in this example are under 1000, enter 1000 in the processing method minimum area.

Alternative: Use the shortest peak of the four in this example to set the Minimum Area. Select the peak by clicking the middle of the peak (the peak turns red). Then click **Set Processing Method Minimum Area**.

Result: Empower calculates 95% of the selected peak's area (the value appears in the Minimum Area field).

11. Click **Integrate** . Note that only four peaks appear because peaks with an area of less than 1000 are not integrated (Figure 6-9).

Note: Adjustments to the processing method parameters are subjective, and you may need to follow your lab's standard operating procedure.

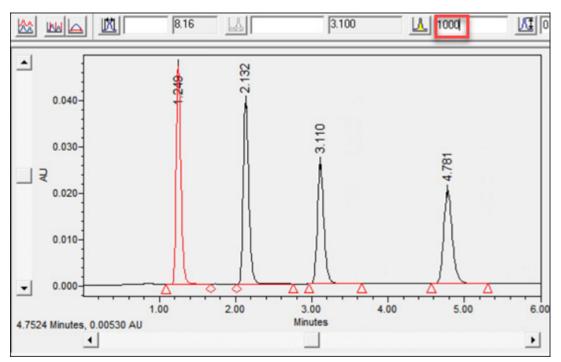
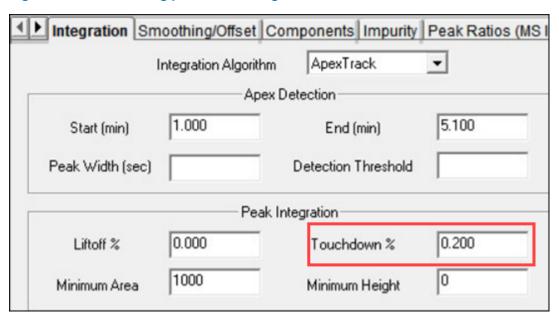


Figure 6–9: Integrated chromatogram with minimum area value

12. The peak start (liftoff) markers are close to the peaks; however, the peak end (touchdown) markers are far from the peaks. To adjust them, click **Processing Parameters** and examine the peak integration parameters (Figure 6-10).

Note: Default values for liftoff percentage and touchdown percentage are 0.000.

Figure 6–10: Processing parameters Integration tab



- 13. Peak integration parameters consist of the following:
 - Liftoff % A baseline start liftoff percentage.
 - Touchdown % A baseline end touchdown percentage.
 - Minimum Area Minimum peak area required for a peak to be reported.
 - Minimum Height Minimum peak height required for a peak to be reported.

In this case, change the peak end by modifying the Touchdown %. The range is 0–100. The default value of 0 produces a touchdown tangent to the baseline. 100 produces a touchdown tangent to the inflection point. If you enter a small number, such as 0.2, it might produce a better touchdown closer to the peak end (Figure 6-11).

14. After you enter the changes, click Integrate , and then Review Main Window ...

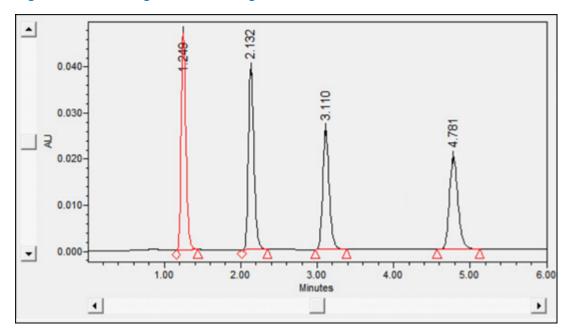
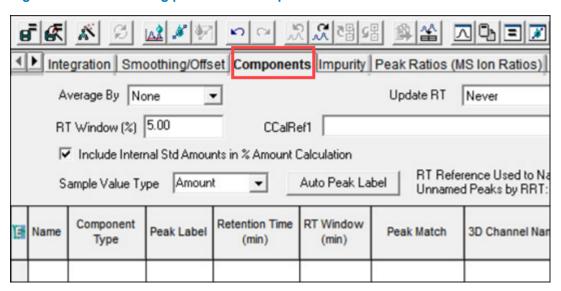


Figure 6-11: Reintegrated chromatogram with touchdown % of 0.2

15. To assign peak names, click **Processing Parameters** , and then select **Components** (Figure 6-12).

Figure 6–12: Processing parameters Components tab



- 16. Click **Fill From Result** to populate the table. This produces one line of information for each integrated peak in the chromatogram.
- 17. A message appears asking whether you want to add channel names to the new components. Click **No**.

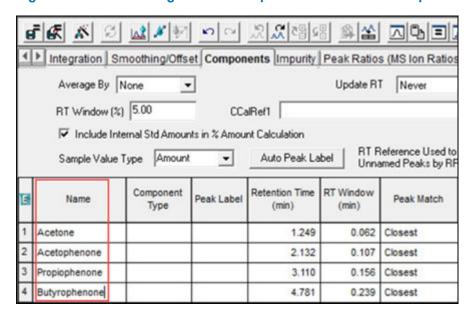
Result: The table is populated with generic peak names (Figure 6-13).

Integration Smoothing/Offset Components Impurity Peak Ratios (M. Average By None Update RT RT Window (%) 5.00 CCalRef1 ✓ Include Internal Std Amounts in % Amount Calculation RT Refere Sample Value Type | Amount Auto Peak Label -Unnamed RT Window Component Retention Time Name Peak Label Peak Match Type (min) (min) Peak1 Closest 1.249 0.062 2 Peak2 2.132 0.107 Closest 3 Peak3 3.110 0.156 Closest Peak4 4.781 0.239 Closest

Figure 6–13: Processing method Components tab with generic peak information

- 18. Specify the following names for the four peaks (Figure 6-14):
 - Acetone
 - Acetophenone
 - Propiophenone
 - Butyrophenone

Figure 6–14: Processing method Components tab with correct peak names

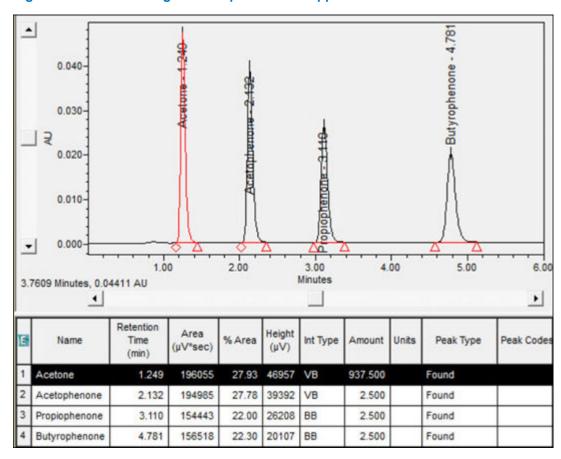


19. Click **Review Main Window** to return to the chromatogram, and then, because this channel of data is a standard, click **Calibrate** to apply the component information.

Note: If Calibrate is not active, the channel of data is not a standard.

Result: The peak names are applied to the peaks (Figure 6-15).

Figure 6-15: Chromatogram with peak names applied



20. Now, examine the channel of data for the sample. Click **Next 2D Channel**, **Integrate**, and then **Quantitate** to produce an integrated chromatogram with peaks (Figure 6-16).

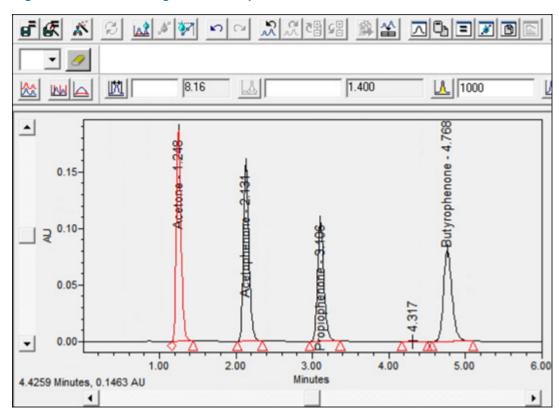
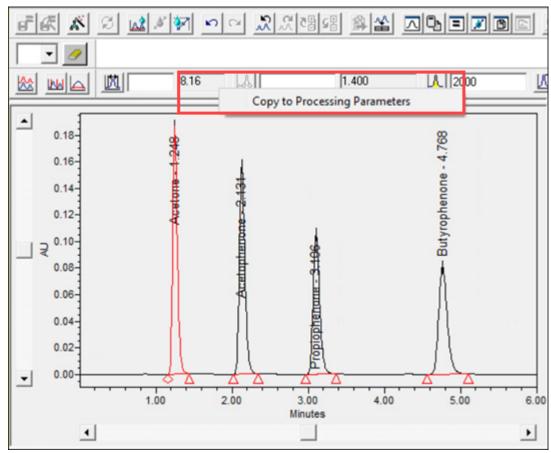


Figure 6–16: Chromatogram for Sample

- 21. Notice that an extra peak that is not of interest is integrated at 4.317 minutes. To prompt Empower to ignore this peak, increase the value for the processing method minimum area to 2000, and then click **Integrate** . Remember to click **Integrate** any time you change an integration parameter.
- 22. Decide which values for Peak Width and Threshold to use in this method. The choices are:
 - To prompt Empower to determine the optimum values for each chromatogram, leave the Processing Method Peak Width and Processing Method Threshold fields empty. If you choose this option, do nothing further to the method.
 - To use the same values for peak width and threshold in every chromatogram, copy the Result Peak Width and Result Threshold values into the method by right-clicking on each field and selecting Copy to Processing Parameters (Figure 6-17).

For this exercise, use the second option to copy the same values for both peak width and threshold.





Result: Empower integrates only the four peaks of interest and applies their correct names (Figure 6-18).

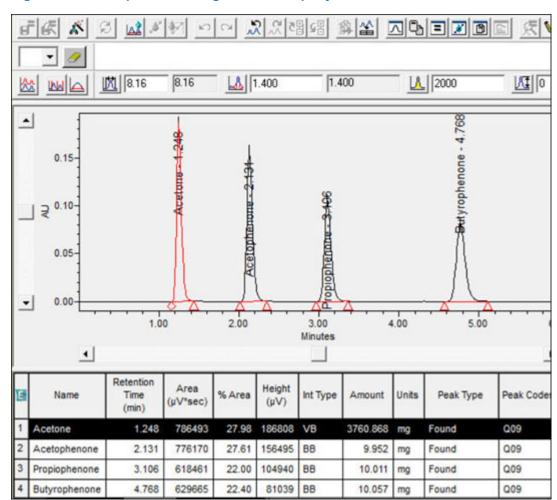
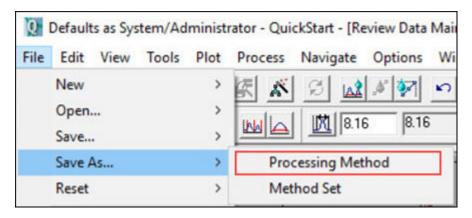


Figure 6–18: Sample Chromatogram with Properly Named Peaks

Note: Refer to the Empower Online Help for column definitions.

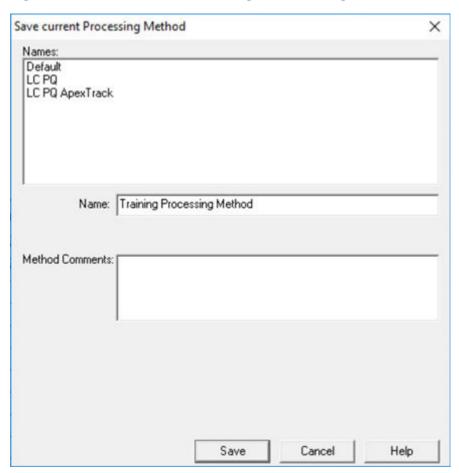
23. Select **File > Save As > Processing Method** (Figure 6-19).

Figure 6-19: Saving the processing method



24. In the Save current Processing Method dialog box, specify Training Processing Method as the name for the method and any comments, and then click **Save**.

Figure 6–20: Save current Processing Method dialog box



Note: You can configure Empower to display Method Comments, as well as general Comments. Refer to the Empower Online Help for more information.

7 Generating and Reviewing Results

After acquiring a sample set, you may want to refine certain characteristics of the samples. The Alter Samples feature helps you accomplish this process efficiently. This chapter shows you how to do the following:

- Alter Samples Use the Alter Sample feature to ensure that the standards and samples include the proper information prior to processing.
- Process the sample set After you have altered the sample set information, you can use the background processing and reporting feature to process the sample set.
- Review the result set After you have processed the sample set, review the result set and calibration curves in the Review Data main window.
- Generate Reports You can print a report from the Results tab of the View Data window.

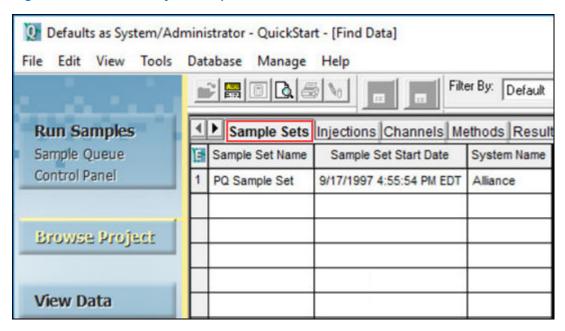
7.1 Altering Samples

After you acquire the data and create the processing method, you can generate results. Before generating the results, use the Alter Sample Set window to verify that your samples include all of the necessary information, and correct or add sample information.

Note: Ensure that View Acquisition is not selected in the Navigation bar.

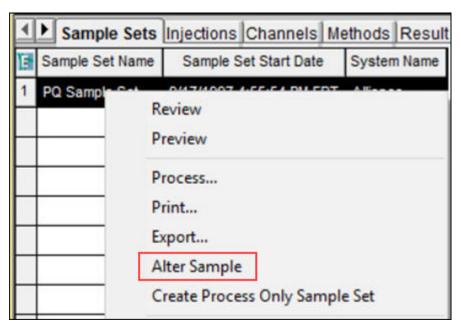
1. In Browse Project, select the **Sample Sets** tab (Figure 7-1).

Figure 7-1: Browse Project Sample Sets tab



2. Right-click the sample set of interest and select **Alter Sample** (Figure 7-2).

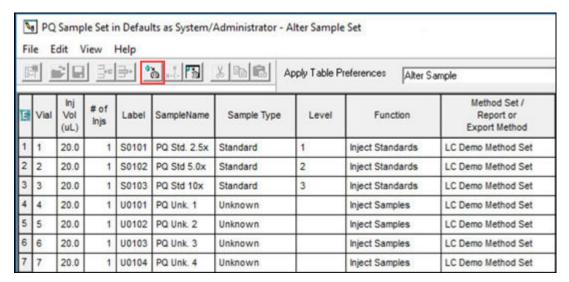
Figure 7–2: Right-click Alter Sample



Note: In the Alter Sample Set window, you can modify user-assigned data, such as Sample Name, Sample Weight, and Dilution values, but you cannot modify the sample set information used to physically collect the data during a chromatography run, such as vial number or injection volume.

3. To generate a calibration curve or curves, use the Component Editor to specify the contents and amount in each standard vial. Click **Amount** (Figure 7-3) to open the Component Editor window (Figure 7-4).

Figure 7–3: Amount tool



4. In this example, we ran three standards at three different levels. To create a multi-level calibration curve or curves follow these steps. For each standard vial, the Component Editor displays the component name and the standard value. You can specify component information before you run the sample set method, as you did in Chapter 5, or after the run, using the Alter Sample Set window.

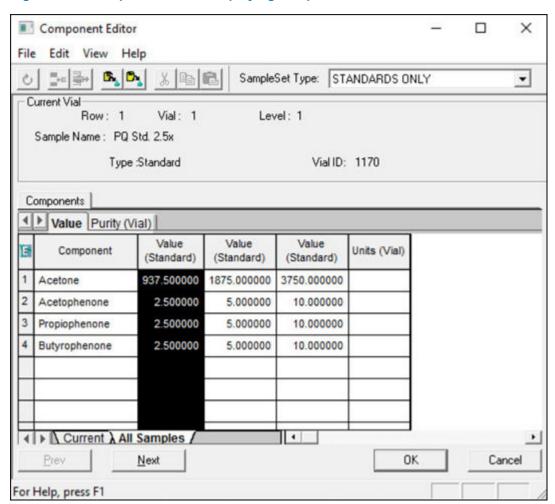


Figure 7–4: Component Editor displaying component names and values

5. To ensure that the component names match the component names in the processing method, copy the names from the processing method by clicking **Copy from Process Method** (Figure 7-5).

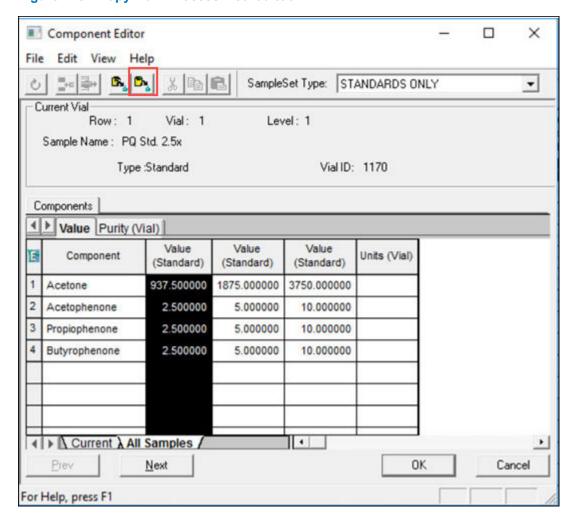


Figure 7–5: Copy from Process Method tool

6. In the Open an existing Processing Method dialog box (Figure 7-6), select the processing method of interest, and then click **Open**.

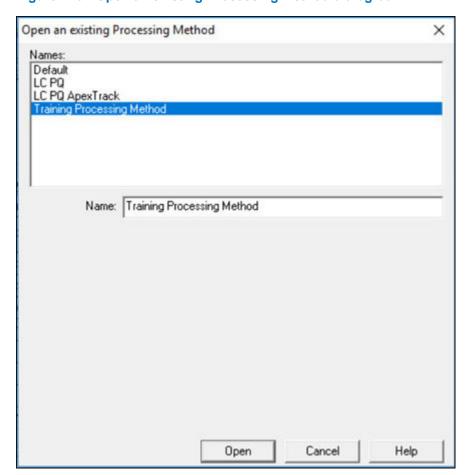


Figure 7–6: Open an existing Processing Method dialog box

- 7. Click **Yes** in the Components warning message.
- 8. If they are not already present, specify units (in this case, mg) by typing the < symbol, followed by the unit, in the Units (Vial) Column (Figure 7-7). The < symbol will not appear in the results.

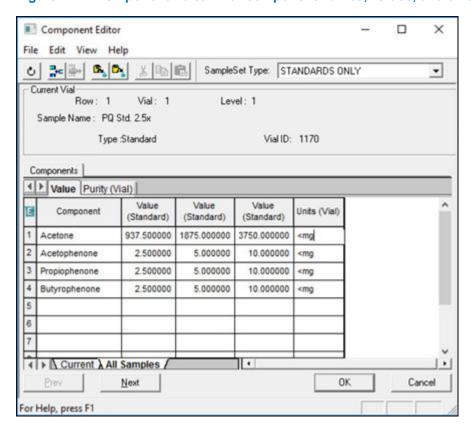


Figure 7–7: Component Editor with component names, values, and units

9. Click the Purity(Vial) tab to enter purity values for the standards. This corrects the standard amounts by the value entered.

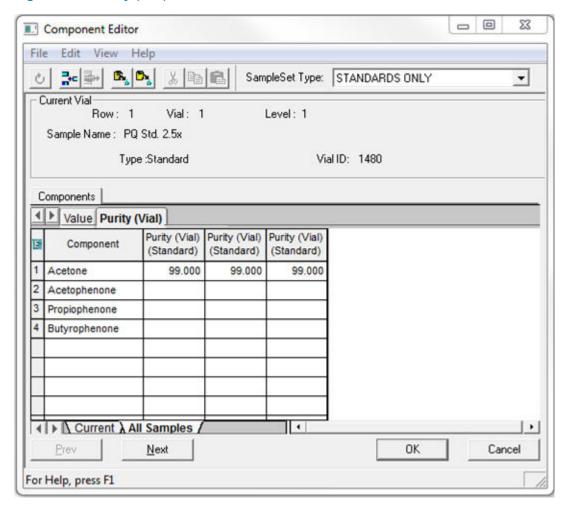


Figure 7-8: Purity (Vial) tab

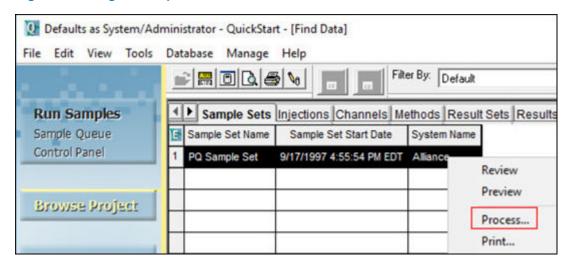
- 10. Click **OK**.
- 11. Save all changes and close the Alter Sample Set window. You are now ready to process the sample set.

7.2 Processing the sample set

After you have altered the sample set information, you can use the background processing and reporting feature to process the sample set.

In the Browse Project window, right-click the sample set and select Process (Figure 7-9).

Figure 7-9: Right-click process

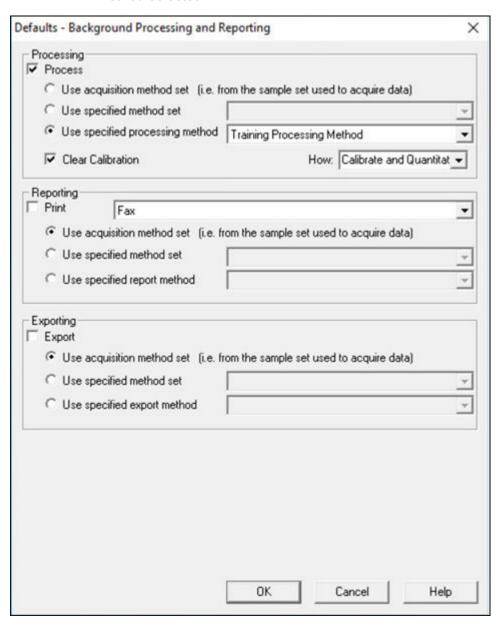


- 2. In the Background Processing and Reporting dialog box, select the appropriate processing options.
 - In the Use specified processing method field, select the new processing method you created in Chapter 6 and click **Clear Calibration**. See Figure 7-10.

If you are processing single-channel 2D data and are not using any bracketing routines, then any of these choices will work. If you are processing multiple channels of data per injection, working with 3D data, or deriving channels, then you must process the data with a method set.

- Use acquisition method set This is the method set used to acquire the data. Ensure
 that you add the processing method to this method set before making this selection.
 This is not used in this example.
- **Use specified method set** Ensure that you pick a method set that contains the proper processing method. This is not used in this example.
- Use specified processing method This allows you to select from a list of previously defined processing methods. Use this selection in this example.
- Clear Calibration Clears any calibration curves associated with your processing method so that you can create a new calibration curve.
- How Calibrate and Quantitate.

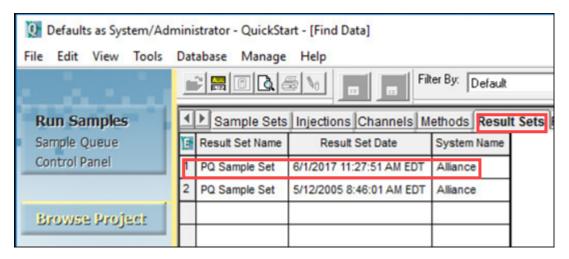
Figure 7–10: Background Processing and Reporting dialog box with processing method selected



- 3. Click OK.
- 4. When you process a sample set (bound collection of raw data), Empower generates a result set (bound collection of results). To review the result set, click **Result Sets** in the Browse Project window (Figure 7-11).

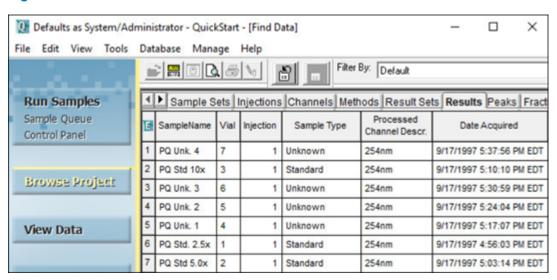
Result: A new result set, with the current date and time stamp, appears at the top of the list. You might have to click **Update** in the toolbar to see the new information.

Figure 7-11: Result Set tab



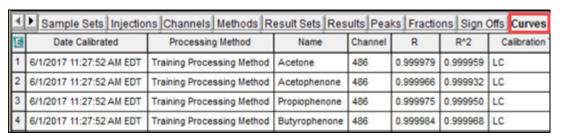
5. Right-click the **Result Set Name**, and then click **View As > Results**. The new results, with the current date and time stamp, appear at the top of the list.

Figure 7-12: Results tab



6. Right-click in the Results table, and then click **View As > Calibration Curves**. Four new calibration curves, with the current date and time stamp, appear at the top of the list.

Figure 7–13: Calibration Curves table



7.3 Reviewing the result set

After you process the sample set, review the data in the Review Data main window.

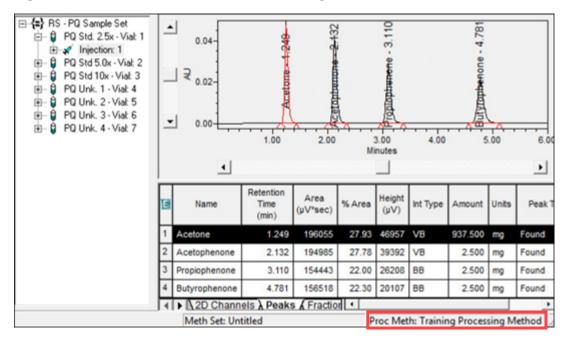
1. Return to **Results Sets**, right-click the new Result Set, and then select **Review** (Figure 7-14).

Figure 7-14: Right-click Result Set, Review

Sample Sets Injections Channels Methods Result Sets Results				
E	Result Set Name	Result Set Date	System Name	Review
1	PQ Sample Set	6/1/2017 11:27:51 AM EDT	Alliance	Preview
2	PQ Sample Set	5/12/2005 8:46:01 AM EDT	Alliance	December

- 2. In the dialog box that appears, click **Yes**.
- 3. The Review Data Main Window appears and shows the Result Set (Figure 7-15). Ensure that the **Peaks** tab is open. The window highlights the first standard and shows the chromatogram and corresponding peak table. The amount field is populated with the numbers you specified earlier in the component editor. In the Result Set tree on the left, you can browse through the entire Result Set. Because these are results, the peaks are integrated and named. Note that the name of the processing method that Empower used to generate the results appears in the lower-right corner of the window.

Figure 7–15: Review Data Main Window showing the result set



4. Select one of the samples in the tree (Figure 7-16).

Result: Empower populates the amount field with values that were calculated from the comparison of peak response to the calibration curve. Because this is an external standard calculation, Empower compares the area under the peak to the calibration curve, and then determines the amount. Empower divides the amount by the sample weight and multiplies the result by the dilution (both values are 1, by default), and then reports the final amount.

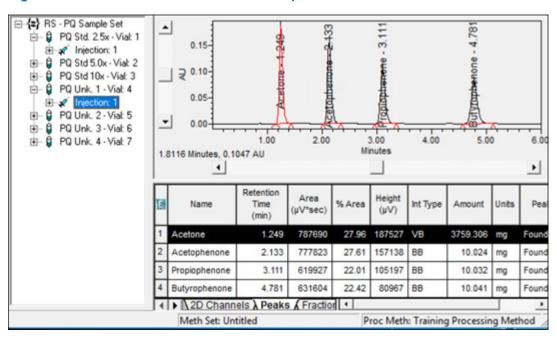
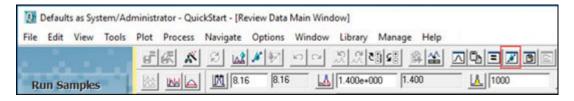


Figure 7–16: Review Data main window sample information

5. Click Calibration Curve 🗾 (Figure 7-17).

Figure 7-17: Calibration Curve tool



6. In the upper portion of the Review Data Calibration Curve Window, review the equation for the line and the R². In the middle portion of the window, review the calibration curve plotting Amount (x-axis) versus Area (y-axis). The point table is in the lower portion of the window. For more information, see the Empower Online Help.

Training Processing Method Date/Time 6/1/2017 11:27:52 AM EDT Method 486 Alliance System Channel Component Acetone • Time (min) 1.249 Y = 2.09e+002 X + 1.43e+003 Equation 0.999959 0.999979 2.725902e+003 R^2 R Standard Error 7.430544e+006 65.262055 RSS RSD None Weighting Codes 0.593946 RSD(E) 800000-500.00 1500.00 2000.00 0.00 1000.00 2500.00 3000.00 3500.00 Amount 3057.3795 Amount, 1.917e+004 Area 1 . ← Calibration / II e I Level % Deviation Manual Point Resu X Value Response Calc. Value Ignore -0.7431 937.500000 196054.928571 930.533406 2 2 1885.449891 0.557 2 1875.000000 395774.750000 3 3750.000000 785015.000000 3746.516703 -0.093

Figure 7–18: Calibration Curve window

7. To view the calibration curve for another component, select the curve from the **Component** list (Figure 7-19).

Figure 7–19: Component list

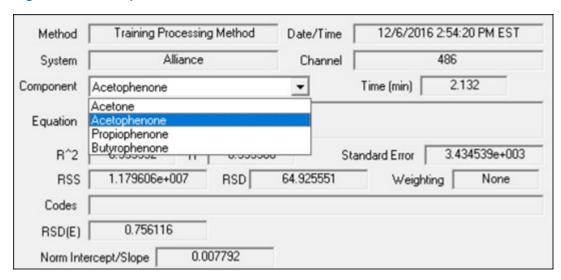
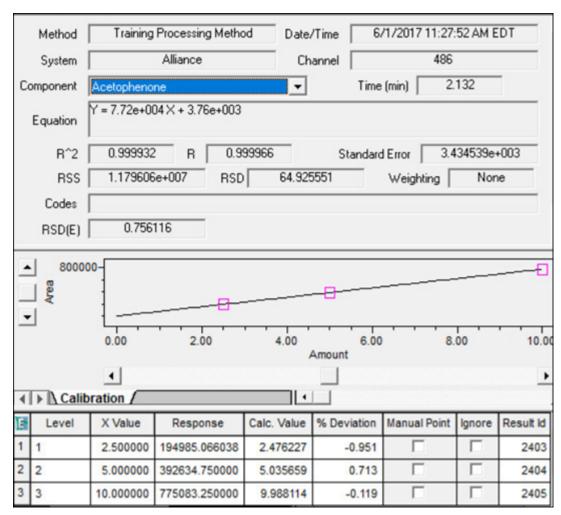


Figure 7–20: Acetophenone Calibration Curve window

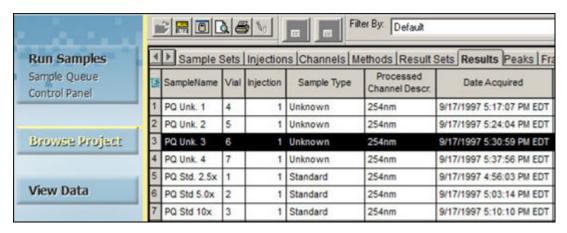


7.4 Reporting

To generate a report after the data has been acquired and processed:

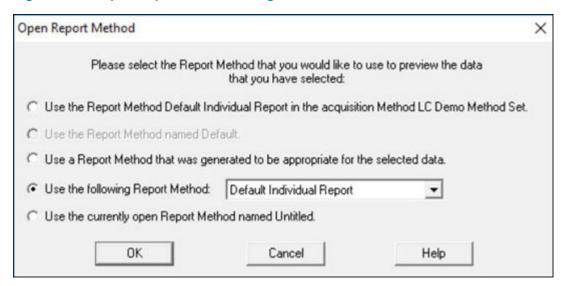
1. From the navigation bar, click **Browse Project**.

Figure 7-21: Browse Project, Results view tab



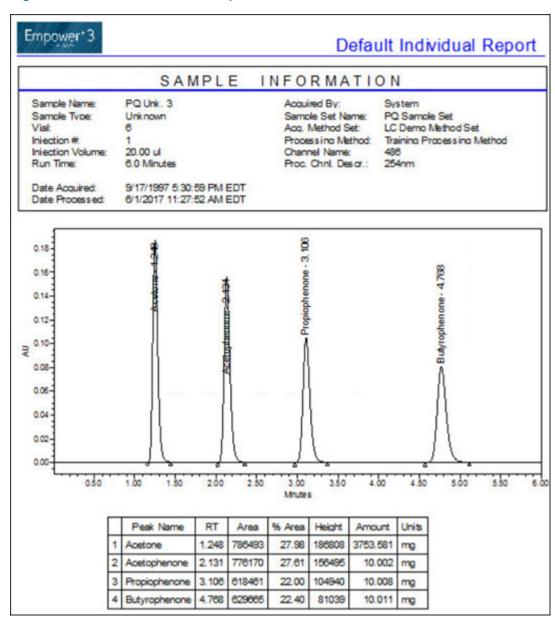
- Click the Results tab.
- 3. Select the result to print.
- 4. Click View Data.

Figure 7–22: Open Report Method dialog box



- 5. In the Open Report Method dialog box, select **Use the following Report Method**, and then **Default Individual Report**. Click **OK**.
- 6. The report opens for you to preview.

Figure 7-23: Default Individual Report



7. Click **Print**

8 Backing Up and Restoring Projects

This chapter describes how to back up and restore projects using the Backup Project Wizard and Restore Project Wizard in Empower software.

The contents of each project (including methods, acquired data, and results) are automatically saved to the Empower database on your computer's hard drive (either the workstation's hard drive, if using an Empower Personal workstation, or the server's hard drive or other external drive, if using an Empower Workgroup or Enterprise system). As you accumulate multiple projects in the database, you need to back up these projects to:

- Keep a copy of current project information in a safe place in case of system failure, which would result in data loss.
- Archive information from an inactive project you want to store for future use. You increase
 free hard disk space by archiving inactive data outside the computer, then deleting the data
 from the hard drive.

Note: Waters strongly recommends that you backup your projects to a destination that is external to the hard drive in your Empower system.

8.1 Backing up projects

When you back up a project, you export all project tablespace information and raw data to a subdirectory that has either a software preset or a path you customize.

You can back up to the following locations:

- Back up to the software's default path (Empower/Projects). This requires a second step of backing up the information in this directory to an external device.
- · Back up to an external device.
- · If you are on a network, back up to a network drive.

Before you begin

Before you back up a project:

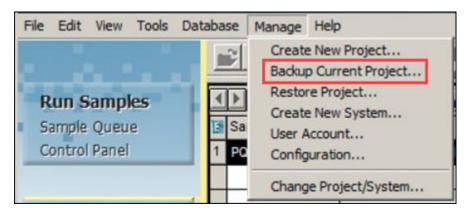
- If you back up your project to a network drive, remember to log in to the network before starting the backup.
- Ensure that your backup device and program are properly installed, powered on, and configured.

8.1.1 Performing a backup

Note: To back up a project, you must log in to Empower software using an account with the Backup Projects privilege.

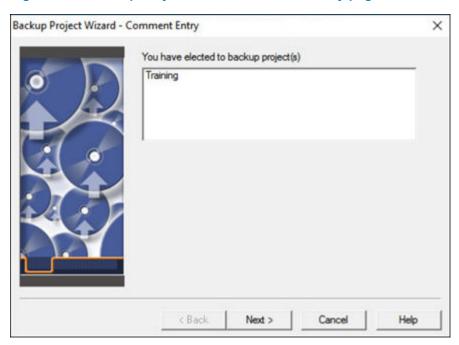
1. Select Manage > Backup Current Project (Figure 8-1).

Figure 8-1: Manage menu



2. In the Backup Project Wizard - Comment Entry page (Figure 8-2), the name of the project appears in the field. Click **Next**.

Figure 8-2: Backup Project Wizard - Comment Entry page



3. In the Select Destination page, you can choose to back up to the current project directory or you can browse to an alternate location.

Click **Browse**, choose the destination, and then click **Next**.

Note: The drive shown in Figure 8-3 must be mapped to a location on your network.

Please choose a destination for the backup files. If you specify a destination other than the default, you only need to enter the root directory - subdirectories will automatically

be created using the project name.

Backup to current project directory

Pressing 'Next' will start the backup process.

When it is completed you will be prompted to backup the appropriate path using your backup software.

@ E:\

X

Browse

Help

Figure 8-3: Backup Project Wizard - Select Destination page

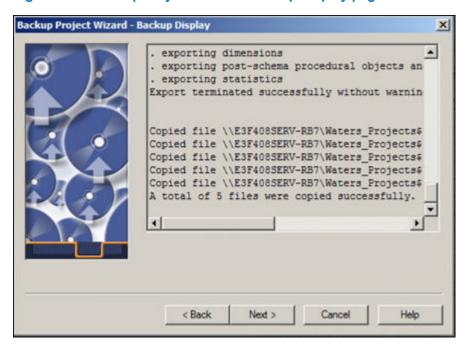
4. This page displays tablespace information as it is exported and raw data files as they are copied. When the process finishes, click **Next**. (This button is available only after the export is complete.)

Next >

Cancel

Figure 8-4: Backup Project Wizard - Backup Display page

< Back



5. Your data is now at the location specified on this page (Figure 8-5). If this is the final destination for your backup, your backup is complete.

Backup Project Wizard - Start Page

This part of the backup process is complete.
Please note the following destination directories:

E:\Training

F you have configured a third party backup application to remove projects from the backup location to external media, click the button below to begin this process. Be sure to label all media properly.

Start Backup Software ...

Figure 8-5: Backup Project Wizard - Start Page

- 6. To move your backed up projects to external media using a third-party application, click **Start Backup Software**.
- 7. Click Finish.

8.2 Restoring Projects

Before you restore a project:

- Ensure that your backup device and program are properly installed, powered up, and configured.
- If you are restoring your project from a network drive, log in to the network before starting the restore process.

8.2.1 Restoring a project

Note: To restore a project, you must log in to Empower software using an account with the Restore Projects privilege.

To restore a project:

1. Select **Manage > Restore Project** (Figure 8-6). If you used backup software, proceed to the next step; otherwise, proceed to step 3.

Figure 8-6: Manage list

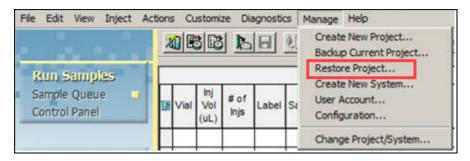
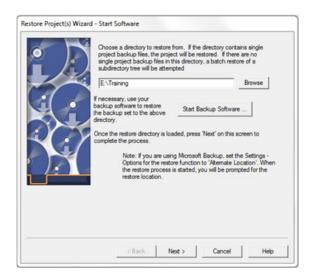


Figure 8–7: Restore Project Wizard - Start Software page



- In the Restore Project Wizard Start Software page, start your chosen backup program to restore the backed up project file to the default directory by clicking **Start Backup Software**.
- 3. Click the **Browse** button and use the Browse for Folder dialog box to locate the appropriate directory structure.
- 4. Click Next.

Project Name: Training
Project Parent: Defaults

Backup Details
Backup Type: Project Backup
Backup Date: 11/3/2016 10:46:18 AM EDT
Database ID: 2842185473

Backup Comments

< Back
Next > Cancel Help

Figure 8-8: Restore Project Wizard - Project Details page

Note: You must specify the exact location of your backed-up data. The last directory in this path is usually Project Name. This directory must contain files named Project Name.exp and Project Name.inf.

Note: If you are using a network drive, it must be mapped on the computer you are using in order to restore projects from it.

5. You can change the project name and the project parent. Make any appropriate changes, and then click **Next**.

Note: You cannot have duplicate project names under the same parent project.

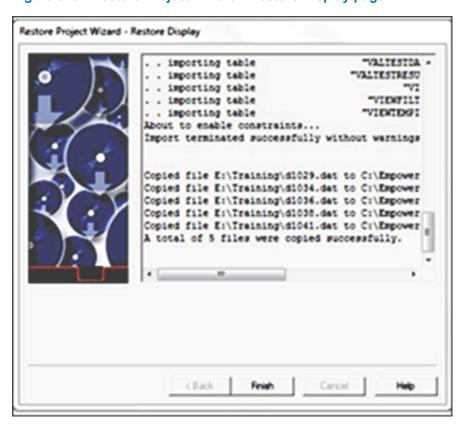


Figure 8-9: Restore Project Wizard - Restore Display page

6. The Restore Display page displays tablespace information as it is imported and the raw data files as they are copied. When the process finishes, click **Finish**. Figure 8-10 shows the restored project in the Configuration Manager. Notice that the project name has been incremented by 1 because there cannot be two projects with the same name.

Figure 8-10: Restored and renamed project Training

76	Training	System	5/17/2017 2:01:16 PM EDT	✓	No Lock
77	Training 1	System	6/2/2017 8:44:23 AM EDT		No Lock

A Creating Projects

A project is a user-defined collection of methods, results, custom fields, view filters, and raw data that resides in the Empower database and appears in Browse Project. Everything except for the raw data is stored in a reserved area of tablespace within the Empower database. Project raw data is stored in a separate directory.

Note: The raw data path for the project can be user-specified using Configuration Manager.

As part of your installation service, the Field Service Engineer will configure the first project for your organization. This appendix describes how to create subsequent projects.

Within Empower, you can:

- · Create any number of projects
- · Import and export data to and from projects
- · Copy selected information from one project to another project

When you create a project, you can define the following parameters:

- Tablespace size size of the logical storage unit within the database specified for the project.
 50 MB is the default value.
- Enabled options the subset of options that you have chosen for the project
- Access privileges the users and groups that have access to the project

A.1 How to create a project

To create a project:

1. Select Manage > Create New Project.

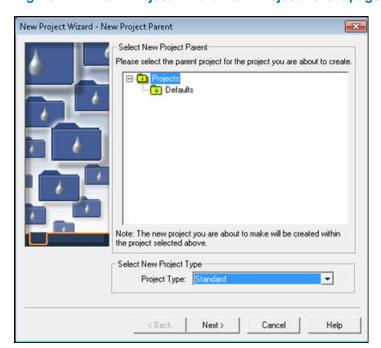
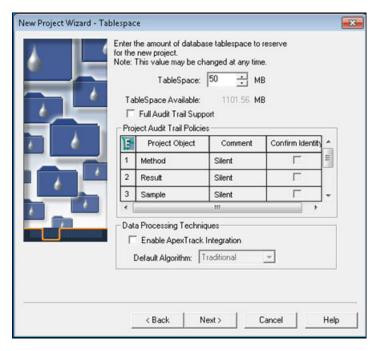


Figure A-1: New Project Wizard-New Project Parent page

2. In the New Project Wizard-New Project Parent page, highlight **Projects** at the root directory. If you want the new project to reside under a different parent project, highlight the parent project from the list. Click **Next**.

Figure A-2: New Project Wizard - Tablespace page



3. In the Tablespace page, note the following:

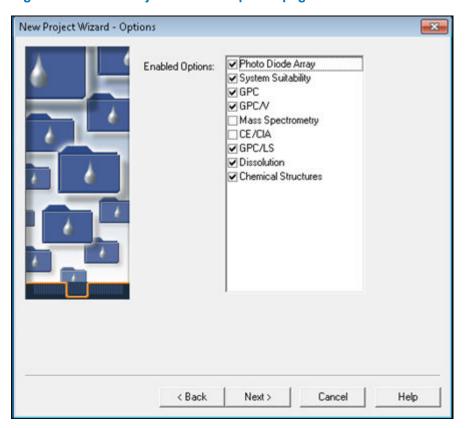
- Notice that the default Tablespace is 50 MB. This is a reasonable starting point; however, if you plan to generate a large volume of results, consider increasing this value.
- Optionally, select the Full Audit Trail Support check box to create a record of all changes made to elements of the project, such as methods and samples.
- Specify whether to require comments on **Methods**, **Results**, **Sample**, and deletion information changes.
- Full Audit Trail Support specifies whether you are prompted for a change description (in the Enter Revision Description dialog box) whenever you save modified methods, results, or samples.

Note: Changes are traceable, whether you have chosen to require comments or not. If you do not require comments, the software will track any changes, but will not issue comments. Empower software retains the state of the Full Audit Trail feature when you back up or restore a project.

Note: You can also set Full Audit Trail Support by using a system policy. For more information on system policies, consult the Empower online help.

4. Click Next.

Figure A-3: New Project Wizard - Options page



On the Options page, select the options that apply to the project, and then click Next.

New Project Wizard - Access Control Allowed Access Select the users that should have access @ Owner Only C Owner and Group to this project. C Owner, Group and World Group User Type Select the type of user access given to the group(s). User's Own Type Allow Access to Groups Administrators Select the group(s) to be given access to the project. Guests World User Type Select the type of access given other users. User's Own Type < Back Next> Cancel Help

Figure A-4: New Project Wizard - Access Control page

 The Access Control page establishes the level of access users and user groups have to the project you create. Determine the appropriate access for the project, and then click Next. Refer to the Empower Online Help for more information.

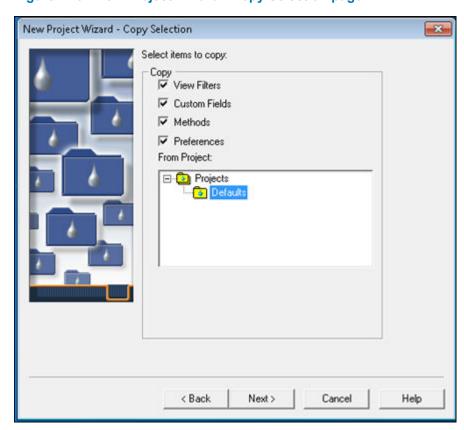


Figure A-5: New Project Wizard - Copy Selection page

- 7. The Copy Selection page allows you to copy certain pieces of information, such as methods, from an existing project into the new project. Select the appropriate items by selecting the check boxes, and then selecting the existing project's name in the **From Project** list.
- 8. Click Next.

Figure A-6: New Project Wizard - Name Entry page

- 9. On the Name Entry page, type the desired name in the **Project Name** field and, if you selected the Full Audit Trail Support option, type a comment in the text box.
- 10. Click Finish.
- 11. In the QuickStart window, select **Manage > Change Project/System**.
- 12. Select the new project, and then click **OK** to open the project.

B Creating Systems

A chromatographic system contains the specific instrumentation configuration you use to acquire data with the Empower software.

As part of your installation service, the Field Service Engineer will configure the first system for your organization. This appendix describes the creation process for subsequent systems.

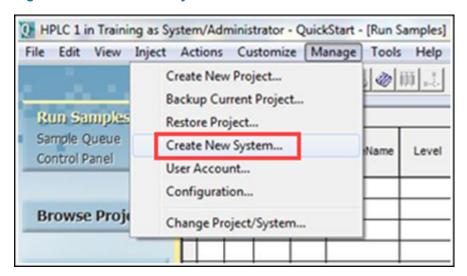
Before you create a system, ensure that instruments are powered on and any calibration and diagnostic routines are complete.

B.1 Creating a chromatographic system

To create a chromatographic system:

Select Manage > Create New System.

Figure B-1: Create New System selection



Choose to define a new chromatographic system, or to connect to a system which already exists.

System Type

Create New System

Connect to Existing System

Figure B-2: New Chromatographic System Wizard - Type Entry page

2. Select Create New System, and then click Next.

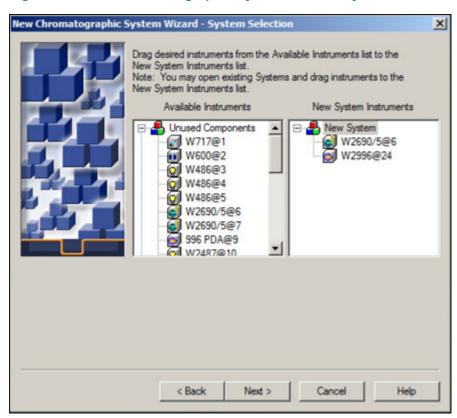


Figure B-3: New Chromatographic System Wizard - System Selection page

- 3. Build your system by moving system instruments from the **Available Instruments** tree pane to the **New System Instruments** tree pane through one of these two methods:
 - Drag and drop the instruments from the Available Instruments tree pane to the New System Instruments tree pane.
 - Double-click the instruments' icons in the Available Instruments tree pane.
 Result: The instruments appear in the New System Instruments tree pane.
- 4. Click Next.

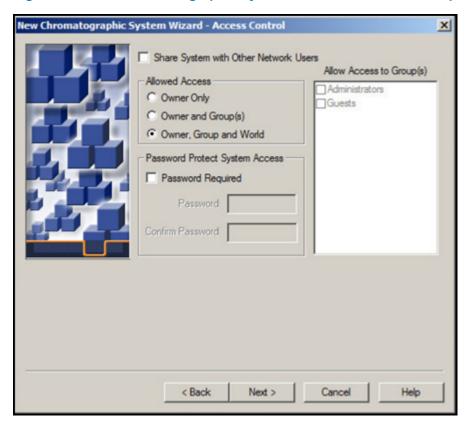


Figure B-4: New Chromatographic System Wizard - Access Control page

5. This page establishes the level of access users, user groups, and all users will have to the system you create. Determine the appropriate access for the system. Refer to the Empower Online Help for more information. Click **Next**.

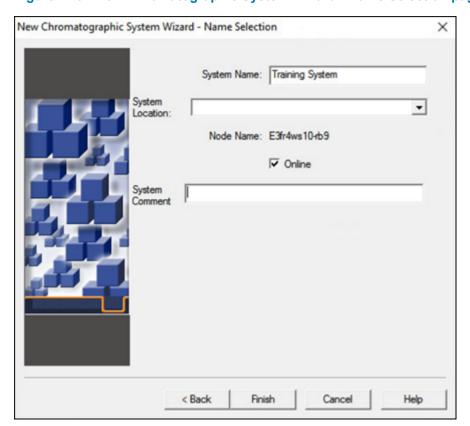


Figure B-5: New Chromatographic System Wizard - Name Selection page

- Enter a descriptive name, select a **System Location** from the list (if any have been created), and any comments about the system, and do not change the default setting of **Online**.
- 7. Click Finish.

Result: The system is created.

Note: After the system is created, it is brought online, where it is active, available to be controlled, and can acquire data through Empower software.

8. When the message indicating that the system was successfully brought online appears, click **OK**. Figure B-6 shows the new system listed in the Configuration Manager.

Figure B-6: New system listed in the Configuration Manager

	System Name	System Location	Node Name	Node Location	OnLine	System Comments
1	HPLC 1	Beverly Lab	Landern-6f01m32	Milford Lab	Yes	Alliance with 2487
2	Training System	Milford Lab	Landern-6f01m32	Milford Lab	Yes	New
3	UPLC 1	Milford Lab	Landern-6f01m32	Milford Lab	Yes	UPLC with PDA