

LabSolutions™

LC Getting Started Guide

1	<i>Start Up</i>	12
2	<i>Set the Instrument Parameters</i> ..	18
3	<i>Single Run</i>	23
4	<i>Data Analysis</i>	25
5	<i>Realtime Batch</i>	31
	Create a Batch Table	31
	Realtime Batch Processing.....	36
6	<i>Multiple Data Analysis</i>	40
7	<i>Data Management</i>	48
8	<i>ShutDown</i>	54

SCL-40 SYSTEM CONTROLLER

CONTROL

ERROR

SHIMADZU

GU-405 DEGASSING UNIT

CE



SHIMADZU

CTO-40S COLUMN OVEN

D-M40 PHOTO DIODE ARRAY DETECTOR

NOTICES

- All rights reserved, including those to reproduce this manual or parts thereof in any form without permission from Shimadzu Corporation.
- The information in this manual is subject to change without notice and does not represent a commitment on the part of the vendor.
- Any errors or omissions which may have occurred in this manual despite the utmost care taken in its production will be corrected as soon as possible, although not necessarily immediately after detection.
- Maintenance parts for this product are provided for seven years after production has stopped. Please note that we may not be able to provide maintenance parts after this period. However, for parts that are not genuine Shimadzu parts, the period of provision is determined by the manufacturer.
- The contents of the hard disk in a PC can be lost due to an accident. Backup your hard disk to protect your important data from accidents.
- If the user or usage location changes, ensure that this Instruction Manual is always kept together with the product.
- Original version is approved in English. SHIMADZU

©2010-2019 Shimadzu Corporation. All rights reserved.

Types of Manuals

Five Instruction Manuals are provided with LabSolutions.
You can also display the [Help] menu to confirm the meanings
and setting ranges of parameters.
The following shows how to make full use of the manuals.

■ Getting Started Guide

This manual is for first-time users.
Follow the sequence of procedures in this guide to gain
an understanding of basic LabSolutions operations.

■ Operators Guide

This manual gives comprehensive
information about overall
data acquisition operations in
LabSolutions, such as system
configuration, data analysis, batch
processing, and report functions.

■ System Users Guide

This manual is for system
administrators.
This manual describes system
administration and data
management.

■ Data Acquisition & Processing Theory Guide

This manual describes peak
detection and quantitation of sample
components (for advanced users).

■ Installation & Maintenance Guide

This manual describes installation
and maintenance of the LabSolutions
software.

■ Help

Refer to [Help] to learn more about
the displayed sub-window.
Click the on-screen [Help] button
or the [F1] key on the keyboard to
display [Help].

The meanings of symbols used in this manual are
as follows.



Useful advice for convenient
instrument operation



Shows where to refer to in the
Operators Guide

What LabSolutions Can Do

LabSolutions software is very easy to use, while incorporating high-grade functions. It provides powerful support for automating and improving the efficiency of sequential data acquisition and analysis operations.

Use LabSolutions to perform the following functions.

- Control of analytical instruments and data acquisition
- Data analysis and viewing of data
- Creation and printing of various customizable reports
- Data management

System Structure

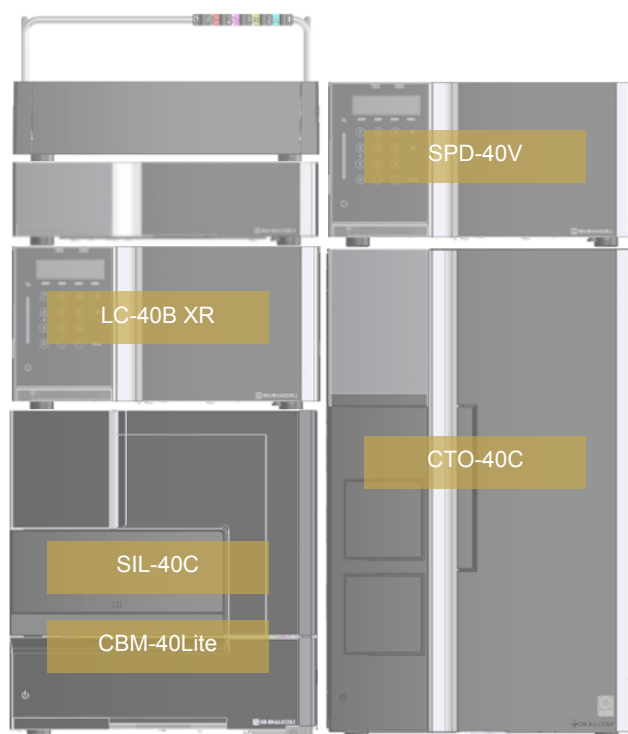
This Getting Started Guide describes data acquisition operations with the assumption that the system includes the following instruments.

• **Detector** SPD-40V

• **Autosampler** SIL-40C

• **Pump** LC-40B XR

• **Column oven** CTO-40C



File Types

Data file (.lcd)

This file contains all analysis results and acquisition information from the following files.

Method file (.lcm)

Acquisition conditions,
analysis conditions,
calibration curve information,
and etc.

Batch file (.lcb)

This file is used for
continuous data acquisition
of sequential samples.

Report format file (.lsr)

This file is used to print
data acquisition results.

-Checks Before Operation-

Data Acquisition Flow

STEP ①

Set Up the Conditions

Set up the data acquisition conditions to suit the component to be measured.

Before starting data acquisition, set up the data acquisition conditions on LabSolutions.

For the data analysis operations described in this manual, set as follows:

Column	Shim-pack VP-ODS (150 mm L × 4.6 mm i.d. 5 µm)
Mobile phase	Pump A = Water, Pump B = Acetonitrile
Flow rate (mobile phase)	1.0 mL/min
Column temperature	40 °C
Detection wavelength	254 nm
Sample Injection volume	10 µL
Sample	Mixtures of para hydroxy benzoic acid ester (paraben mixed sample) 10, 20 and 40 ppm standard samples, and 2 unknown samples



STEP ②

Data Acquisition

When you have finished setting up the data acquisition conditions,

start off by acquiring the data.

On LabSolutions, the operation of analysis samples one at a time is called "**single run**".

To evaluate the data acquisition conditions, change the data acquisition conditions, measure standard samples and unknown samples, and check the separation state of the target component.

Perform data acquisition on other samples using the data acquisition conditions that provided the optimum separation state.



3 Single Run P.23



Setting up the data acquisition conditions and optimizing the data processing parameters are important for obtaining better data acquisition results. This section describes the basic flow of data analysis.

STEP ③ Analysis

Process the acquired data, and **apply the analysis conditions.**

Normally, multiple data is analyzed to determine peak integration conditions so that consistent results (e.g. repeatability of retention time and peak area, detection limits of target components, and linearity) can be acquired.

When the data analysis conditions have been fixed, quantitative calculation (i.e. investigation as to how much of the target component is contained in the sample) is performed on the unknown sample based on the data analysis results of the acquired standard sample.

To perform quantitation, a calibration curve must be made from the known concentrations and peak area values of the standard samples. This calibration curve is used to calculate the concentration of the unknown sample.



4 Data Analysis P.25



STEP ④ Realtime Batch

Perform data acquisition on sequential samples together.

Realtime batch is performed to measure sequential samples continuously when the data acquisition conditions have been fixed by performing a single run.



5 Realtime Batch P.31



6 Multiple Data Analysis P.40



STEP ⑤ Data Management

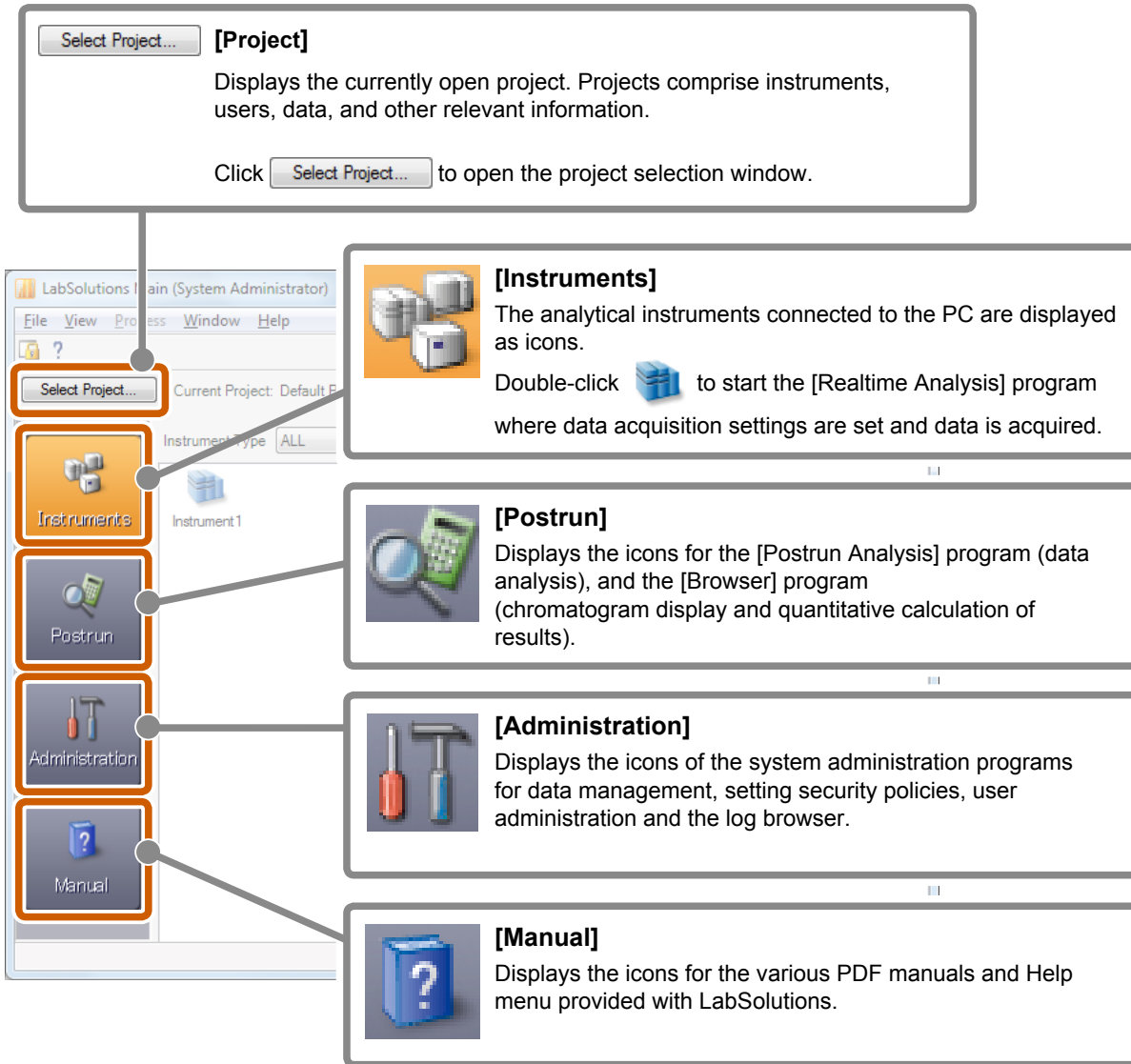
Display the data files acquired using realtime batch in step ④ by specifying filtering conditions in the Data Manager.

The Data Manager can display PDF files created during data acquisition.

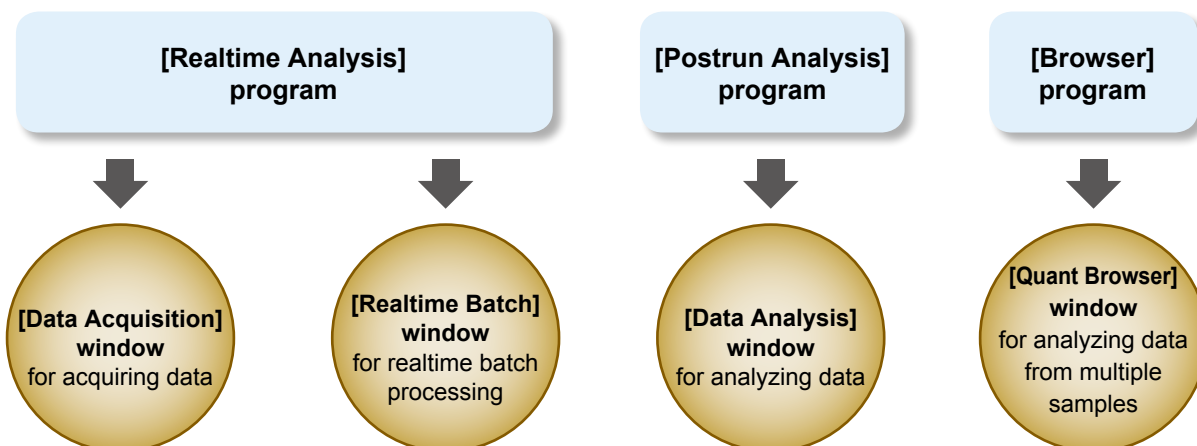


7 Data Management P.48

LabSolutions Main Window

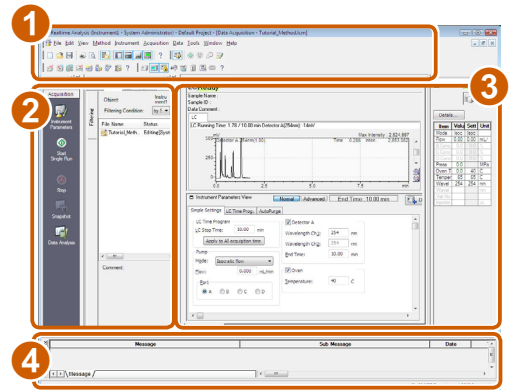


LabSolutions Main Programs and Main Windows



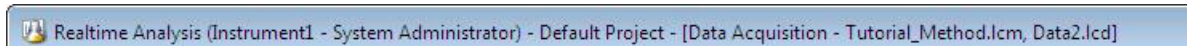
LabSolutions Windows

The following example describes the [Realtime Analysis] program window.



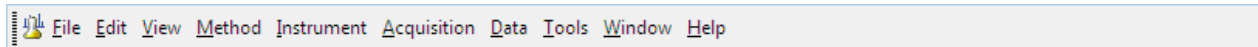
1 Title Bar

This bar displays the names of the current program, window, project, loaded file, and other information.



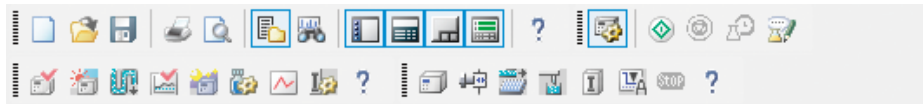
Menu Bar

This bar displays the current window and menus that are available based on the operating rights of the current user.



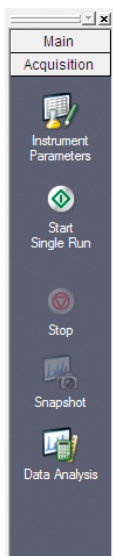
Toolbar

This bar displays icons of frequently used menu items and icons for operating analytical instruments.



2 Assistant Bar

This bar displays icons for frequently used data acquisition operations.



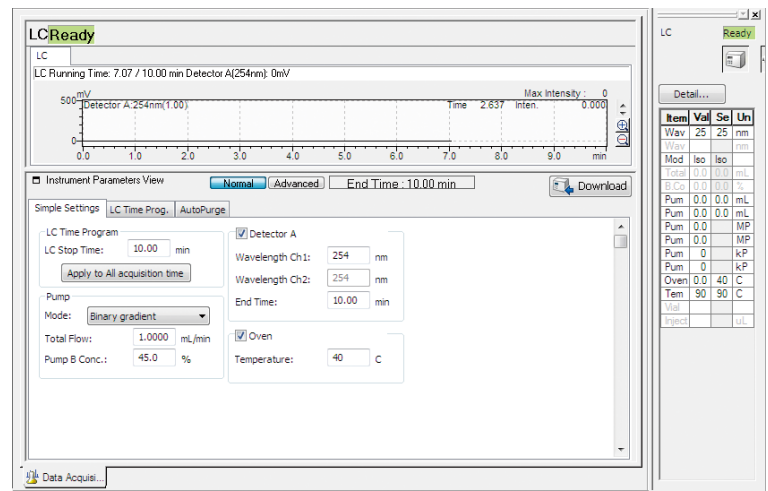
Data Explorer

This sub-window displays files for the selected project and instruments.



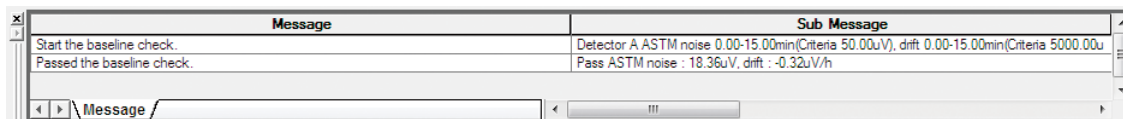
3 Window

In the [Realtime Analysis] program, [Data Acquisition], [Realtime Batch] and other windows are displayed as icons on the assistant bar. In the [Postrun Analysis] program, [Data Analysis], [PDA Data Analysis], [Calibration Curve], [Report Format] and other windows are displayed. Switch the windows by clicking the icons on the assistant bar. Instrument Monitor (right side of the window) check the acquisition conditions and connections.



4 Output Window

This window displays an operation history and error messages that occur.



How to Open Windows

Note that a project must be selected in order to open windows.

Reference **1 Start Up P.12**

Set the Data Acquisition Parameters and Execute a Single Run:

Open the [Data Acquisition] window from the main window.

1 Instruments **2** Instrument1 **3** Data Acquisition

▼ [Realtime Analysis] program

▼ [Data Acquisition] window

▲ Main Window

Reference **2 Set the Instrument Parameters P.18**

Reference **3 Single Run P.23**

The screenshot shows the LabSolutions Main window with three numbered callouts: 1 points to the 'Instruments' icon, 2 points to 'Instrument1', and 3 points to the 'Data Acquisition' icon. A dashed arrow points from the 'Data Acquisition' icon to a larger screenshot of the 'Data Acquisition' window. This window shows a chromatogram with a peak at 2.828 min and an intensity of 2.828. Below the chromatogram is the 'Instrument Parameters View' with fields for 'LC Stop Time' (00:00 min), 'Wavelength Ch1' (254 nm), 'Wavelength Ch2' (254 nm), 'End Time' (00:00 min), 'Purge' (Normal), 'Detector A' (Detector A), 'Height' (10000 mAU), 'Flow' (1.000 mL/min), 'Oven' (40 C), and 'Temperature' (25 C).

Continuous Data Acquisition of Sequential Samples:

Open the [Realtime Batch] window from the main window.

Reference **5 Realtime Batch P.31**

1 Instruments **2** Instrument1 **3** Realtime Batch

▼ [Realtime Analysis] program

▼ [Realtime Batch] window

▲ Main Window

The screenshot shows the LabSolutions Main window with three numbered callouts: 1 points to the 'Instruments' icon, 2 points to 'Instrument1', and 3 points to the 'Realtime Batch' icon. A dashed arrow points from the 'Realtime Batch' icon to a larger screenshot of the 'Realtime Batch' window. This window shows a table with columns: Analysis, Valid, Tray Name, Sample Name, Sample ID, Sample Type, and Me. The table contains 10 rows of data for various samples like 'Paraben Mixture' and 'Sample A'. Below the table is the 'Details' section with fields for 'Flow' (0.000 mL/min), 'Press' (0.0 MPa), 'Oven T' (40 C), 'Temper' (25 C), and 'Wavelength' (254 nm).

Data Analysis and Quantitative Calculations:

Open the [Data Analysis] window from the main window.

Reference **4** Data Analysis P.25

▲Main Window

▼[Postrun Analysis] program

[Data Analysis] window ▶

Peak#	Ret. Time	Area	Height
1	3.327	2722	1076
2	3.344	522516	1076
3	3.334	222209	976
4	5.508	327123	830
5	3.267	461919	114
6		212872	2843

Multiple Data Analysis and Quantitative Calculations:

Open the [Quant Browser] window from the main window.

Reference **6** Multiple Data Analysis P.40

▲Main Window

▼[Browser] program

[Quant Browser] window ▶

Object	Instrument	Sample Name	Method
1	Tutorial_L1400	Sample 1	StandardCalo.Pol
2	Tutorial_L1400	Sample 2	StandardCalo.Pol
3	Tutorial_L1400	Sample 3	StandardCalo.Pol
4	Tutorial_L1400	Sample 4	StandardCalo.Pol
5	Tutorial_L1400	Sample 5	StandardCalo.Pol
6	Tutorial_L1400	Sample 6	StandardCalo.Pol
7	Tutorial_L1400	Sample 7	StandardCalo.Pol
8	Tutorial_L1400	Sample 8	StandardCalo.Pol
9	Tutorial_L1400	Sample 9	StandardCalo.Pol
10	Tutorial_L1400	Sample 10	StandardCalo.Pol

Chapter

1

Start Up

This chapter describes how to start up LabSolutions.

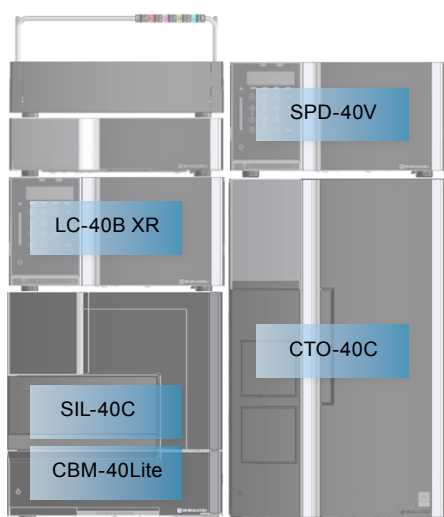


Refer to "LC Data Acquisition" in *Operators Guide* for details on the "Data Acquisition" window.

1 Check the connections.

Ensure that all of the units (pump, autosampler, column oven, and detector) of the analytical instruments are connected to the system controller and optical link cables.

2 Turn the power on for each of the instruments.

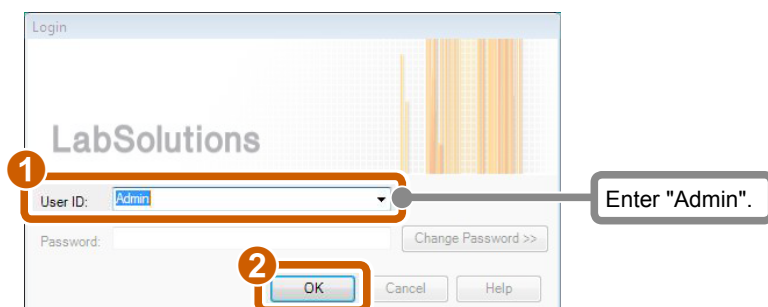


3 Turn the PC and printer on.

4 Double-click on the desktop.

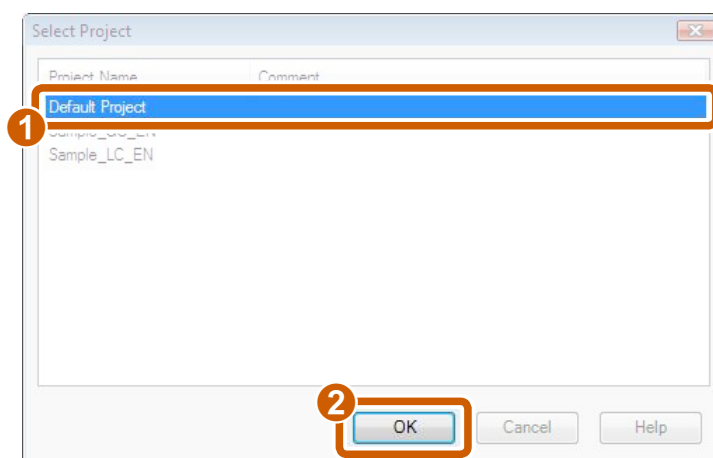
The [Login] sub-window opens.


5 Log in.



6 Select a project.

Upon initial startup, the project selection window is displayed after logging in. In this case, select the desired project. For subsequent startups, the [Realtime Analysis] program opens using the project selected when the previous session was closed.

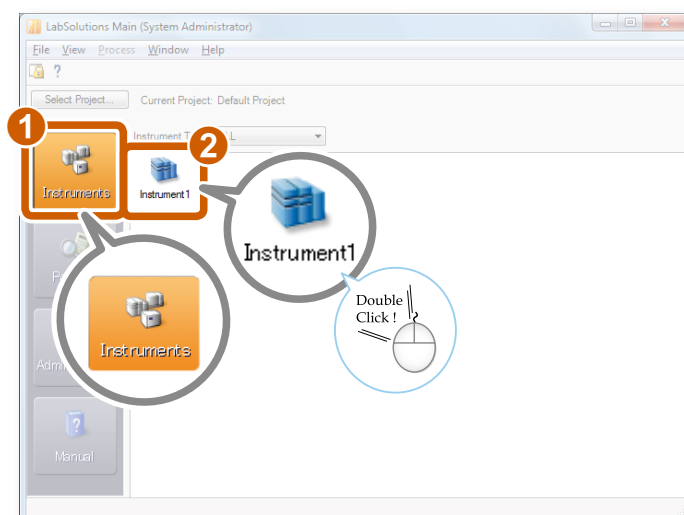


 **Hint** The [Select Project] window is also displayed when logging in for the first time using a newly created user.




Reference Refer to "System Management" in the *Operators Guide* for details on creating users.

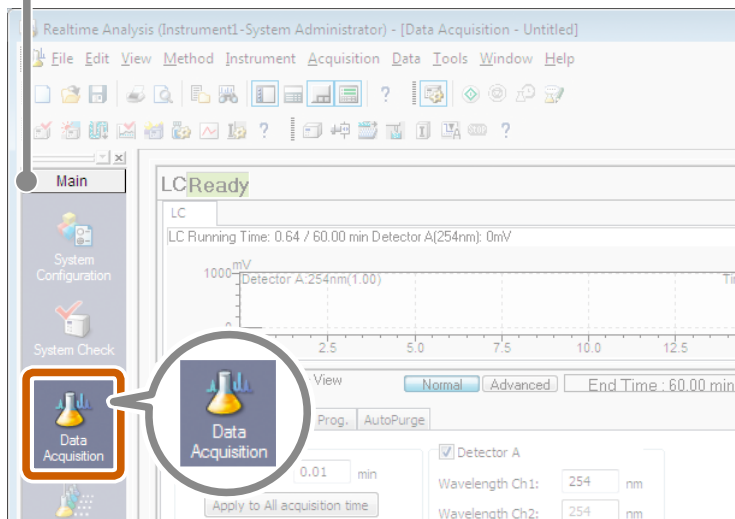
7 Open the [Realtime Analysis] program.



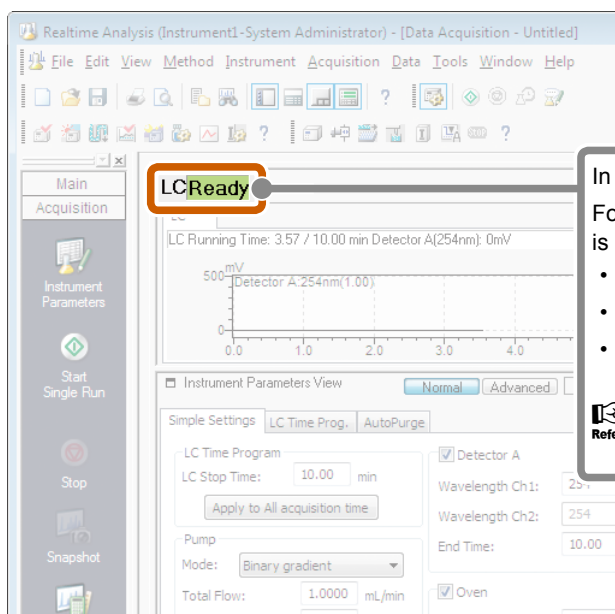
Continued on the following page 

8 Open the [Data Acquisition] window.

 **Hint** Click here if the [Main] assistant bar is not displayed.



9 Confirm the status.



In a normal state, [Ready] is displayed for the status. Follow the recommendations below if [Not Connected] is displayed.

- Ensure that the power is ON.
- Ensure that instruments are connected correctly.
- Ensure that the system configuration settings are correct.



Reference [Re-Set the System Configuration] P.15 for details.

LabSolutions



"I want to connect to the system."

"I want to change the system configuration."

In such cases

Re-Set the System Configuration.

1

Open the [System Configuration] sub-window.

Hint Click here if the [Main] assistant bar is not displayed.

The screenshot shows the LabSolutions software interface. The main window is titled "Realtime Analysis (Instrument1 - System Administrator) - [Data Acquisition - Untitled]". The left sidebar contains several buttons: "Main", "System Configuration" (highlighted with a red box), "System Check", "Data Acquisition", "Realtime Batch", "Report Format", "Calibration Curve", "Batch Edit", and "Acquisition". A callout bubble points to the "System Configuration" button in the main window area. The main window displays "LCReady" status, a chromatogram plot, and various system settings like "LC Time Program", "Pump", and "Oven".

Item	Val	Se	Un
Wav	25	25	nm
Wav			nm
Mod	Iso	Iso	
Total	0.0	0.0	mL
B.Co	0.0	0.0	%
Pum	0.0	0.0	mL
Pum	0.0	0.0	mL
Pum	0.0		MP
Pum	0.0		MP
Pum	0		kP
Pum	0		kP
Oven	0.0	40	C
Tem	90	90	C
Val			
Inject			uL

The [System Configuration] sub-window opens.

2 Open the [Data Acquisition] window.

1 Double Click!

The [Instrument] sub-window opens.

Select the system controller to use.

Click [Settings...]

2

3

4 Select [RS-232C] or [Ethernet]. For an [Ethernet] connection, enter [IP Address].

5

Click here to display each instrument currently connected to the system controller at [Modules Used for Analysis] in the [System Configuration] sub-window.

Hint When using a photodiode array (PDA) detector, select the desired detector in the [Model] list on the [PDA] row, and select [SCSI Port] or [IP Address] at [Communication Settings].

Instrument	Model	Communication	Settings
LC	CBM-40Lite	Ethernet	192.168.200.99
LHS	None	None	None
PDA	None	None	None
ELSD	None	None	None
MWD	None	None	None
ADC	None	None	None

3 Check that the system configuration is correct.

1

Double-click the unit, and set the properties of each unit.

2

Click here to send the settings to the LC.

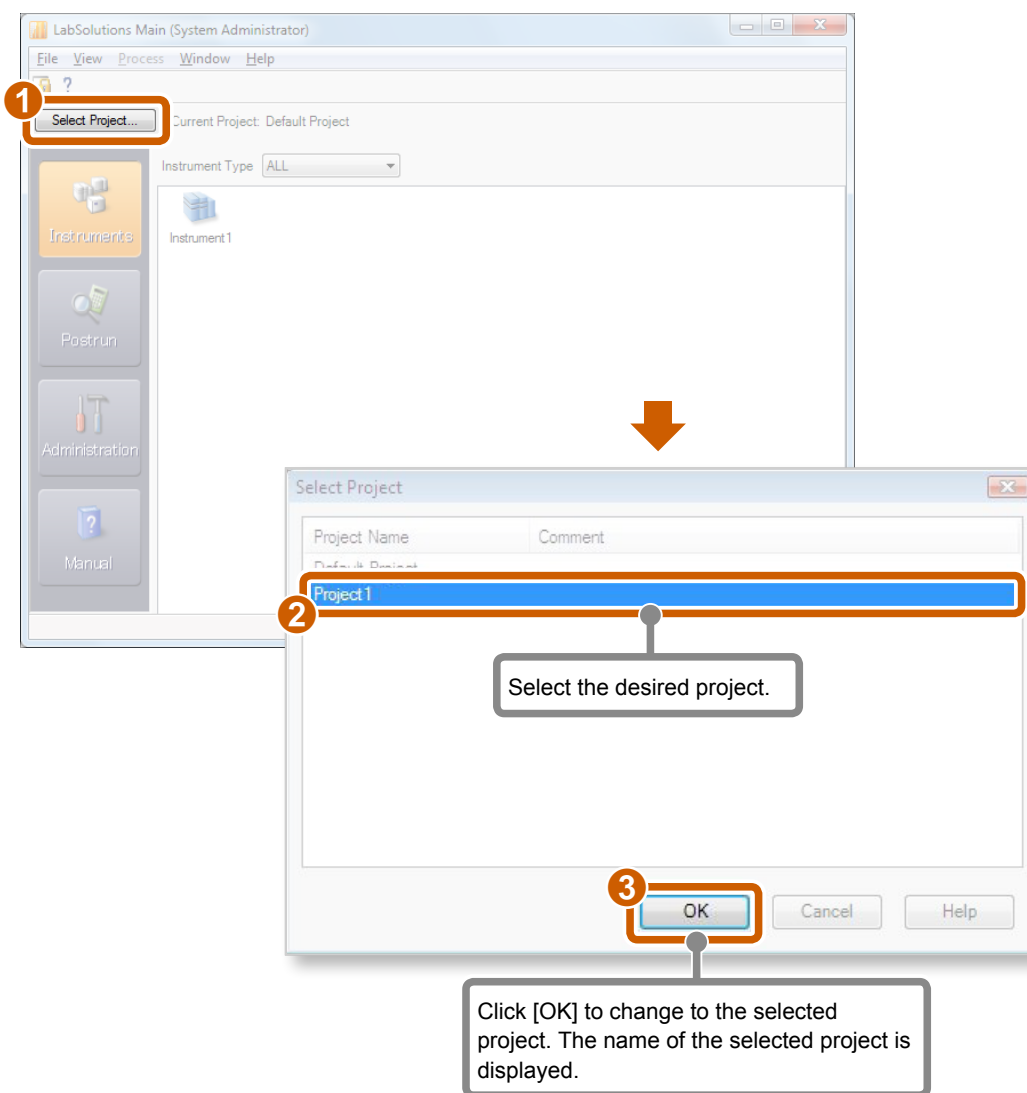
LabSolutions



"I want to change to another project."

In such cases

Click [Select Project].



Chapter 2

Set the Instrument Parameters

The data acquisition method (instrument parameters) are saved to the method file after they have been set in [Instrument Parameters View] in the [Data Acquisition] window. This chapter explains how to set the instrument parameters.

1 Open the [Data Acquisition] window.

2 Set each of the parameters on the [Simple Settings] tab.

Realtime Analysis (Instrument1-System Administrator) - [Data Acquisition - Untitled]

File Edit View Method Instrument Acquisition Data Tools Window Help

Main Acquisition

Instrument Parameters

Start Single Run

Stop

Snapshot

Data Analysis

LCReady

LC

LC Running Time: 3.57 / 10.00 min Detector A(254nm): 0mV

500 mV

Time

Max Intensity : 0

LC Stop Time : 10.00 min

1 Normal

2 Simple Settings

3 LC Time Program

LC Stop Time: 10.00 min

4 Pump

Mode: Binary gradient

Total Flow: 1.0000 mL/min

Pump B Conc.: 45.0 %

5

6

Set [Detector A] to .

Wavelength Ch1 : 254 nm

End Time : 10.00 min

Set [Oven] to .

Temperature : 40 °C

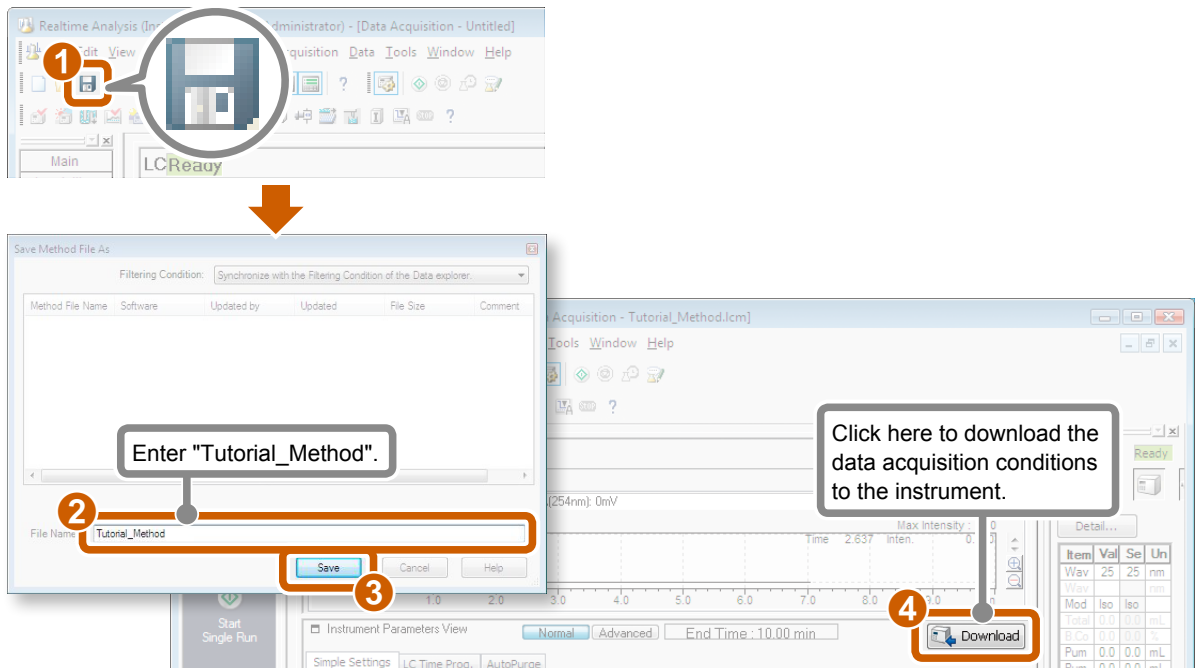
Item	Val	Se	Un
Wav	25	25	nm
Wav			nm
Mod	Iso	Iso	
Total	0.0	0.0	mL
El Co	0.0	0.0	%
Pum	0.0	0.0	mL
Pum	0.0	0.0	mL
Pum	0.0	0.0	MP
	0	0	MP
	0	0	kP
	0	40	C
	90	90	C
			uL

C: 115GB Free NUM

Reference Refer to P.6 for details on data acquisition conditions.

Reference Refer to "Set the Instrument Parameters" of the "LC Data Acquisition" chapter in the *Operators Guide* for details on instrument parameters.

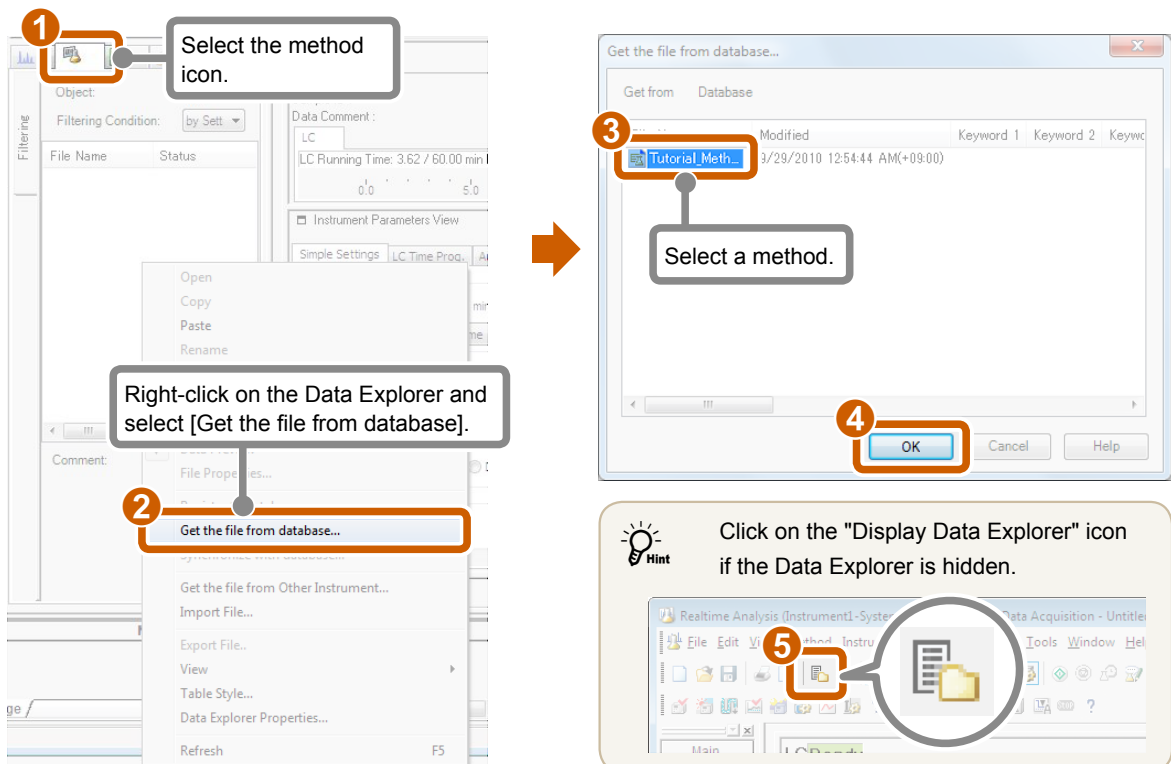
3 Save the data acquisition conditions.



LabSolutions



Retrieve a method from the database using the Data Explorer and perform analysis.



Control Panel

Using the control panel, you can edit data acquisition conditions (instrument parameters), check instrument status, and control the instrument. This section describes how to set instrument parameters using the control panel.

1 This part is called control panel. The instrument status can be checked.

2 Set data acquisition conditions (instrument parameters).

3 Click here to download the data acquisition conditions to the instrument and to close this sub-window.



Switching Display Settings

In the [Display Settings of Instrument Parameter View] sub-window, you can select displaying either the control panel or the instrument parameter view.

1 Display Settings of Instrument Parameter View...

2 Display Control Panel

3 OK

LabSolutions



Baseline Check

By the baseline check, you can check whether or not noise and drift values on the baseline are within the preset time and at the threshold or below.

Baseline check parameters are saved in the method file.

1 Set [Baseline Check Parameters].

Set both [Noise] and [Drift] to , and enter [Start], [End] and [Threshold].



In the [Baseline Check] sub-window, the noise calculation method can be changed, and the maximum delay time when the result of the baseline check is [Fail] within the preset time. [Help](#) for details.

2 Perform the baseline check.

After measurement ends, the check results are displayed in Baseline Check Results sub-window and Output Window.

Output Window

Message	Sub Message
Start the baseline check.	Detector A ASTM noise 0.00-15.00min(Criteria 50.00uV), drift 0.00-15.00min(Criteria 5000.00uV/h)
Passed the baseline check.	Pass ASTM noise : 18.36uV, drift : -0.32uV/h

Baseline Check Results

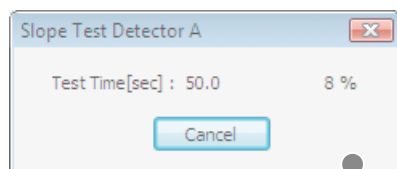
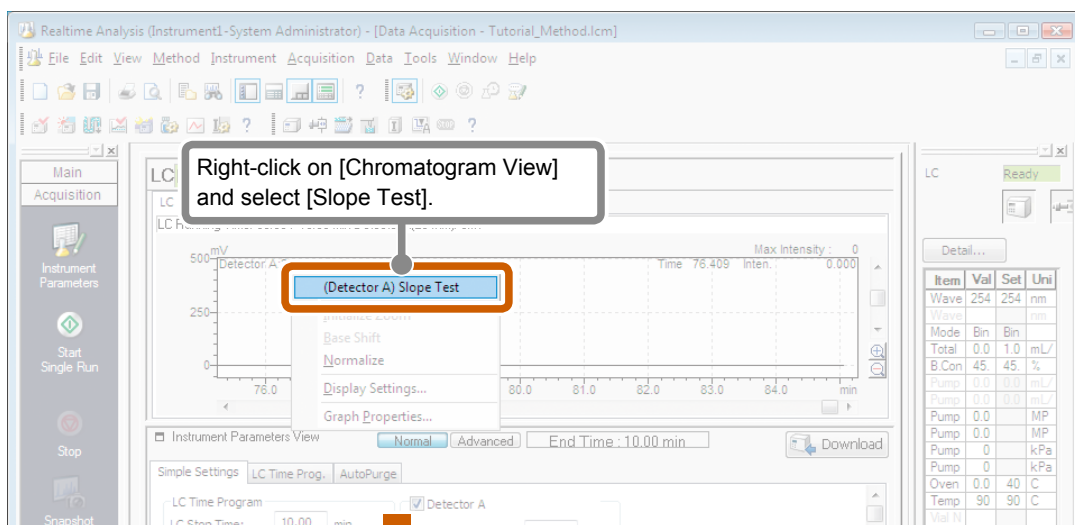
Slope Test

By performing the Slope Test, the peak detection sensitivity (Slope value) of peak integration parameters can be automatically set from the status of the noise and drift appearing on the chromatogram before data acquisition.

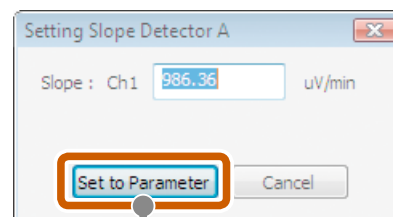
This section describes the Slope Test.



- Slope values refer to the numerical values for determining the peak start and end points. To be more precise, the peak start point is judged when an ascent slope exceeds the preset value, and, alternatively, the peak end point is judged when a descent slope falls below the preset value.
- Optimum Slope values can be obtained from the data by the Slope Test.



The measurement result is displayed when the test ends.



To apply the measurement result to the peak integration parameters, click here.



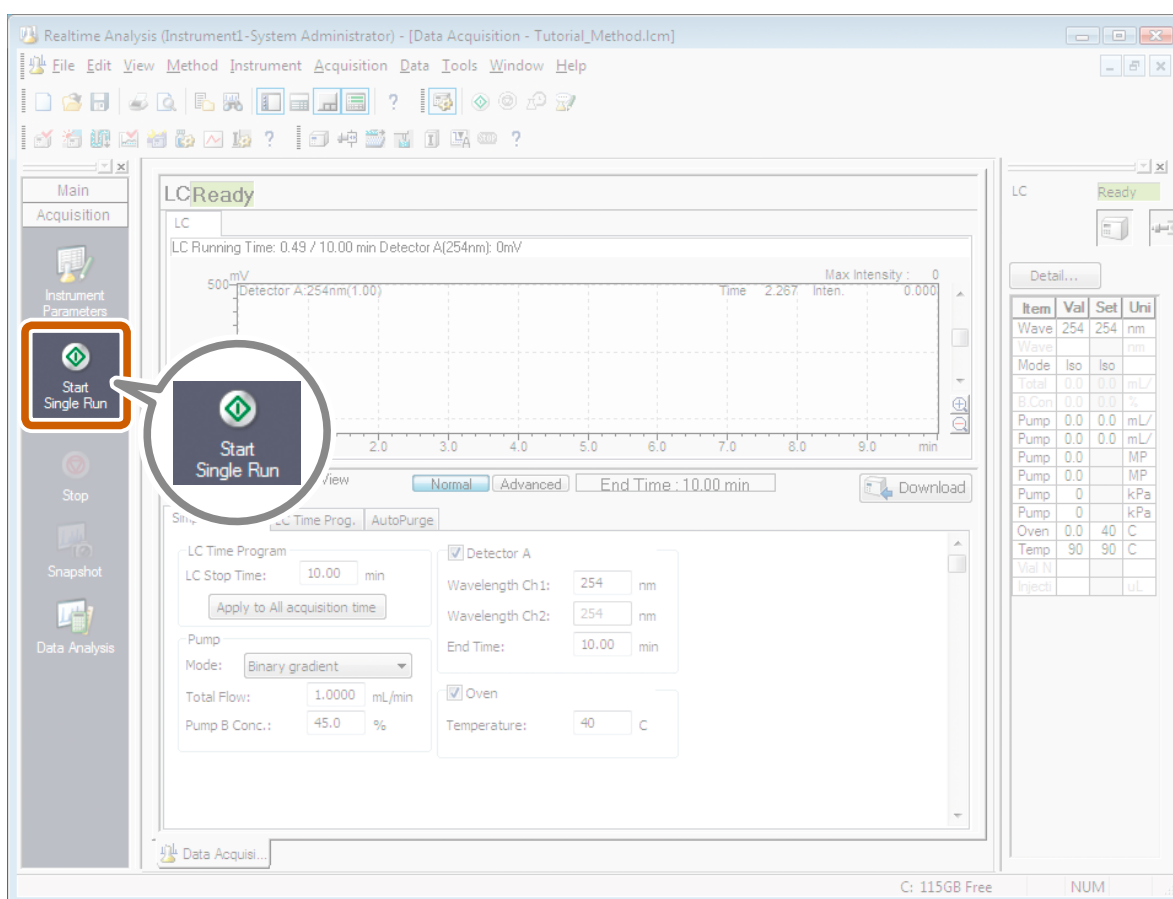
To make preset values clearer, set a value rounded up to the nearest integer larger than the displayed slope value. For example, set "1000" for "986.36".

Chapter 3 Single Run

This chapter describes the operation of measuring a standard sample once only (single run) using a saved method file "Tutorial_Method.lcm".
First, perform single run using a standard sample.

1 Open the [Data Acquisition] window.

2 Open the [Single Run] sub-window.



The [Single Run] sub-window opens.

3

Set the conditions for a single run.

In this example, set the conditions for pouring 10 ppm of paraben mixed sample into vial No.1 on the autosampler, and injecting 10 μL of that sample.

The 'Single Run' dialog box is shown with the following settings and annotations:

- Acquisition Information:** Sample Name: Paraben Mixture, Sample ID: (empty), Method File: Tutorial_Method.lcm.
- Data File:** Create into: Test (highlighted with a red box and '1', with a callout 'Enter "Test"'). Auto-Increment: 1, 2, ...
- Sampler:** Vial#: 1, Tray: 1, Injection Volume: 10 μL (highlighted with a red box and '2').
- Buttons:** OK (highlighted with a red box and '3', with a callout 'Click here to start the acquisition.'), Cancel, Help.

Hint Data acquisition automatically ends when the [LC Stop Time] set in the method file is exceeded.

The status changes to **Ready** when data acquisition ends.

The Realtime Analysis software interface shows the status 'LCRunning' in a red box. A callout points to the 'Stop' button in the 'Start Single Run' section, with a callout 'Click here to cancel data acquisition midway.'

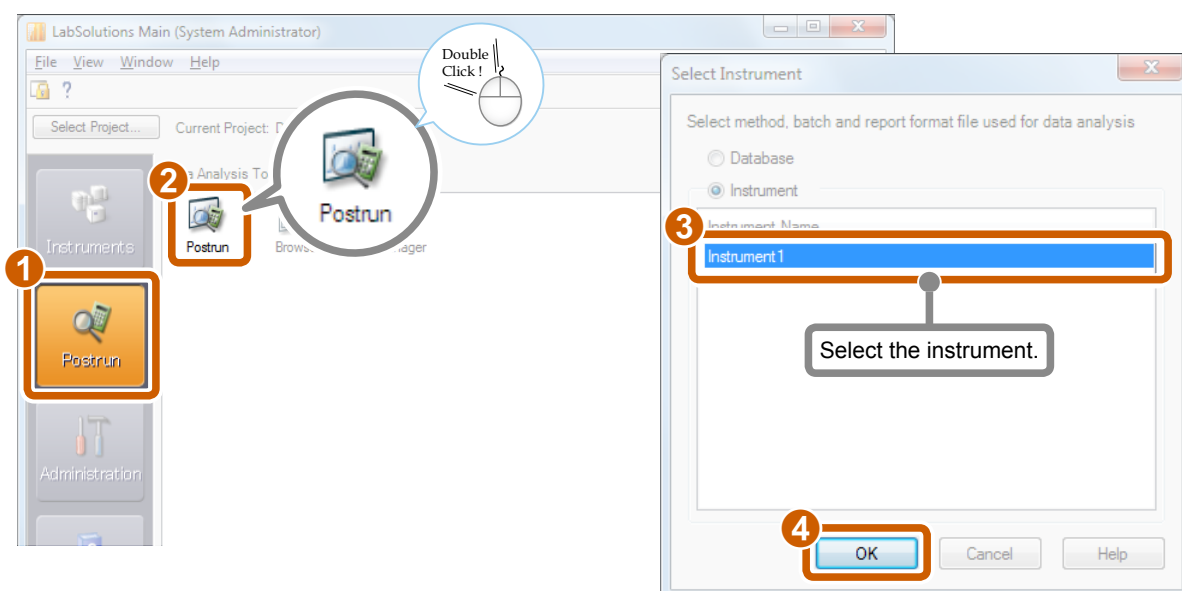


The Realtime Analysis software interface shows the status 'LCReady' in a green box. The 'Start Single Run' button is now green, indicating the system is ready for the next run.

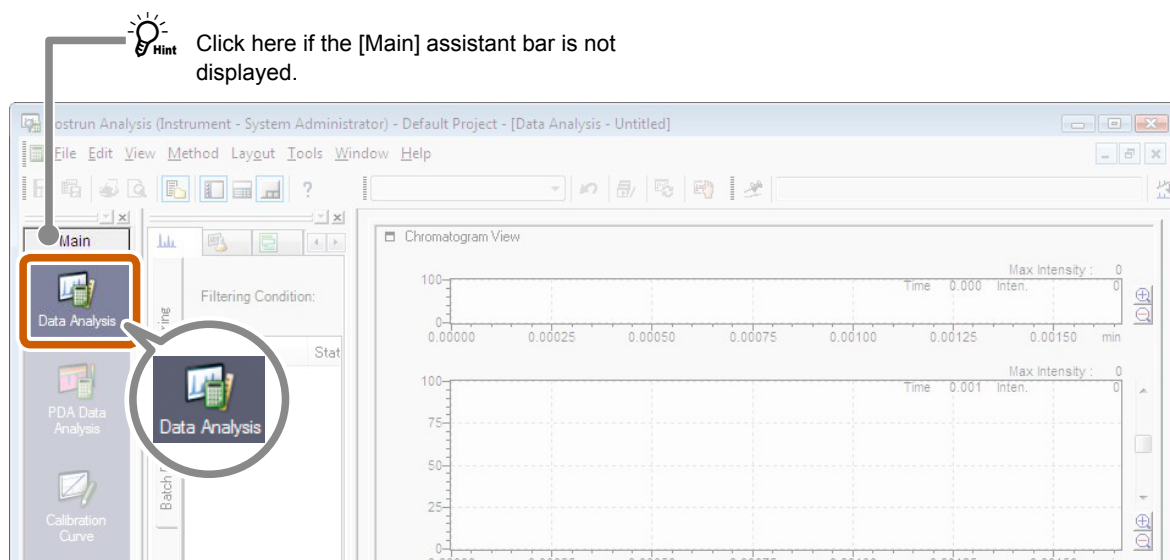
Chapter 4 Data Analysis

After single run ends, check the data to see if the peaks have been detected correctly. This chapter describes how to change the peak integration conditions of the data file "Test.lcd" obtained by performing single run to optimize the peak integration parameters.

1 Open the [Postrun Analysis] program.




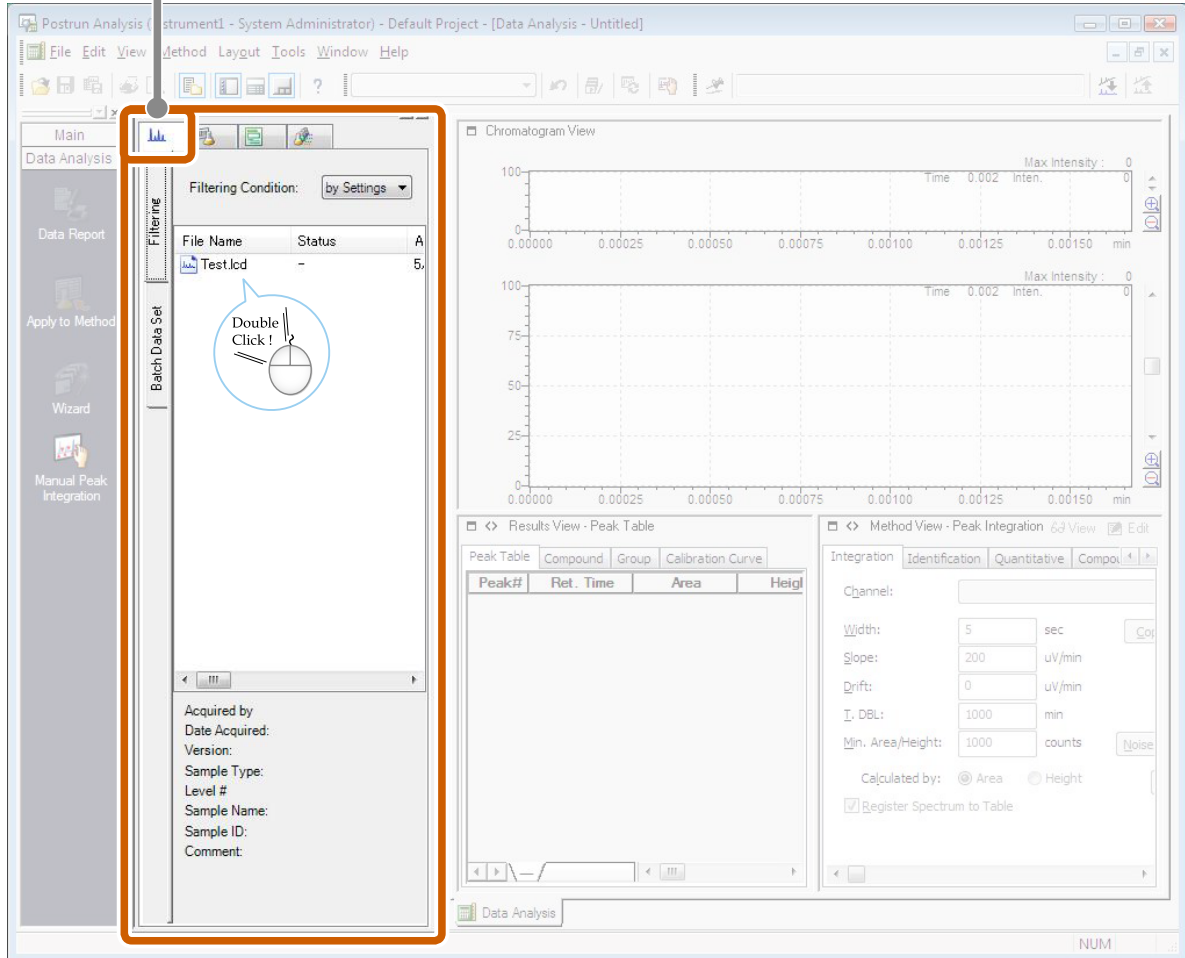
2 Open the [Data Analysis] window.



The [Data Analysis] window opens.


3 Display "Test.lcd".

Click  on the upper section of the Data Explorer and then double-click "Test.lcd".



The screenshot shows the 'Data Analysis' window with the following components:

- Data Explorer (left):** A table with columns 'File Name' and 'Status'. It contains one row: 'Test.lcd' with status '5.'. A callout bubble with a double-click icon and the text 'Double Click!' points to this row.
- Chromatogram View (top right):** Two plots showing intensity vs. time (min). The x-axis ranges from 0.00000 to 0.00150. The y-axis ranges from 0 to 100. The plots are currently empty.
- Results View - Peak Table (bottom left):** A table with columns: Peak#, Ret. Time, Area, Heigl.
- Method View - Peak Integration (bottom right):** A panel with various settings: Channel, Width (5 sec), Slope (200 uV/min), Drift (0 uV/min), T. DBL (1000 min), Min. Area/Height (1000 counts). It also has radio buttons for 'Area' and 'Height' and a checkbox for 'Register Spectrum to Table'.

 **Reference** Refer to "Data Analysis" chapter in *Operators Guide* for details on the "Data Analysis" window.

Continued on the following page 

4 Enter the peak integration parameters.

Click **Edit** to edit each parameter value.

Click **View** to perform processing on the data, and the processing results are displayed in [Chromatogram View] and [Results View - Peak Table].

Peak#	Ret. Time	Area	Height	Mark
1	1.657	4782	332	
2	3.046	582518	107698	
3	3.924	524530	81818	
4	5.505	527123	63083	
5	8.267	494019	41447	
Total		2132972	294378	

Integration

Width: 5 sec

Slope: 1000 uV/min

Width : 5 sec



Width values refer to the minimum half-width value (height 1/2 width) of the peak to detect.

Noise peaks are removed by optimizing the Width value.

Determine the start and end points of the peak by the Slope value.

The positions where the absolute values of the baseline slope become these values are the start and end points of the peak.



Reference

Refer to "Peak Integration Parameters" of the "Data Analysis" chapter in *Operators Guide* for details on the Peak Integration Parameters.

5 Enter the quantitative parameters.

Chromatogram View

Peak Table

Peak#	Ret. Time	Area	Height	Max
1	1.857	2792	332	
2	2.044	522518	107698	
3	3.924	524530	81818	
4	6.505	527123	63883	
5	8.257	494018	41447	
Total		2132972	294378	

Method View - Quantitative Parameters

Hint Click to enlarge the window.

Method View - Quantitative Parameters

1. View/Edit buttons

2. Quantitative Parameters tab

3. Quantitative Method: External Standard

4. Calibration Curve: # of Calib. Levels: 3

5. X Axis of Calib. Curve: Conc.

- Hint
- The [External Standard] method involves calculating concentrations from the peak area (height) of unknown samples using a calibration curve made based on a standard sample.
 - At [# of Calib. Levels], set the number of concentration points for the standard sample required for creating the calibration curve.
 - When creating calibration curves with the least squares method, set [X Axis of Calib. Curve] to [Conc.].

Continued on the following page

6 Fill in the Compound Table.

The screenshot shows the software interface with two main windows. The top window is 'Chromatogram View' showing two chromatograms. The bottom window is 'Method View - Compound Table' which contains a table with columns: ID#, Name, Type, Channel, Ret. Time, Conc.(1), Conc.(2), and Conc.(3). A magnifying glass labeled 'ZOOM UP' is positioned over the table.

Peak#	Ret. Time	Area	Height
1	3.046	502878	107638
2	3.924	524530	81818
3	5.505	527123	63063
4	8.267	484019	41447
Total		2132872	284378

This section provides a detailed view of the 'Method View - Compound Table'. Callout 1 points to the 'Compound' column header. Callout 2 points to the table rows. Callout 3 points to the 'View' button. A zoomed-in table below shows the data for the first four rows.

ID#	Name	Type	Channel	Ret. Time	Conc.(1)	Conc.(2)	Conc.(3)
1	Methylparaben	Target	Detector A - C	3.046	10.000	20.000	40.000
2	Ethylparaben	Target	Detector A - C	3.924	10.000	20.000	40.000
3	Propylparaben	Target	Detector A - C	5.505	10.000	20.000	40.000
4	Butylparaben	Target	Detector A - C	8.267	10.000	20.000	40.000

Click View to change the cell background color to yellow to fix the newly edited parameters.



- The result obtained by performing data acquisition is used for [Ret. Time].
- Selecting the [Ret. Time] cell, and clicking the peak in [Chromatogram View] automatically enters the retention time of that peak to the currently selected [Ret. Time] cell. The retention time can be set by simply clicking the mouse.



Refer to "Compound Table Retention Times Using the Mouse" of the "Data Analysis" chapter in the *Operators Guide* for details on setting retention times.

7 Save the processing results to a data file.

Click here to save the processing results to "test.lcd".



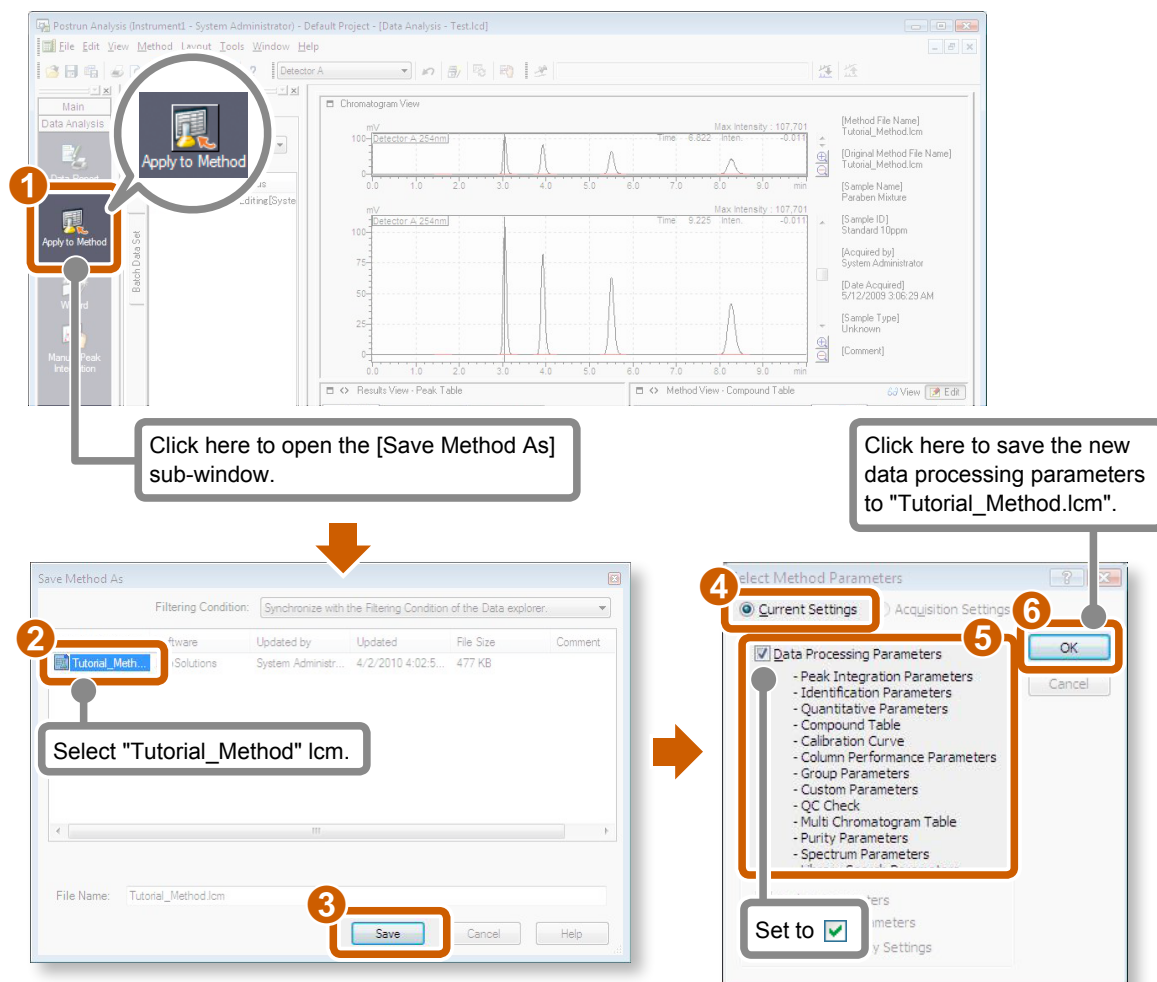
8 Save the method file.

Click here to open the [Save Method As] sub-window.


Click here to save the new data processing parameters to "Tutorial_Method.lcm".

Select "Tutorial_Method" lcm.

Set to Data Processing Parameters



To use saved data processing parameters for other data, perform either of the following operations to save the new data processing parameters to the method file (in this example, "Tutorial_Method.lcm").

- Click [Save Data and Method File] on the [File] menu.
- Click  (Apply to Method) on the [Data Analysis] assistant bar (operation in step 8 above).

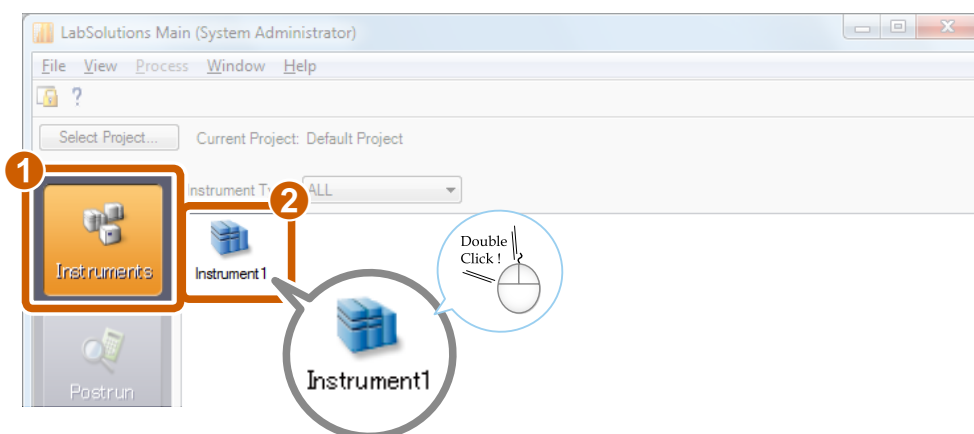
Chapter 5 Realtime Batch

To perform data acquisition continuously on multiple samples (realtime batch), a Batch Table must first be created. Batch Tables can be easily created by using the table easy setting feature of LabSolutions.

5.1 Create a Batch Table

In the following example, create a Batch Table with standard samples set to 1st to 9th rows, and unknown samples set to the 10th and 11th rows.

1 Open the [Realtime Analysis] program.



2 Open the [Realtime Batch] window.



The [Realtime Batch] window opens.

3 Edit the Batch Table.

1 Table Easy Settings...

2 Select [New].

3 Set [Standard] to .

Vial# : 1 to 3
Injection Volume : 10 µL
Repetitions : 3
Data File : Tutorial_Std

4 Set [Unknown] to .

Vial# : 4 to 5
Injection Volume : 10 µL
Data File : Tutorial_Unk

5 Click here to create a Batch Table made up of 11 rows.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Inj. Volume	I
1	1	1			1:Standard (I)	Tutorial_Method.lcm	Tutorial_Std001.lcd	1	10	
2	1	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std002.lcd	1	10	
3	1	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std003.lcd	1	10	
4	2	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std004.lcd	2	10	
5	2	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std005.lcd	2	10	
6	2	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std006.lcd	2	10	
7	3	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std007.lcd	3	10	
8	3	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std008.lcd	3	10	
9	3	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std009.lcd	3	10	
10	4	1			0:Unknown	Tutorial_Method.lcm	Tutorial_Unk001.lcd	0	10	
11	5	1			0:Unknown	Tutorial_Method.lcm	Tutorial_Unk002.lcd	0	10	

- Hint** • In Batch Tables, you can set the sample information of each sample and output of reports.
- Reference** • Refer to "Edit Batch Tables" of the "Realtime Batch" chapter, "Edit Batch Tables" of the "Calibration Curves" chapter in *Operators Guide* for details on the editing batch tables.
- Enter "-1" in [Vial#] to acquire data without injecting samples from the autosampler.

Continued on the following page

4 Copy a cell.

1 Select here.

2 Fill Down

3 9

4 Paraben Mixture

5 OK

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1	1	1	Paraben Mixture	1:Standard:()	1:Standard	Tutorial_Method.lcm	Tutorial_Std001.lcd	1
2	1	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std002.lcd	1
3	1	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std003.lcd	1
4	2	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std004.lcd	2
5	2	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std005.lcd	2
6	2	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std006.lcd	2
7	3	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std007.lcd	3
8	3	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std008.lcd	3
9	3	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std009.lcd	3
10	4	1	Sample A	0:Unknown	0:Unknown	Tutorial_Method.lcm	Tutorial_Unk001.lcd	0
11	5	1	Sample B	0:Unknown	0:Unknown	Tutorial_Method.lcm	Tutorial_Unk002.lcd	0

5 Enter a numbered series.

1 Select here.

2 Fill Series

3 11

4 Unknown01

5 OK

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1	1	1	Paraben Mixture	1:Standard:()	1:Standard	Tutorial_Method.lcm	Tutorial_Std001.lcd	1
2	1	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std002.lcd	1
3	1	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std003.lcd	1
4	2	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std004.lcd	2
5	2	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std005.lcd	2
6	2	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std006.lcd	2
7	3	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std007.lcd	3
8	3	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std008.lcd	3
9	3	1	Paraben Mixture	1:Standard	1:Standard	Tutorial_Method.lcm	Tutorial_Std009.lcd	3
10	4	1	Sample A	Unknown01	Unknown	Tutorial_Method.lcm	Tutorial_Unk001.lcd	0
11	5	1	Sample B	Unknown02	Unknown	Tutorial_Method.lcm	Tutorial_Unk002.lcd	0

6

Directly enter remaining items to the Batch Table to create the Batch Table shown below.

Folder: C:\LabSolutions\Sample\LC

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1	1	1	Paraben Mixture	Standard 10ppm	1:Standard.()	Tutorial_Method.lcm	Tutorial_Std001.lcd	1
2	1	1	Paraben Mixture	Standard 10ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std002.lcd	1
3	1	1	Paraben Mixture	Standard 10ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std003.lcd	1
4	2	1	Paraben Mixture	Standard 20ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std004.lcd	2
5	2	1	Paraben Mixture	Standard 20ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std005.lcd	2
6	2	1	Paraben Mixture	Standard 20ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std006.lcd	2
7	3	1	Paraben Mixture	Standard 40ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std007.lcd	3
8	3	1	Paraben Mixture	Standard 40ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std008.lcd	3
9	3	1	Paraben Mixture	Standard 40ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std009.lcd	3
10	4	1	Sample A	Unknown01	0:Unknown	Tutorial_Method.lcm	Tutorial_Unk001.lcd	0
11	5	1	Sample B	Unknown02	0:Unknown	Tutorial_Method.lcm	Tutorial_Unk002.lcd	0

7

Save the batch file.

1

2

3

Enter "Tutorial_Batch".

File Name: Tutorial_Batch

Save Cancel Help

LabSolutions



Create a Batch Table Using Quick Batch

You can also create a Batch Table using quick batch.

1 Quick Batch... F6

2 Enter the sample information.

3 Select a sample type and vials.

4 Add Batch Table

5 Start

Click here to add them to a Batch Table. With the settings shown in this figure, a Batch Table for the standard sample is created. Also, for the unknown sample, perform the procedures (2) and (3) shown in this figure to add them to the Batch Table.

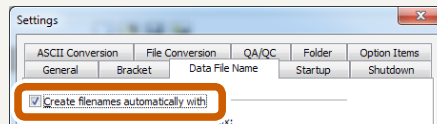
Editor	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Inj. Volume	Report Output
1	1	1	Paraben Mixture	Standard 10pp	1 Standard (I)	LC:Tutorial_Method.Icm	(Auto Filename)	1	10	<input checked="" type="checkbox"/>
2	1	1	Paraben Mixture	Standard 10pp	1 Standard	LC:Tutorial_Method.Icm	(Auto Filename)	1	10	<input checked="" type="checkbox"/>
3	1	1	Paraben Mixture	Standard 10pp	1 Standard (I)	LC:Tutorial_Method.Icm	(Auto Filename)	1	10	<input checked="" type="checkbox"/>
4	2	1	Paraben Mixture	Standard 20pp	1 Standard (I)	LC:Tutorial_Method.Icm	(Auto Filename)	2	10	<input checked="" type="checkbox"/>
5	2	1	Paraben Mixture	Standard 20pp	1 Standard	LC:Tutorial_Method.Icm	(Auto Filename)	2	10	<input checked="" type="checkbox"/>
6	2	1	Paraben Mixture	Standard 20pp	1 Standard (I)	LC:Tutorial_Method.Icm	(Auto Filename)	2	10	<input checked="" type="checkbox"/>
7	3	1	Paraben Mixture	Standard 40pp	1 Standard (I)	LC:Tutorial_Method.Icm	(Auto Filename)	3	10	<input checked="" type="checkbox"/>
8	3	1	Paraben Mixture	Standard 40pp	1 Standard	LC:Tutorial_Method.Icm	(Auto Filename)	3	10	<input checked="" type="checkbox"/>
9	3	1	Paraben Mixture	Standard 40pp	1 Standard (I)	LC:Tutorial_Method.Icm	(Auto Filename)	3	10	<input checked="" type="checkbox"/>
10	4	1	Sample A	Unknown01	0 Unknown	LC:Tutorial_Method.Icm	(Auto Filename)	0	10	<input checked="" type="checkbox"/>
11	5	1	Sample B	Unknown02	0 Unknown	LC:Tutorial_Method.Icm	(Auto Filename)	0	10	<input checked="" type="checkbox"/>



Reference Refer to Help for details on operations and the applicable models.



Hint When [(Auto Filename)] is displayed in the [Data File Name] field, you cannot directly enter a data file name. To enter a data file name directly, click [Settings] in the [Quick Batch] sub-window. On the [Data File Name] tab page in the displayed [Settings] sub-window, clear the [Create filenames automatically] checkbox.



5.2 Realtime Batch Processing

Execute realtime batch using the Batch Table you created.

1 Place the samples in the autosampler.

Vial 1 (level 1)	Paraben mixed sample	10 ppm solution (standard solution)
Vial 2 (level 2)	Paraben mixed sample	20 ppm solution (standard solution)
Vial 3 (level 3)	Paraben mixed sample	40 ppm solution (standard solution)
Vial 4	Unknown sample (to be quantitated)	
Vial 5	Unknown sample (to be quantitated)	

2 Start realtime batch processing.

Click here to open the [Realtime Batch] and [Data Acquisition] windows simultaneously, and starts data acquisition from the 1st row of the Batch Table.

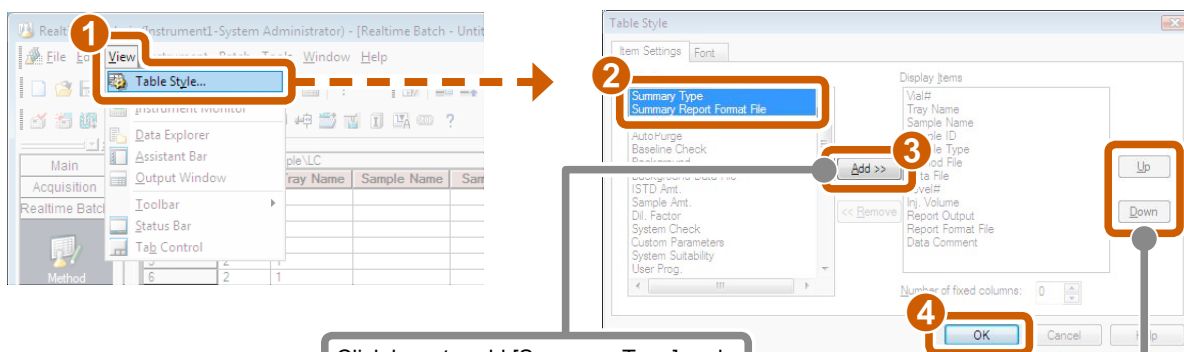
Click here to cancel data acquisition midway. To edit the content of the Batch Table during realtime batch, click to pause realtime batch.

LabSolutions



Print a Summary Report

1 Add items to display in the Batch Table.

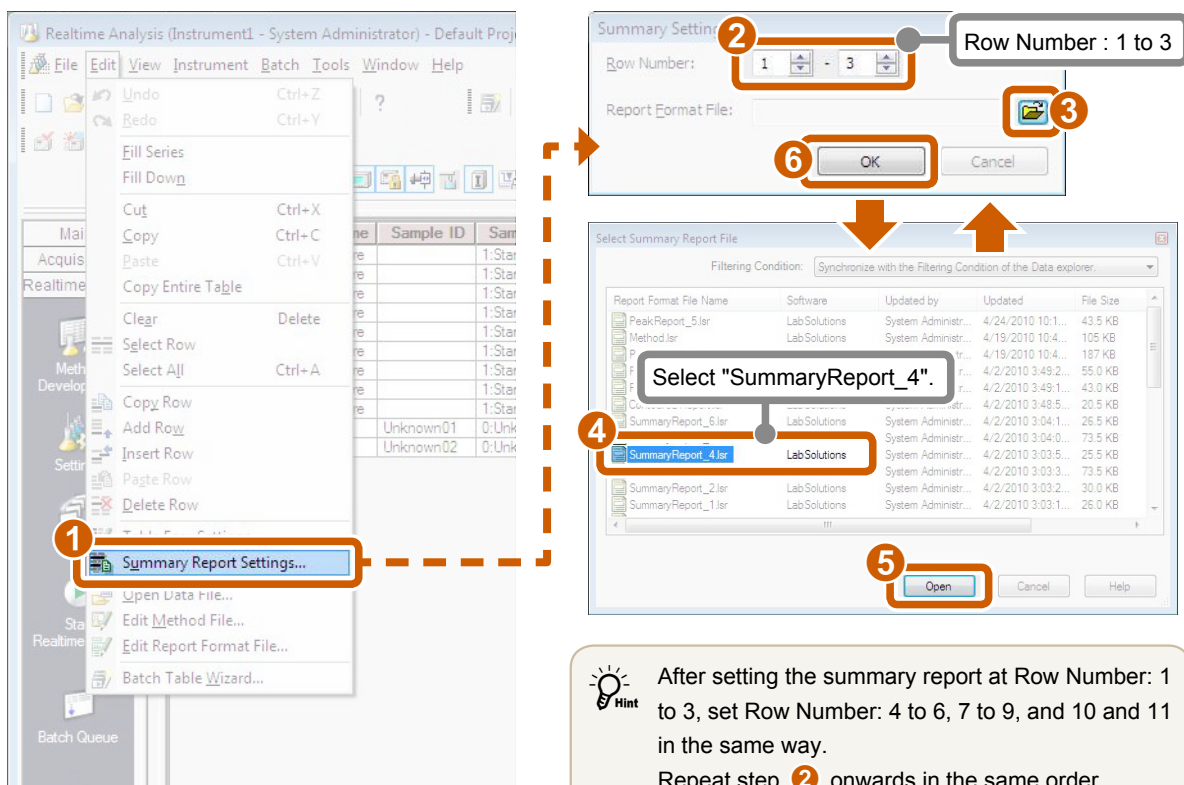


Click here to add [Summary Type] and [Summary Report Format File] to the items to display in the Batch Table.



The order of display items in the Batch Table can be changed by clicking [Up] or [Down].

2 Set up the summary report.



After setting the summary report at Row Number: 1 to 3, set Row Number: 4 to 6, 7 to 9, and 10 and 11 in the same way. Repeat step 2 onwards in the same order.

Continued on the following page

3

Check the output configuration of the summary report.

Analysis	Vial#	Tray Name	Sample Name	Summary Type	Summary Report Format File	Sample ID	Sample Type	Method File	Data File
1	1	1	Paraben Mixtu	Summary Start	SummaryReport_4.lsr		1:Standard:(I)	Tutorial_Method.lcm	Tutorial_Std001.lcd
2 >>	1	1	Paraben Mixtu	Summary Run			1:Standard	Tutorial_Method.lcm	Tutorial_Std002.lcd
3	1	1	Paraben Mixtu	Summary End			1:Standard	Tutorial_Method.lcm	Tutorial_Std003.lcd
4	2	1	Paraben Mixtu	Summary Start	SummaryReport_4.lsr		1:Standard	Tutorial_Method.lcm	Tutorial_Std004.lcd
5	2	1	Paraben Mixtu	Summary Run			1:Standard	Tutorial_Method.lcm	Tutorial_Std005.lcd
6	2	1	Paraben Mixtu	Summary End			1:Standard	Tutorial_Method.lcm	Tutorial_Std006.lcd
7	3	1	Paraben Mixtu	Summary Start	SummaryReport_4.lsr		1:Standard	Tutorial_Method.lcm	Tutorial_Std007.lcd
8	3	1	Paraben Mixtu	Summary Run			1:Standard	Tutorial_Method.lcm	Tutorial_Std008.lcd
9	3	1	Paraben Mixtu	Summary End			1:Standard	Tutorial_Method.lcm	Tutorial_Std009.lcd
10	4	1	Sample A	Summary Start	SummaryReport_1.lsr	known01	0:Unknown	Tutorial_Method.lcm	Tutorial_Unk001.lcd
11	5	1	Sample B	Summary End		known02	0:Unknown	Tutorial_Method.lcm	Tutorial_Unk002.lcd

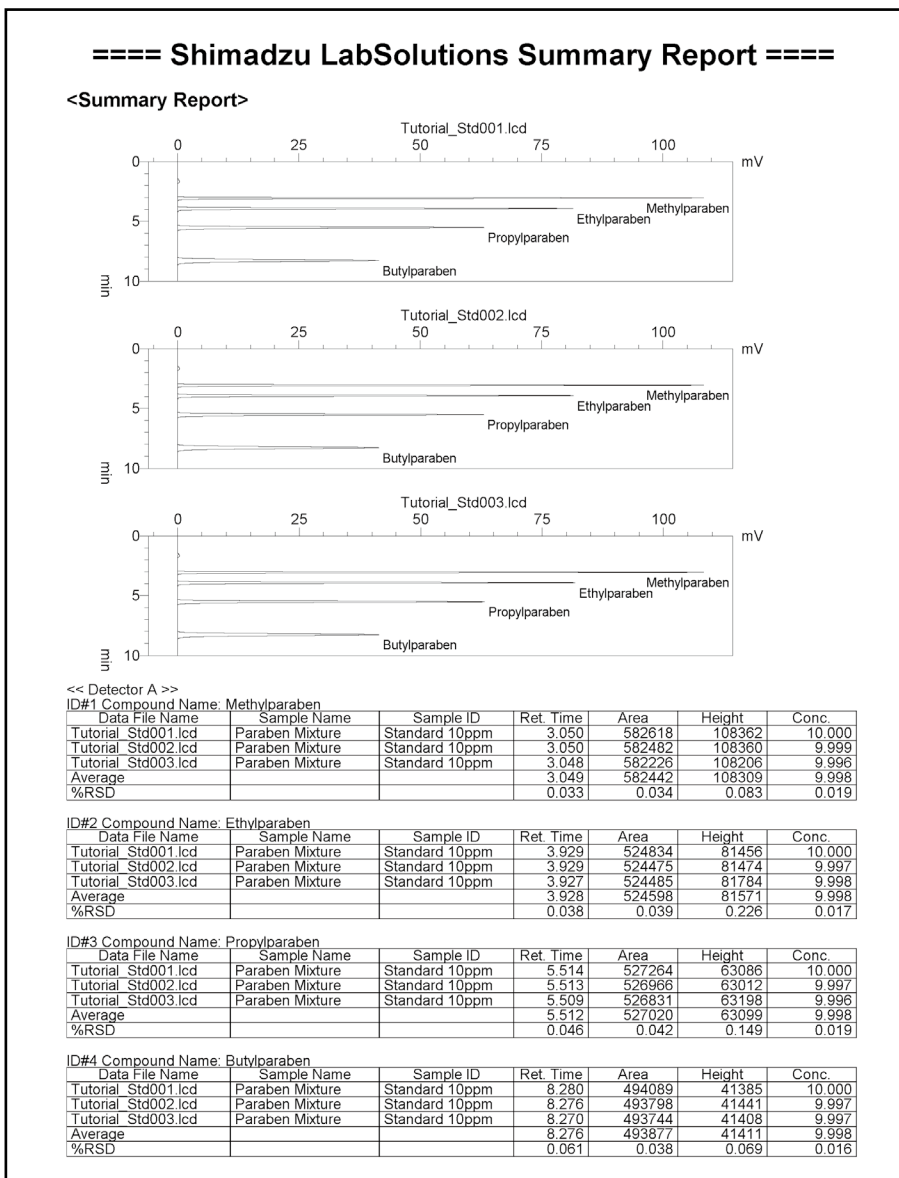
When you have finished the output configuration of the summary report, execute realtime batch to print the summary report.



Refer to "5.2 Realtime Batch Processing" P.36 for details on executing realtime batch.

[Printout Example]

Standard samples

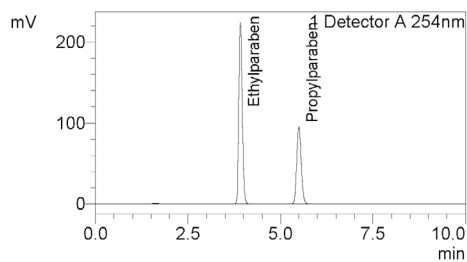


Unknown samples

==== Shimadzu LabSolutions Summary Report ====

Sample Name : Sample A
 Sample ID : Unknown01
 Data Filename : Tutorial_Unk001.lcd
 Method Filename : Tutorial_Method.lcm
 Batch Filename : Tutorial_Batch.lcb
 Vial # : 1-4
 Injection Volume : 10 uL
 Date Acquired : 5/12/2009 4:54:52 AM
 Date Processed : 7/13/2010 3:45:30 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator

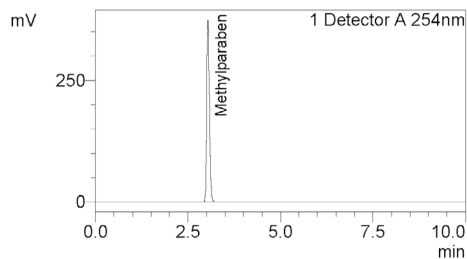


Peak#	Ret. Time	Area	Height	ID#
1	1.630	7980	521	
2	2.048	2420	262	
3	3.925	1431436	224742	2
4	5.503	790700	95203	3
Total		2232536	320730	

ID#	Name	Conc.	Unit
1	Methylparaben	--	mg/L
2	Ethylparaben	27.361	mg/L
3	Propylparaben	14.965	mg/L
4	Butylparaben	--	mg/L

Sample Name : Sample B
 Sample ID : Unknown02
 Data Filename : Tutorial_Unk002.lcd
 Method Filename : Tutorial_Method.lcm
 Batch Filename : Tutorial_Batch.lcb
 Vial # : 1-5
 Injection Volume : 10 uL
 Date Acquired : 5/12/2009 5:05:26 AM
 Date Processed : 7/13/2010 3:45:32 PM

Sample Type : Unknown
 Acquired by : System Administrator
 Processed by : System Administrator



Peak#	Ret. Time	Area	Height	ID#
1	1.609	9804	599	
2	2.098	6145	476	
3	3.046	1940550	373550	1
Total		1956500	374624	

ID#	Name	Conc.	Unit
1	Methylparaben	33.449	mg/L
2	Ethylparaben	--	mg/L
3	Propylparaben	--	mg/L
4	Butylparaben	--	mg/L

Chapter 6

Multiple Data Analysis

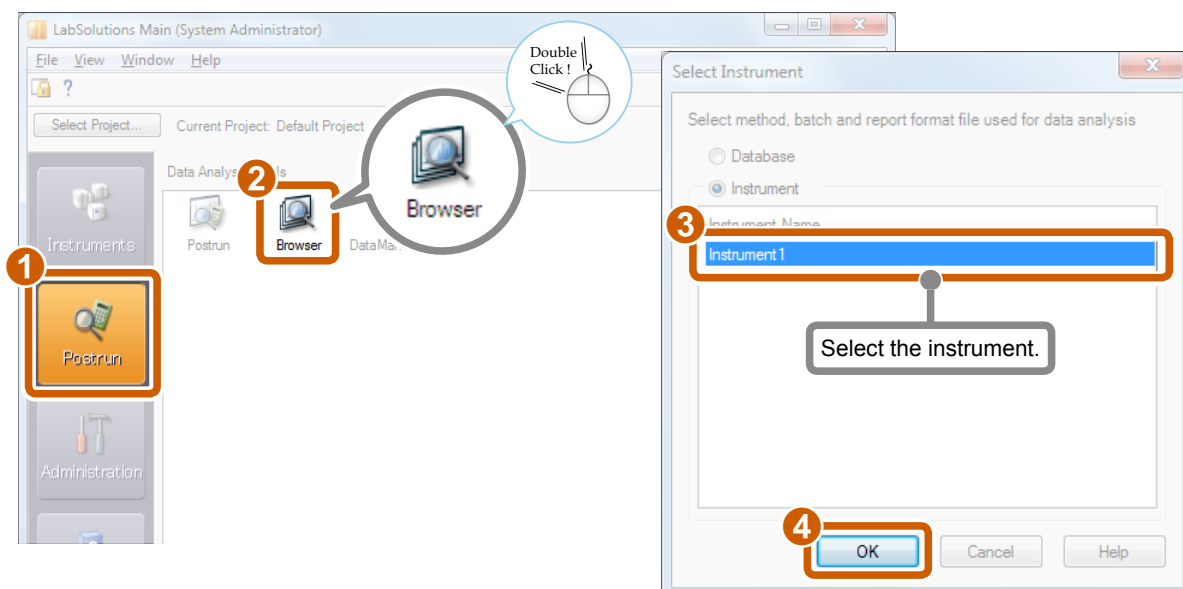
The LabSolutions [Browser] program is handy for checking the quantitative calculation results and chromatograms of multiple data.

In the [Quant Browser] window of the [Browser] program, you can check multiple data, and change the data processing parameters of the currently displayed method file to modify calibration curves and perform postrun batch on multiple data.

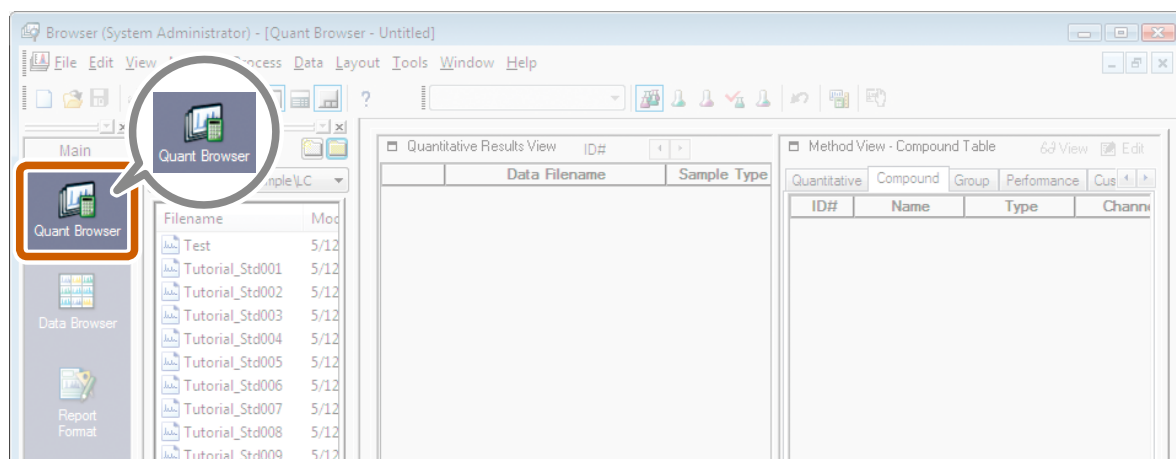


Reference Refer to "Quant Browser" chapter in *Operators Guide* for details on the "Quant Browser" window.

1 Open the [Browser] program.



2 Open the [Quant Browser] window.



Open the [Quant Browser] window.

3 Load the batch file.

1

2

Drag and drop this file to display the quantitative results data.

Quantitative Results View

Data Filename	Sample Type	Level#	Res
---------------	-------------	--------	-----

Method View - Compound Table

Integration	Identification	Quantitative	Compound	Group	Performance
ID#	Name	Type	Channel	ISTD Group	

Chromatogram View

Chromatogram | Sample Info

Time: 0.001 Inten. Max Intensity: 0

Calibration Curve/Spectrum View

Calb Curve | Spectrum

Continued on the following page 

4 Confirm the quantitative results.

The screenshot displays a software interface for chromatography data analysis. A table in the center lists data files and their corresponding sample types and levels. Below the table, a chromatogram shows detector response over time with several peaks. To the right, a calibration curve plot shows the relationship between peak area and concentration.

	Data Filename	Sample Type	Level#	Rt
1	Tutorial_Std001.lcd	Standard/Calc. Poi	1	
2	Tutorial_Std002.lcd	Standard/Calc. Poi	1	
3	Tutorial_Std003.lcd	Standard/Calc. Poi	1	
4	Tutorial_Std004.lcd	Standard/Calc. Poi	2	
5	Tutorial_Std005.lcd	Standard/Calc. Poi	2	
6	Tutorial_Std006.lcd	Standard/Calc. Poi	2	
7	Tutorial_Std007.lcd	Standard/Calc. Poi	3	
8	Tutorial_Std008.lcd	Standard/Calc. Poi	3	
9	Tutorial_Std009.lcd	Standard/Calc. Poi	3	
10	Tutorial_Unk001.lcd	Unknown	0	
11	Tutorial_Unk002.lcd	Unknown	0	

Method View - Compound Table

Integration	Identification	Quantitative	Compound	Group	Performance
	Methylparaben	Target	Detector A - C		3.046
	Ethylparaben	Target	Detector A - C		3.924
	Propylparaben	Target	Detector A - C		5.505
	Butylparaben	Target	Detector A - C		8.267

Chromatogram View

Chromatogram: mV (Detector A: 254nm) vs Time (min). Max Intensity: 108,369 Inten.

Calibration Curve/Spectrum View

Calib Curve: $Y = 57642.98X + 12444.51$
 $R^2 = 0.9993066$ $r = 0.999533$

LabSolutions



Modify Calibration Curves

1

Confirm peak integration parameters.

Confirm the peak integration parameters when peak detection is inappropriate.

The screenshot displays the LabSolutions software interface. The main window shows a 'Quantitative Results View' with a table of data files. A 'Method View - Peak Integration Parameters' dialog box is open, showing settings for 'Detector A - Ch1(254nm)'. The parameters are:

Parameter	Value	Unit
Width	5	sec
Slope	1000	uV/min
Drift	0	uV/min
I. DBL	1000	min
Min. Area/Height	1000	counts

The 'Calculated by' option is set to 'Area'. A 'Zoom UP' callout points to the 'Program' button. A 'Click here to perform postrun batch on all data.' callout points to the 'Post Run' button. A 'Make sure that these values are appropriate.' callout points to the 'Width', 'Slope', and 'Min. Area/Height' fields. A 'Calibration Curve/Spectrum View' window is also visible, showing a linear plot with the equation $Y = 57642.99X + 12444.51$ and $r^2 = 0.9999066$.

Continued on the following page

2

Confirm identification parameters.

Confirm the identification parameters and Compound Table when peaks are not identified correctly.

The screenshot shows the 'Method View - Identification Parameters' window. A magnifying glass labeled 'ZOOM UP' points to the 'Identification' tab. A callout box with a '2' points to the 'Window/Band' settings, and another callout box with a '1' points to the 'View' and 'Edit' buttons. A third callout box with a '3' points to the 'View' and 'Edit' buttons in the 'Compound' tab. A text box says 'Make sure that these values are appropriate.' To the right, a 'Calibration Curve/Spectrum View' window shows a linear plot of Area vs. Conc. with the equation $Y = 57642.89X + 12444.51$ and $r^2 = 0.9999066$.

3

Confirm the Compound Table.

The screenshot shows the 'Method View - Compound Table' window. A magnifying glass labeled 'ZOOM UP' points to the 'Compound' tab. A callout box with a '2' points to the 'Compound' tab, and another callout box with a '1' points to the 'View' and 'Edit' buttons. A third callout box with a '4' points to the 'View' and 'Edit' buttons. A text box says 'Make sure that these values are appropriate.' To the right, a 'Calibration Curve/Spectrum View' window shows a linear plot of Area vs. Conc. with the equation $Y = 57642.89X + 12444.51$ and $r^2 = 0.9999066$.

ID#	Name	Type	Channel	Ret. Time
1	Methylparaben	Target	Detector A - C	3.046
2	Ethylparaben	Target	Detector A - C	3.924
3	Propylparaben	Target	Detector A - C	5.505
4	Butylparaben	Target	Detector A - C	8.267

4 Confirm calibration points.

ZOOM UP

Confirm the calibration curve.

1

2

Make sure that the calibration point on the 1st row is set to .

ID#	Name	Type	Channel	Ret. Time
1	Methylparaben	Target	Detector A - C	3.046
2	Ethylparaben	Target	Detector A - C	3.934
3	Propylparaben	Target	Detector A - C	5.506
4	Butylparaben	Target	Detector A - C	8.267

Data Filename	Height	Conc. (mg/L)	Std. Conc.	Area%	Height%	Accuracy	Cal. Point
Tutorial_Std001.lcd	108.362	9.891	10	27.299	36.777	100.0	<input checked="" type="checkbox"/>
Tutorial_Std002.lcd	108.360	9.889	10	27.309	36.778	100.0	<input checked="" type="checkbox"/>
Tutorial_Std003.lcd	108.206	9.885	10	27.309	36.690	98.8	<input checked="" type="checkbox"/>
Tutorial_Std004.lcd	218.591	20.172	20	27.398	36.765	100.0	<input checked="" type="checkbox"/>
Tutorial_Std005.lcd	218.192	20.168	20	27.396	36.719	100.0	<input checked="" type="checkbox"/>
Tutorial_Std006.lcd	218.269	20.162	20	27.393	36.76	100.0	<input checked="" type="checkbox"/>
Tutorial_Std007.lcd	430.746	39.955	40	27.324	36.71	100.0	<input checked="" type="checkbox"/>
Tutorial_Std008.lcd	430.983	39.933	40	27.322	36.71	100.0	<input checked="" type="checkbox"/>
Tutorial_Std009.lcd	431.190	39.944	40	27.326	36.71	100.0	<input checked="" type="checkbox"/>
Tutorial_Unk001.lcd	-----	-----	-----	-----	-----	-----	<input type="checkbox"/>
Tutorial_Unk002.lcd	373.550	33.449	-----	99.185	99.71	-----	<input type="checkbox"/>

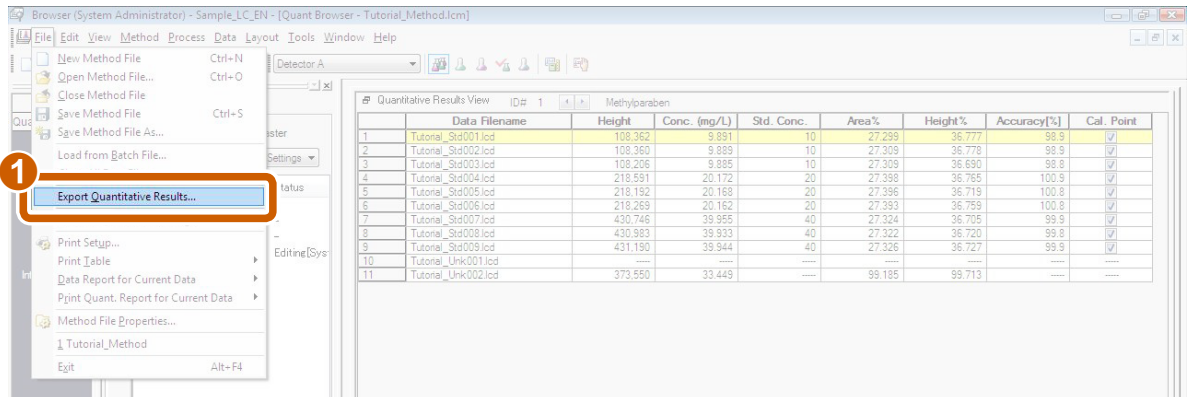
Calibration Curve: $Y = 57642.3x + 12444.51$
 $r^2 = 0.9999066$ $r = 0.9999533$

5 Save the method file and data file.

Save the method file and data file.

Export Quantitative Calculation Results

This section describes how to save quantitative calculation results as a text file.



Export to

Copy to Clipboard

Output File:

Items to Output

All Items

Items Displayed on the Screen

IDs to Output

All IDs

Designate IDs:

Delimiter

Select [Output File], and enter "QuantitativeResult" as the file name.

Select [Items Displayed on the Screen].

Select [All IDs].

Click here to save the "QuantResult.txt" file in the Sample folder.



Refer to "Export the Quantitative Results" of the "Quant Browser" chapter in *Operators Guide* for details on exporting quantitative results.

LabSolutions

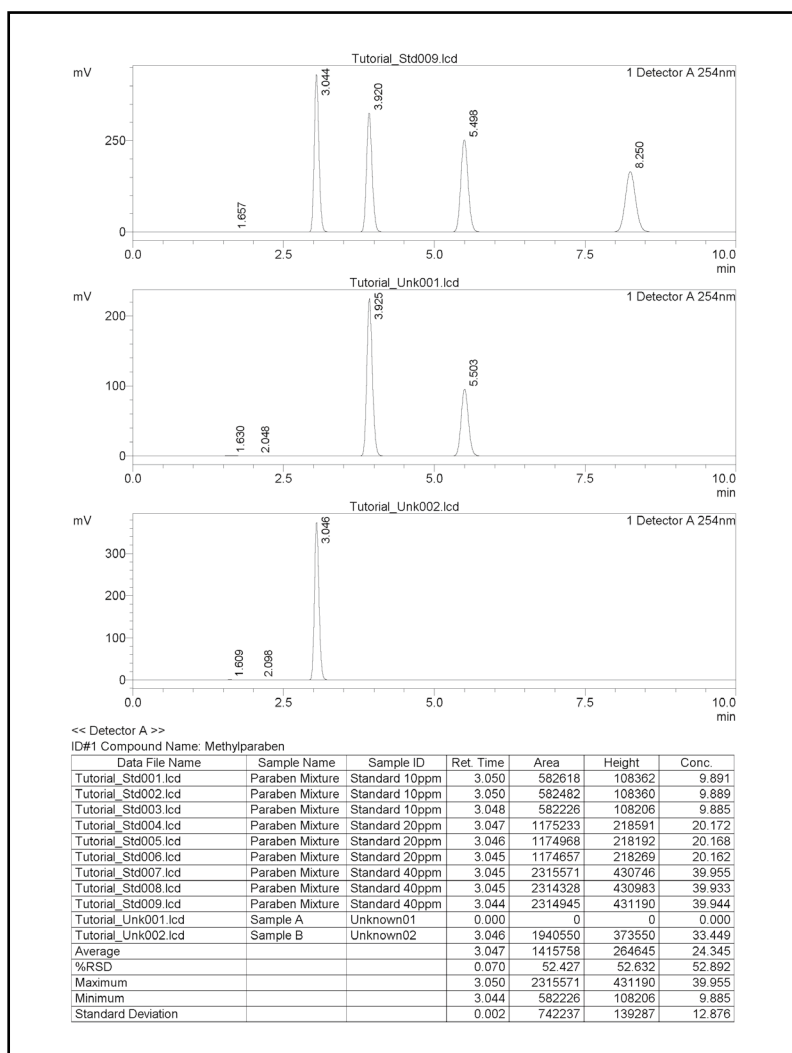


Print the Quantitative Results Table

To print a browser report, select [Print] at [Print Table] on the [File] menu.

The screenshot shows the 'File' menu with 'Print Table' selected. The 'Print Table' sub-menu is open, showing 'Print' (Ctrl-P) as the primary option. Other options include 'Print Quant. Report for Current Data', 'Method File Properties...', 'Tutorial_Method', and 'Exit'. The background shows a 'Quantitative Results View' table for 'Methylparaben' and a 'Method View - Compound' table.

ID#	Name	Type
1	Methylparaben	Target
2	Ethylparaben	Target
3	Propylparaben	Target
4	Butylparaben	Target



Select [Edit Format] from [Print Table] on the [File] menu to edit the report format.

Chapter 7

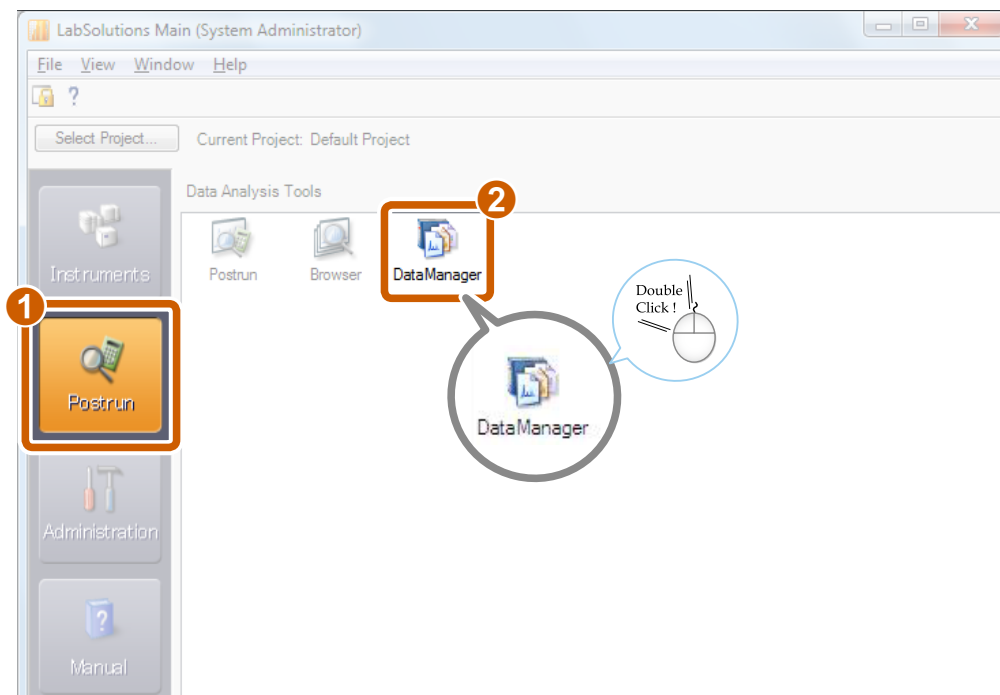
Data Management

The [DataManager] program in LabSolutions provides a convenient way to filter and view the files used by LabSolutions, which include data files, method files, batch files, and report format files, by specifying filtering conditions, such as the instrument name.



Reference Refer to the *System Users Guide* for details on the [DataManager] window.

1 Open the [DataManager] program.



2 Select [Data] for [Files of type].



The Data Manager can be used to view information on methods, batches, and report format files.

To view such information, clicking on [Show Method/Batch/Report Format in Database] in the [Tools] menu allows you to select method, batch, or report for [Files of type].

3 Filter the data using the [Instrument Name] condition.

The screenshot shows the 'DataManager (System Administrator)' application window. The 'Filtering' dialog box is open, showing various filter criteria. The 'Instrument Name' dropdown is highlighted with a red box and a '2', with a callout box pointing to it containing the text 'Enter "Instrument1" for [Instrument Name]'. The 'Start' button is circled with a red box and a '3', and the 'Clear' button is circled with a red box and a '1'. The 'Batch Data Set' section on the left contains several dropdown menus and checkboxes, including 'Max. # to List', 'Instrument Type', 'Data No.', 'Data File Name', 'Sample Name', 'Sample ID', 'Last Signature Status', 'Acquired by', 'Updated by', 'Date Acquired', 'Modified', and 'Comment'. An 'Advanced...' button is at the bottom of the dialog.

Continued on the following page 

4 Check the filtered data.

Check the filtered data file names.

The screenshot shows the Data Manager interface with a list of data files. The 'Data File Name' column is highlighted with a red box. The list includes files like Tutorial_Std005.lcd, Tutorial_Std004.lcd, Tutorial_Std008.lcd, Tutorial_Std003.lcd, Tutorial_Std009.lcd, Tutorial_Std006.lcd, Tutorial_Std007.lcd, Tutorial_Std002.lcd, Tutorial_Std001.lcd, Tutorial_Unk002.lcd, Tutorial_Unk001.lcd, and Test.lcd.

Data No.	Date Registered	Registered by	Date Acquired	Acquired by	Modified	Updated by	Instrument Type
1	9/13/2010 12090	System Administr	5/12/2009 40200	System Administr	9/13/2010 12085	System Administr	LC
2	9/13/2010 12085	System Administr	5/12/2009 35120	System Administr	9/13/2010 12085	System Administr	LC
3	9/13/2010 12090	System Administr	5/12/2009 43342	System Administr	9/13/2010 12085	System Administr	LC
4	9/13/2010 12085	System Administr	5/12/2009 34039	System Administr	9/13/2010 12085	System Administr	LC
5	9/13/2010 12090	System Administr	5/12/2009 44416	System Administr	9/13/2010 12085	System Administr	LC
6	9/13/2010 12090	System Administr	5/12/2009 41235	System Administr	9/13/2010 12085	System Administr	LC
7	9/13/2010 12090	System Administr	5/12/2009 42309	System Administr	9/13/2010 12085	System Administr	LC
8	9/13/2010 12085	System Administr	5/12/2009 33004	System Administr	9/13/2010 12085	System Administr	LC
9	9/13/2010 12085	System Administr	5/12/2009 31925	System Administr	9/13/2010 12085	System Administr	LC
10	9/13/2010 12072	System Administr	5/12/2009 50526	System Administr	9/13/2010 12072	System Administr	LC
11	9/13/2010 12072	System Administr	5/12/2009 45452	System Administr	9/13/2010 12072	System Administr	LC
12	8/18/2011 11370	System Administr	5/12/2009 30629	System Administr	4/2/2010 40028	System Administr	LC

5 Check the information of the selected data.

Click on "Tutorial_Std002.lcd".

The screenshot shows the Data Manager interface with the selected data file 'Tutorial_Std002.lcd' highlighted. A callout box points to the file name. Below the main table, there is a zoomed-in view of the chromatogram data for the selected file.

Check the information contained in the data.

ZOOM UP

Detector N	Channel/W	Line	Peak#	ID#	Retention	Relative R	Concentrati	Unit	Area	Height	Peak Start	Peak End
1	Detector A	Detector A 2	1	1	1.650	0.000	0.000		5207	345	1.417	1.842
2	Detector A	Detector A 2	2	1	3.050	9.889	mg/L	582482	108360	2.883	3.350	
3	Detector A	Detector A 2	3	2	3.929	9.905	mg/L	524475	81474	3.725	4.275	
4	Detector A	Detector A 2	4	3	5.513	9.924	mg/L	526966	63012	5.275	5.858	
5	Detector A	Detector A 2	5	4	8.276	9.931	mg/L	493798	41441	7.950	8.708	

6 Display the PDF result file for the data file.

The screenshot shows the DataManager (System Administrator) interface. The main window displays a list of data files with columns for File Name, Date Acquired, Acquired by, Modified, Updated by, and Instrument Type. A callout box with a red circle '1' points to the file 'Tutorial_Std002.lcd' in the list, with the text 'Click on "Tutorial_Std002.lcd".'. Below the list, a chromatogram (LC) is displayed with a table of peaks. A callout box with a red circle '2' points to the PDF file 'Tutorial_Std002.pdf' in the file list below the chromatogram, with the text 'Double-click on " Tutorial_Std002.pdf *".'.

File Name	Date Acquired	Acquired by	Modified	Updated by	Instrument Type	
2 Tutorial_Unk001.lcd 0-26	9/13/2010 1:09:12	System Administr	5/12/2009 5:05:26	System Administr	LC	
3 Tutorial_Std009.lcd 0-26	9/13/2010 1:09:17	System Administr	5/12/2009 4:54:52	System Administr	LC	
4 Tutorial_Std006.lcd 0-24	9/13/2010 1:09:17	System Administr	5/12/2009 4:44:16	System Administr	LC	
5 Tutorial_Std007.lcd 0-23	9/13/2010 1:09:16	System Administr	5/12/2009 4:33:42	System Administr	LC	
6 Tutorial_Std006.lcd 0-22	9/13/2010 1:09:16	System Administr	5/12/2009 4:23:09	System Administr	LC	
7 Tutorial_Std005.lcd 0-21	9/13/2010 1:09:16	System Administr	5/12/2009 4:12:35	System Administr	LC	
9 Tutorial_Std003.lcd 0-19	9/13/2010 1:09:15	System Administr	5/12/2009 4:02:00	System Administr	LC	
10 Tutorial_Std002.lcd 0-18	9/13/2010 1:09:14	System Administr	5/12/2009 3:51:20	System Administr	LC	
11 Tutorial_Std001.lcd 0-17	9/13/2010 1:09:14	System Administr	5/12/2009 3:40:39	System Administr	LC	
11370	System Administr	5/12/2009 3:08:29	System Administr	4/2/2010 4:00:28	System Administr	LC

Detector	Channel/W	Line	Peak#	ID#	Retention	Relative R	Concentra	Unit	Area	Height	Peak Start	Peak End
1	Detector A	Detector A	1		1.650		0.000		5207	345	1.417	1.842
2	Detector A	Detector A	2	1	3.160		9.989	mg/L	520492	103930	2.883	3.320
3	Detector A	Detector A	3	2	3.920		9.905	mg/L	524475	81474	3.725	4.275
4	Detector A	Detector A	4	3	5.513		9.924	mg/L	526966	63012	5.275	5.869
5	Detector A	Detector A	5	4	8.276		9.931	mg/L	493799	41441	7.950	8.709

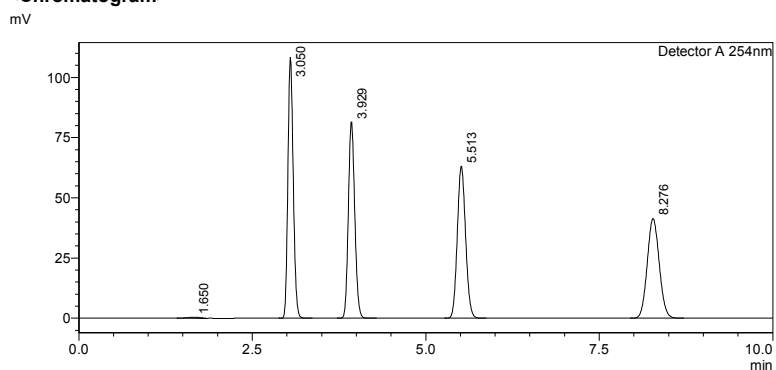


Analysis Report

<Sample Information>

Sample Name	: Paraben Mixture	Sample Type	: Standard
Sample ID	: Standard 10ppm	Level	: 1
Data Filename	: Tutorial_Std002.lcd	Acquired by	: System Administrator
Method Filename	: Tutorial_Method.lcm	Processed by	: System Administrator
Batch Filename	: Tutorial_Batch.lcb		
Vial #	: 1-1		
Injection Volume	: 10 uL		
Date Acquired	: 5/12/2009 3:30:04 AM		
Date Processed	: 9/13/2010 1:11:30 PM		

<Chromatogram>



<Peak Table>

Detector A 254nm							
Peak#	Ret. Time	Area	Height	Conc.	Unit	Mark	Name
1	1.650	5207	345	0.000			
2	3.050	582482	108360	9.889	mg/L		Methylparaben
3	3.929	524475	81474	9.905	mg/L		Ethylparaben
4	5.513	526966	63012	9.924	mg/L		Propylparaben
5	8.276	493798	41441	9.931	mg/L		Butylparaben
Total		2132927	294631				

LabSolutions



Open the [Postrun Analysis] Program.

The procedure for opening the [Postrun Analysis] program from the Data Manager is described below.

Select "Tutorial_Std002.lcd", right-click on the file name, and then click [Open with Related Application].

Registered by	Date Acquired	Acquired by	Modified	Updated by	Instrument Type
em Administr	5/12/2009 5:06:26	System Administr	9/13/2010 1:09:12	System Administr	LC
em Administr	5/12/2009 4:54:52	System Administr	9/13/2010 1:09:11	System Administr	LC
em Administr	5/12/2009 4:44:16	System Administr	9/13/2010 1:09:17	System Administr	LC
System Administr	5/12/2009 4:33:02	System Administr	9/13/2010 1:09:16	System Administr	LC
System Administr	5/12/2009 4:12:35	System Administr	9/13/2010 1:09:15	System Administr	LC
System Administr	5/12/2009 4:02:00	System Administr	9/13/2010 1:09:15	System Administr	LC
System Administr	5/12/2009 3:51:20	System Administr	9/13/2010 1:09:14	System Administr	LC
System Administr	5/12/2009 3:40:39	System Administr	9/13/2010 1:09:14	System Administr	LC
System Administr	5/12/2009 3:30:04	System Administr	9/13/2010 1:09:57	System Administr	LC
System Administr	5/12/2009 3:19:25	System Administr	9/13/2010 1:09:13	System Administr	LC
System Administr	5/12/2009 3:08:29	System Administr	4/2/2010 4:00:28	System Administr	LC

Detector	Channel/W	Line	Peak#	ID#	Retention	Relative R	Concentra	Unit	Area	Height	Peak Start	Peak End
1	Detector A	Detector A	1	1	1.650		0.000		5207	345	1.417	1.842
2	Detector A	Detector A	2	1	3.050		9.988	mg/L	582492	108360	2.983	3.950
3	Detector A	Detector A	3	2	3.929		9.905	mg/L	524475	81474	3.725	4.275
4	Detector A	Detector A	4	3	5.513		9.924	mg/L	526966	63012	5.275	5.888
5	Detector A	Detector A	5	4	8.276		9.931	mg/L	493798	41441	7.960	8.708



The [Postrun Analysis] program opens.

Peak#	Ret. Time	Area	Height	Mark	Co
1	1.650	5207	345		
2	3.050	582492	108360		
3	3.929	524475	81474		
4	5.513	526966	63012		
5	8.276	493798	41441		
Total		2132927	294631		

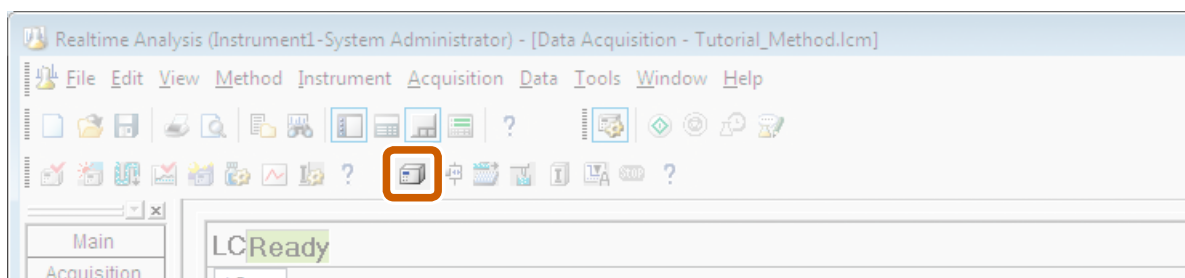
Chapter 8 ShutDown

Last of all, this chapter describes how to exit LabSolutions.

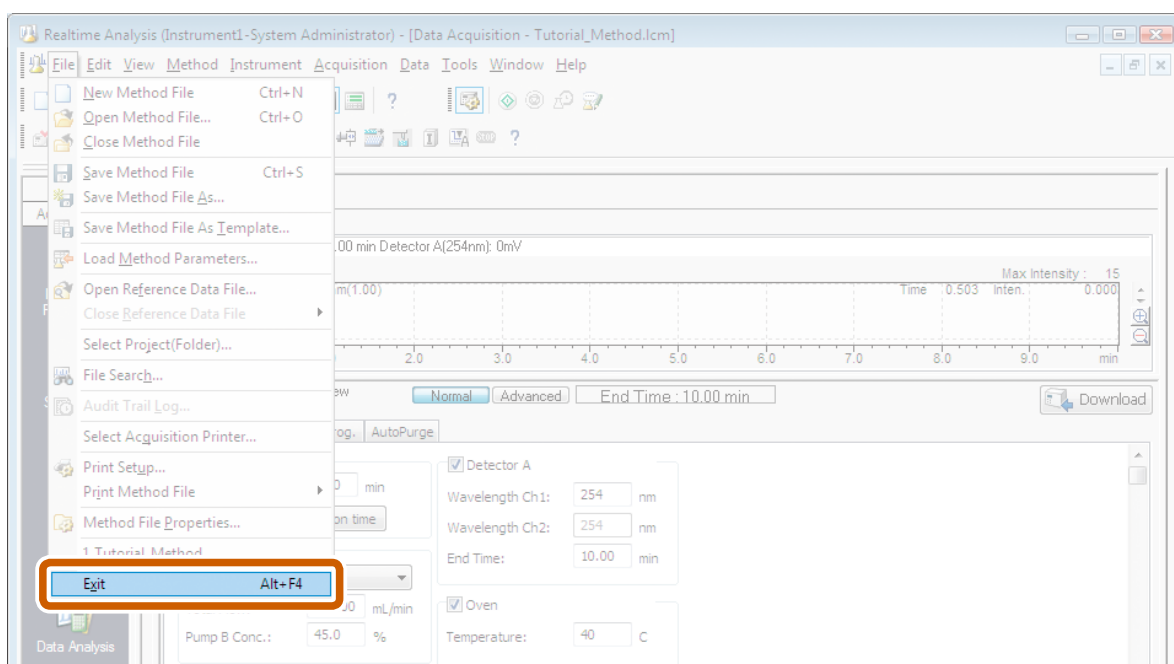
1 Stop instrument operation.

Stop pump solvent delivery and heating of the column oven.

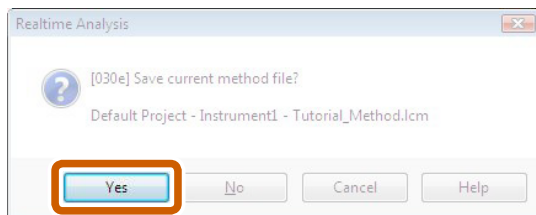
2 Set to OFF.



3 Select [Exit] when the oven has cooled down.



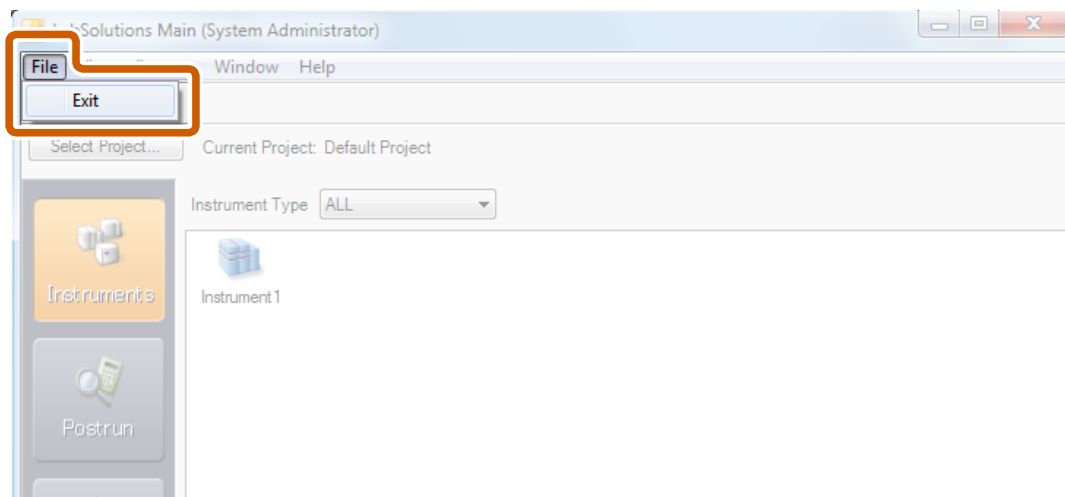
4 Click [Yes].



When there is a file that has not yet been saved, a window to confirm whether or not to save the file when exiting the [Realtime Analysis] program opens.

5 Exit LabSolutions.

If the [Postrun Analysis] program or [Browser] program is open, click [Exit] on the [File] menu of each program to exit the respective program.



6 Shutdown Windows, and turn the PC and printer off.

7 Turn each instrument off.