

# LabSolutions

## LC Getting Started Guide

<b>1</b>	<i>Start Up</i> .....	<b>12</b>
<b>2</b>	<i>Set the Instrument Parameters</i> ..	<b>16</b>
<b>3</b>	<i>Single Run</i> .....	<b>20</b>
<b>4</b>	<i>Data Analysis</i> .....	<b>22</b>
<b>5</b>	<i>Realtime Batch</i> .....	<b>28</b>
	Create a Batch Table .....	<b>28</b>
	Realtime Batch Processing.....	<b>32</b>
<b>6</b>	<i>Multiple Data Analysis</i> .....	<b>36</b>
<b>7</b>	<i>ShutDown</i> .....	<b>44</b>



## 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.

©2010 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

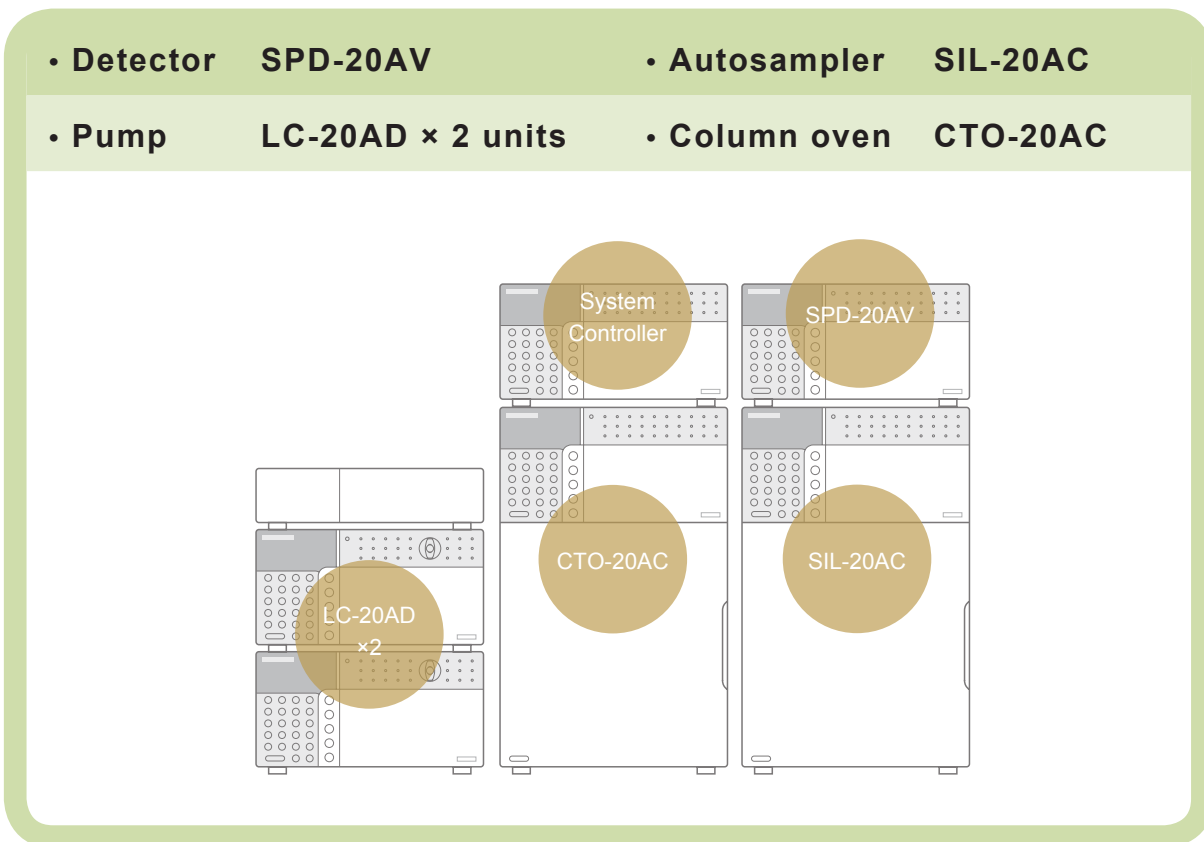
LabSolutions software is very easy to use, while incorporating high-grade functions. It provides powerful support for automating and improving the efficiency of sequential data acquisition and analysis operations.

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

## System Structure

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



# 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.20

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.22

## STEP ④

# Realtime Batch


**Perform data acquisition on sequential samples together.**

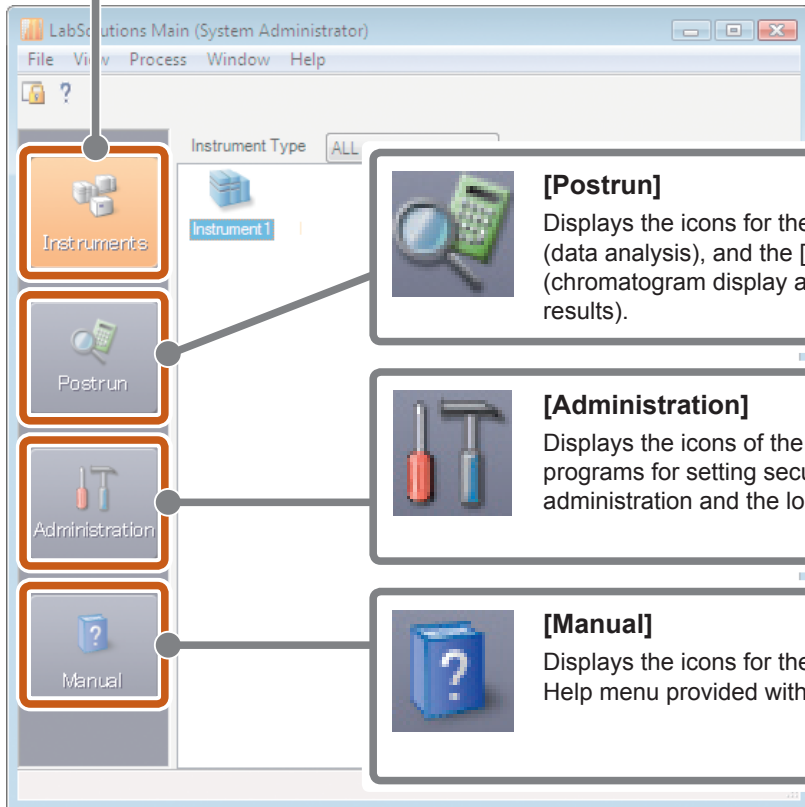
Realtime batch is performed to measure sequential samples continuously when the data acquisition conditions have been fixed by performing a single run.

 **5 Realtime Batch** P.28

 **6 Multiple Data Analysis** P.36

# LabSolutions Main Window

**[Instruments]**  
The analytical instruments connected to the PC are displayed as icons. Double-click  to start the [Realtime Analysis] program where data acquisition settings are set and data is acquired.

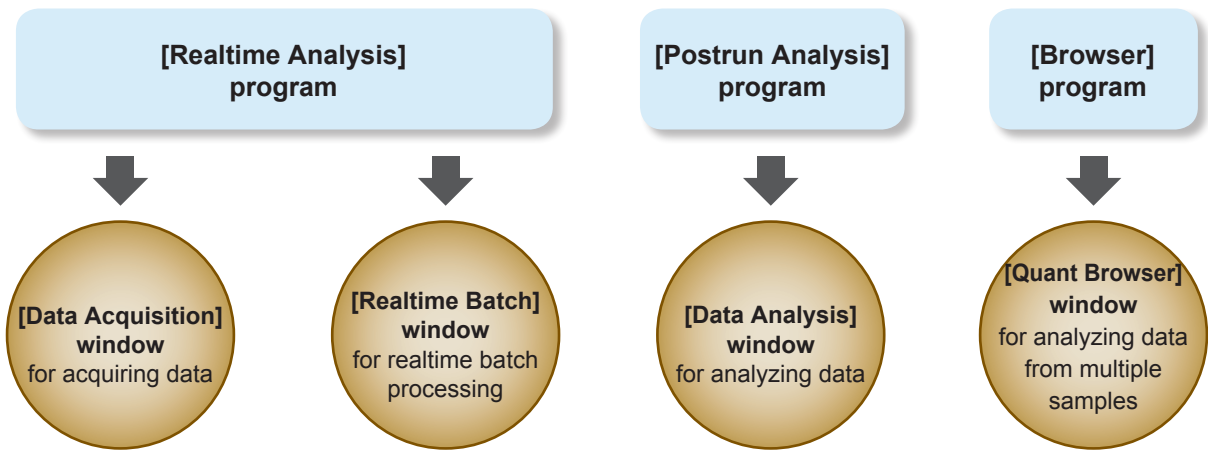


**[Postrun]**  
Displays the icons for the [Postrun Analysis] program (data analysis), and the [Browser] program (chromatogram display and quantitative calculation of results).

**[Administration]**  
Displays the icons of the system administration programs for setting security policies, user administration and the log browser.

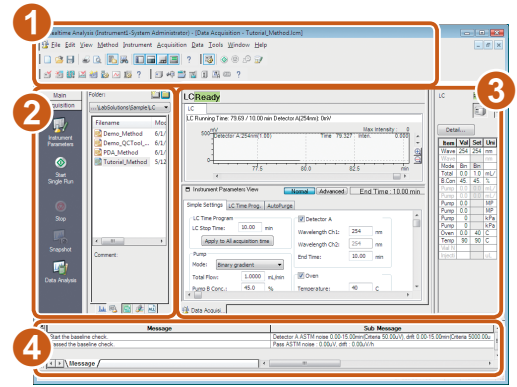
**[Manual]**  
Displays the icons for the various PDF manuals and Help menu provided with LabSolutions.

## LabSolutions Main Programs and Main Windows



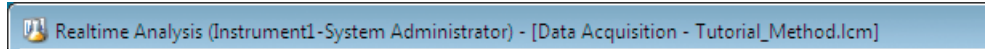
# LabSolutions Windows

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



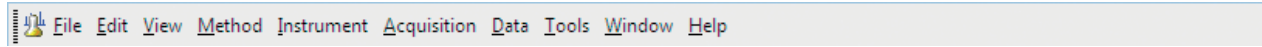
## 1 Title Bar

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



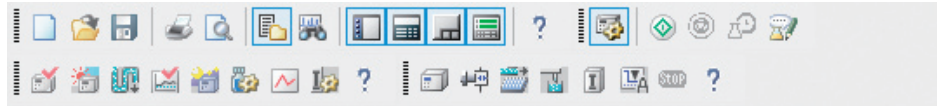
## Menu Bar

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



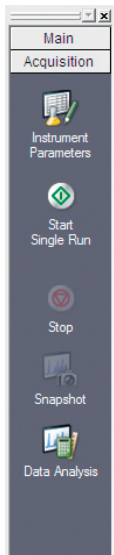
## Toolbar

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.



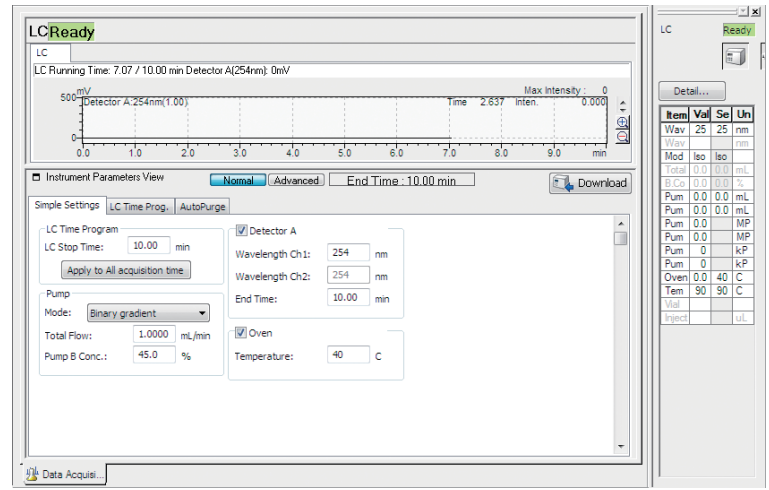
## Data Explore

This sub-window displays the names of files in the selected folder.



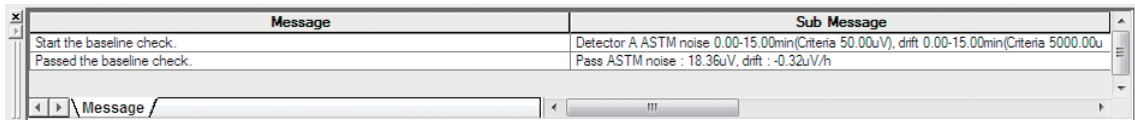
## 3 Window

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

## Set the Data Acquisition Parameters and Execute a Single Run:

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

- Reference** 2 **Set the Instrument Parameters** P.16
- Reference** 3 **Single Run** P.20

▼ [Realtime Analysis] program

▼ [Data Acquisition] window

▲ Main Window

The screenshot shows the LabSolutions Main window with three numbered callouts: 1. 'Instruments' button, 2. 'Instrument1' window, and 3. 'Data Acquisition' button. The 'Data Acquisition' window is open, showing a graph of 'LCReady' and 'LC Running Time: 2:57 / 10:00 min Detector A(254nm) Only'. The 'Instrument Parameters View' is also visible, showing settings for 'LC Time Program', 'LC Stop Time', 'Pump', 'Wavelength Ch1', 'Wavelength Ch2', 'End Time', 'Total Flow', 'Pump B Conc.', 'Detector A', 'Oven', and 'Temperature'.

## Continuous Data Acquisition of Sequential Samples:

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

- Reference** 5 **Realtime Batch** P.28

▼ [Realtime Analysis] program

▼ [Realtime Batch] window

▲ Main Window

The screenshot shows the LabSolutions Main window with three numbered callouts: 1. 'Instruments' button, 2. 'Instrument1' window, and 3. 'Realtime Batch' button. The 'Realtime Batch' window is open, displaying a table of sample data.

Analysis	Val#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Lot
1	1		Paraben Mixture	Standard 10ppm	1 Standard	Tutorial_Method.lcm	Tutorial_Seq001.lcd	
2	1		Paraben Mixture	Standard 10ppm	1 Standard	Tutorial_Method.lcm	Tutorial_Seq002.lcd	
3	1		Paraben Mixture	Standard 10ppm	1 Standard	Tutorial_Method.lcm	Tutorial_Seq003.lcd	
4	2		Paraben Mixture	Standard 20ppm	1 Standard	Tutorial_Method.lcm	Tutorial_Seq004.lcd	
5	2		Paraben Mixture	Standard 20ppm	1 Standard	Tutorial_Method.lcm	Tutorial_Seq005.lcd	
6	2		Paraben Mixture	Standard 20ppm	1 Standard	Tutorial_Method.lcm	Tutorial_Seq006.lcd	
7	3		Paraben Mixture	Standard 40ppm	1 Standard	Tutorial_Method.lcm	Tutorial_Seq007.lcd	
8	3		Paraben Mixture	Standard 40ppm	1 Standard	Tutorial_Method.lcm	Tutorial_Seq008.lcd	
9	3		Paraben Mixture	Standard 40ppm	1 Standard	Tutorial_Method.lcm	Tutorial_Seq009.lcd	
10	4		Sample A	Unknown01	0 Unknown	Tutorial_Method.lcm	Tutorial_Unk001.lcd	
11	5		Sample B	Unknown02	0 Unknown	Tutorial_Method.lcm	Tutorial_Unk002.lcd	

## Data Analysis and Quantitative Calculations:

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



4 Data Analysis P.22

▼ [Postrun Analysis] program

▼ [Data Analysis] window

▲ Main Window

Peak#	Ret. Time	Area	Height
1	1.857	4792	
2	3.040	52518	1076
3	3.924	524930	918
4	5.505	527123	630
5	8.267	484219	414
Total		2132972	2943

## Multiple Data Analysis and Quantitative Calculations:

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



6 Multiple Data Analysis P.36

▼ [Browser] program

▼ [Quant Browser] window

▲ Main Window

Peak#	Ret. Time	Area	Height
1	1.857	4792	
2	3.040	52518	1076
3	3.924	524930	918
4	5.505	527123	630
5	8.267	484219	414
Total		2132972	2943

# Chapter 1

## Start Up

This chapter describes how to start up LabSolutions.

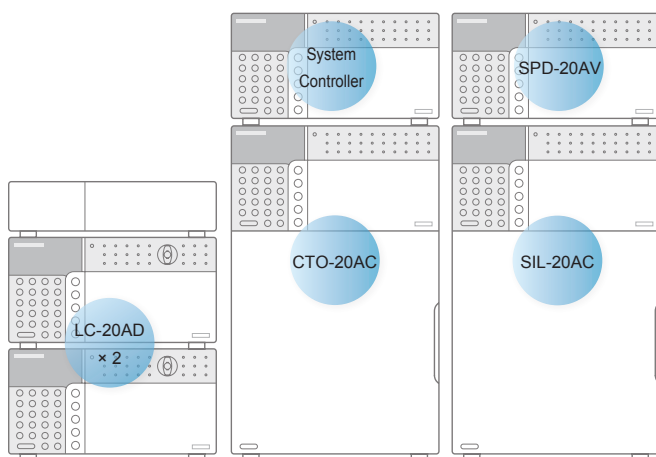


Refer to "LC Data Acquisition" in *Operators Guide* for details on the "Data Acquisition" window.

### 1 Check the connections.

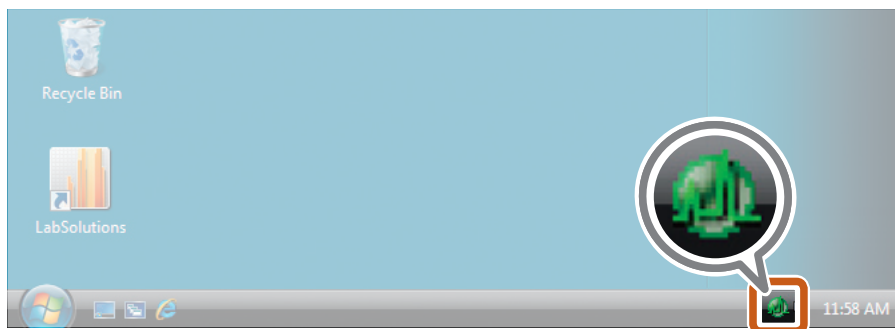
Ensure that all of the units (pump, autosampler, column oven, and detector) of the analytical instruments are connected to the system controller and optical link cables.

### 2 Turn the power on for each of the instruments.



### 3 Turn the PC and printer on.

Verify that the [LabSolutions Service] icon in the systray on the taskbar is green after the PC starts up.

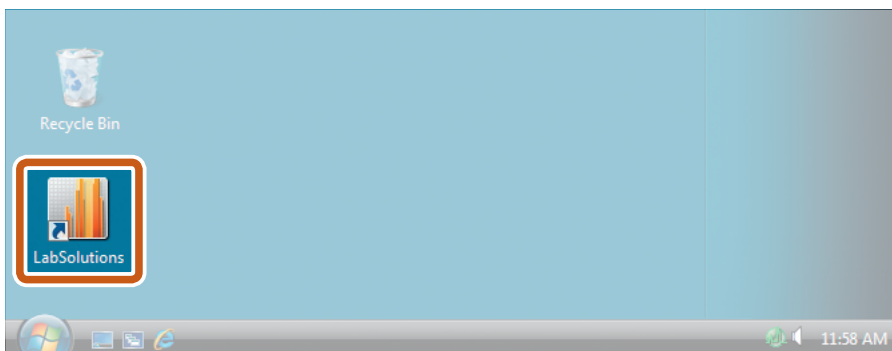


If the icon is yellow, this means that LabSolutions is in the process of starting up. Wait a while.

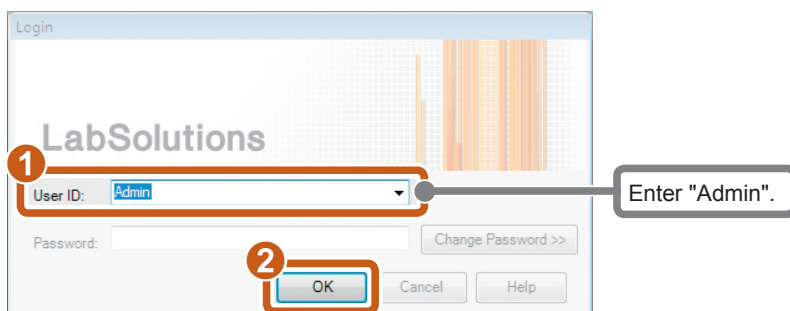
If the icon is red, this means that an error has occurred. Restart the PC.

## 4 Double-click on the desktop.

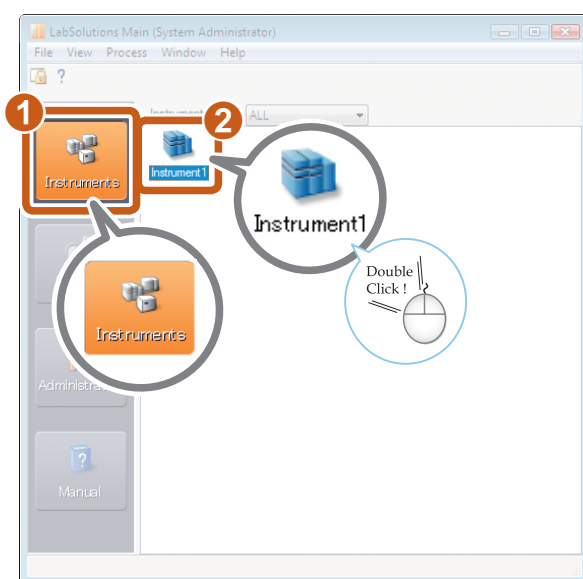
The [Login] sub-window opens.



## 5 Log in.




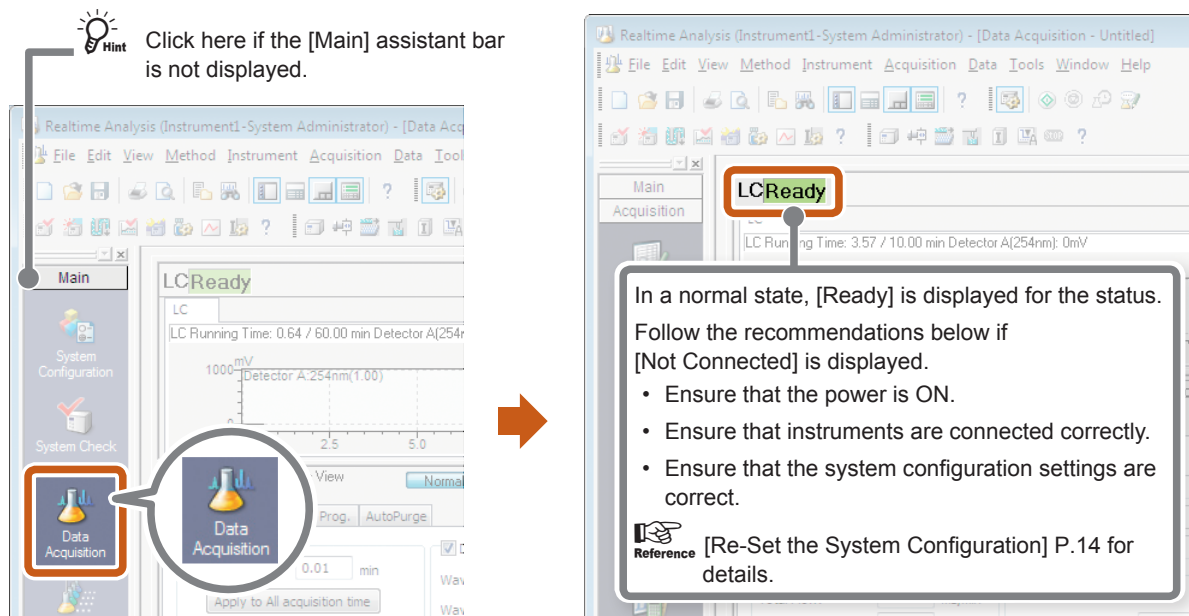
## 6 Open the [Realtime Analysis] program.



Continued on the following page 


# 7 Open the [Data Acquisition] window.

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



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.14 for details.

LabSolutions




"I want to connect to the system."

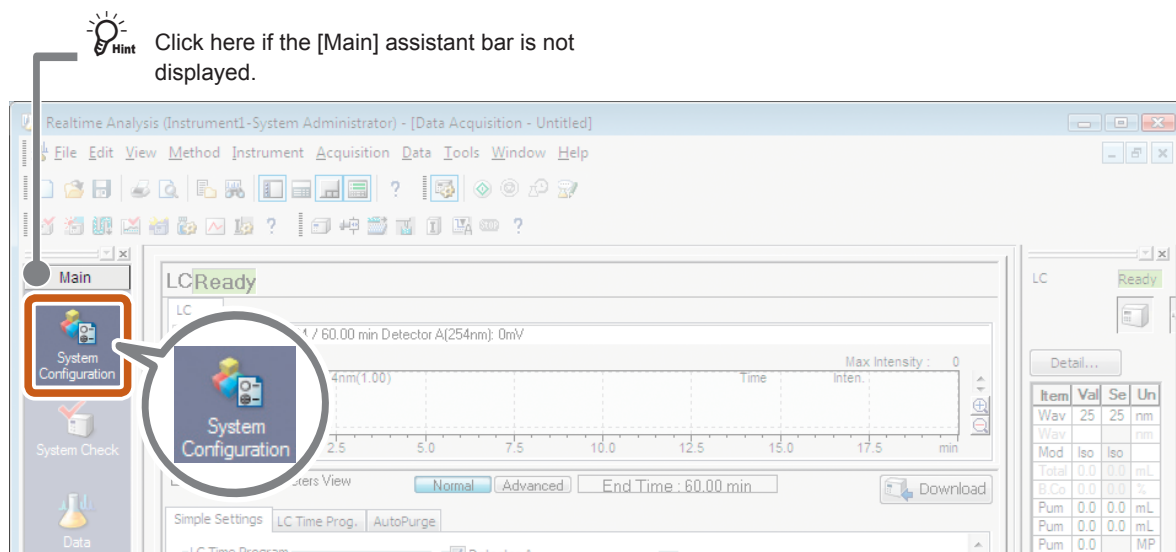
"I want to change the system configuration."

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.



Item	Val	Se	Un
Wav	25	25	nm
Mod	Iso	Iso	mL
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

The [System Configuration] sub-window opens.

## 2 Set up communications.

**1** Double Click!

The [Instrument] sub-window opens.

Select the system controller to use.

Click [Settings...]

Instrument	Model	Communication	Settings
LC	CBM-20A	rsnet	192.168.200.99
PDA	None	rs Type	None ConnectInfo
ELSD	None	rs Type	None ConnectInfo

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

**4**

Communication: Ethernet

IP Address : 192 . 168 . 200 . 99

**5** OK

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].

## 3 Check that the system configuration is correct.

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

**2** OK

Click here to send the settings to the LC.

# 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.

LC Ready

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

500 mV  
Time Inten.

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 Detector A  
Wavelength Ch1: 254 nm  
Wavelength Ch2: 254 nm  
End Time: 10.00 min

6 Oven  
Temperature: 40 °C

Set [Detector A] to .  
Wavelength Ch1 : 254 nm  
End Time : 10.00 min

Mode : Binary gradient  
T.Flow : 1.0000 mL/min  
B.Conc : 45 %

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
B.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

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.

1

The folder initially displayed here is the default folder. To change the default folder, Reference "Default Folder and Change the Default Folder" P.17

Enter "Tutorial\_Method".

2

3

4

Click here to download the data acquisition conditions to the instrument.

File name: Tutorial\_Method

Save as type: LC Method File (\*.lcm)

Save

Download

Item Val Set Uni  
Wave 254 254 nm  
Wave 254 254 nm  
Mode Iso Iso  
Total 0.0 0.0 mL  
B.Con 45. 45. %  
Pump 0.0 0.0 mL/L  
Pump 0.0 0.0 mL/L  
Pump 0.0 0.0 MP  
Pump 0.0 0.0 MP  
Pump 0 kPa  
Oven 0.0 40 C  
Temp 90 90 C  
Val N  
Inject

LabSolutions



## Default Folder and Change the Default Folder

1

Set this sub-window when changing the folder or creating a new folder.

Folder: ... \LabSolutions\Sample\LC

Filename Mod  
Tutorial\_method 6/19

This folder is the default folder.

Look in: C:\LabSolutions\Sample\LC

Computer  
Local Disk (C:)  
LabSolutions  
Common  
Data  
Manual  
MSLibrary  
Sample  
Sample  
GC  
System  
LC  
Template

Apply to All acquisition time

Wavelength Ch1: 254 nm  
Wavelength Ch2: 254 nm

Item Val Set Uni  
Wave 254 254 nm  
Wave 254 254 nm  
Mode Bin Bin  
Total 0.0 1.0 mL/L  
B.Con 45. 45. %  
Pump 0.0 0.0 mL/L  
Pump 0.0 0.0 mL/L  
Pump 0.0 0.0 MP  
Pump 0.0 0.0 MP  
Pump 0 kPa  
Oven 0.0 40 C  
Temp 90 90 C  
Val N  
Inject

# 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].

**Hint** 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. **Reference** 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

LabSolutions



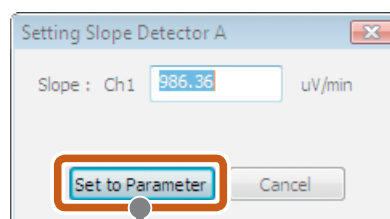
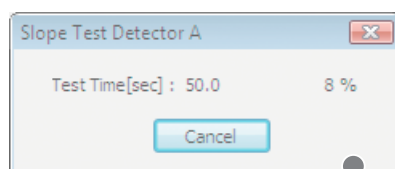
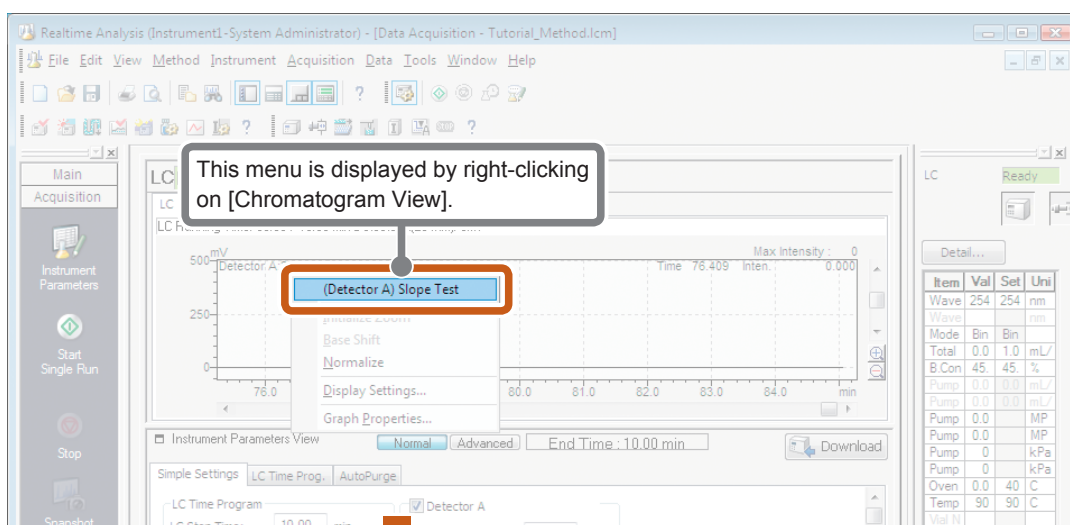
## Slope Test

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.



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".

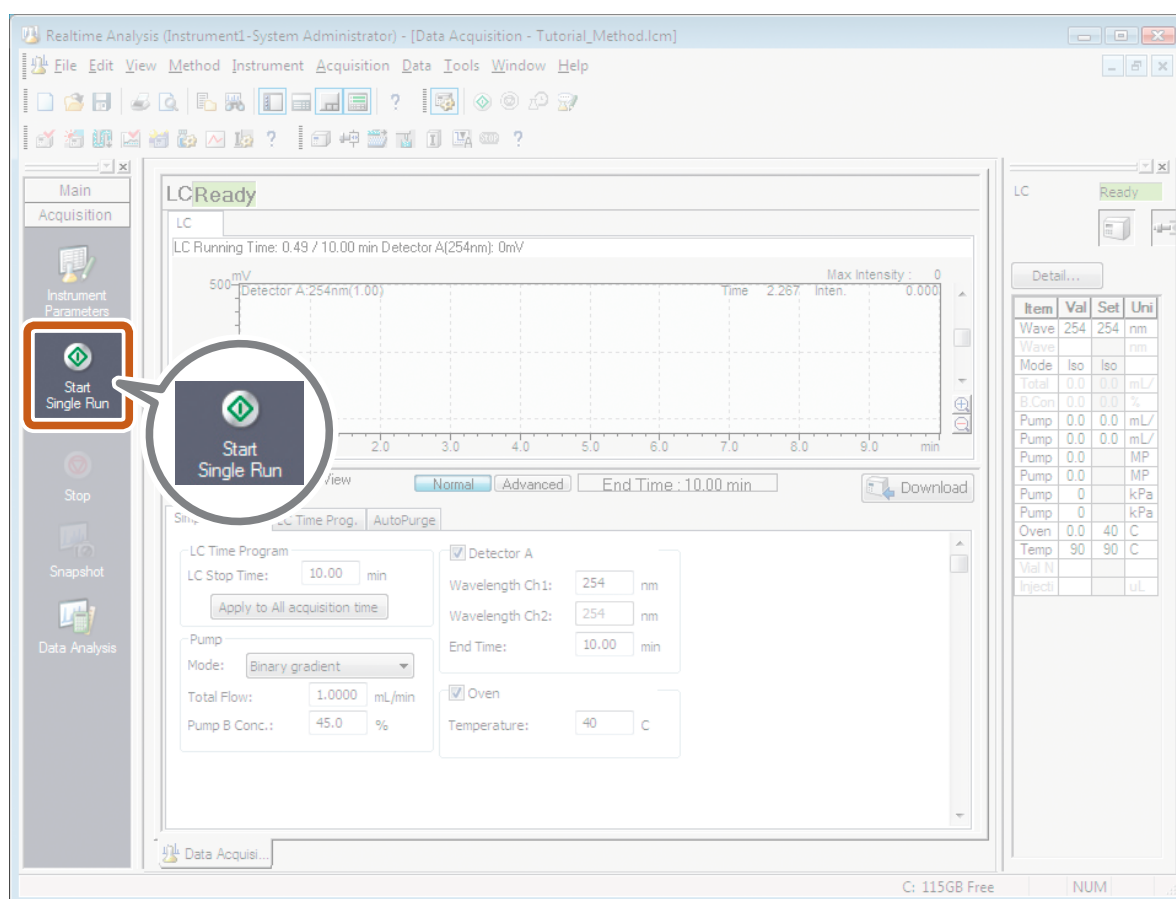
# Chapter 3

## 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.

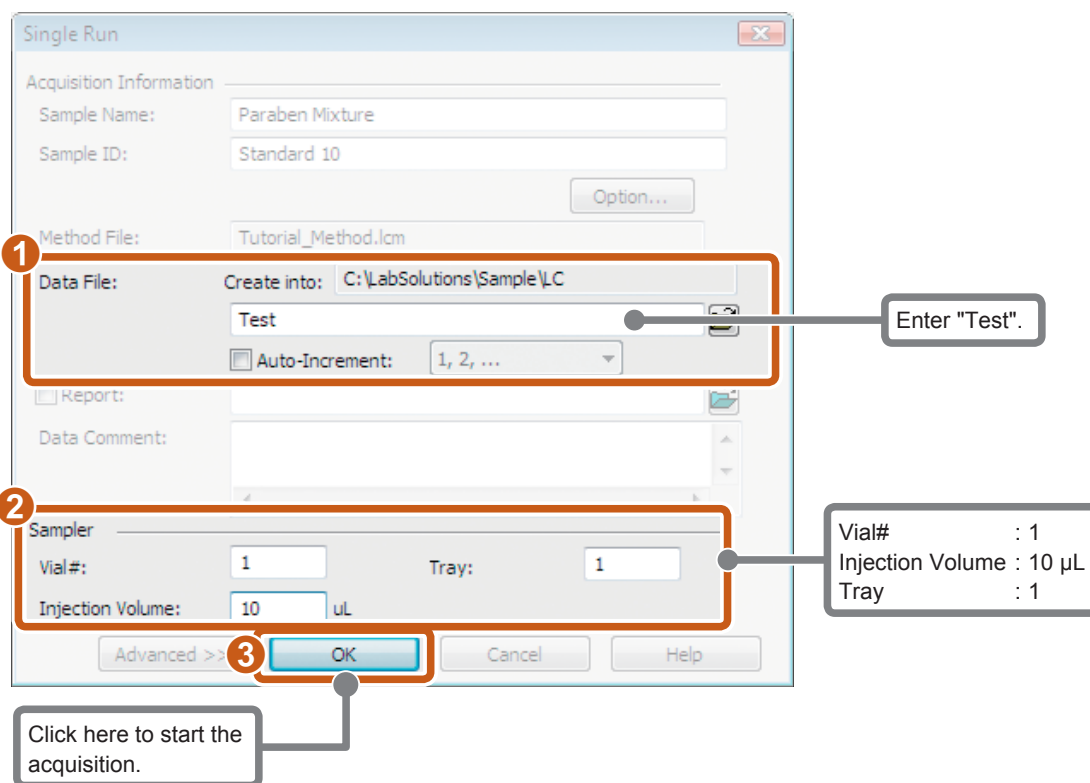
2 Open the [Single Run] sub-window.



The [Single Run] sub-window opens.

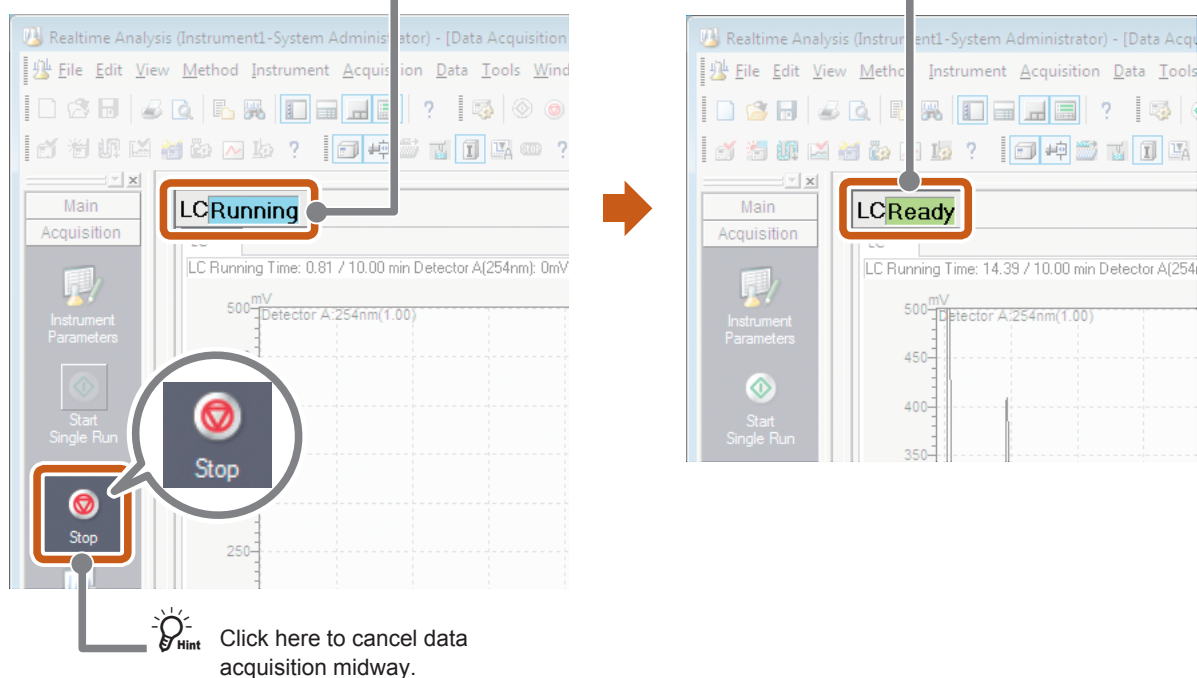
# 3 Set the conditions for a single run.

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



**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.

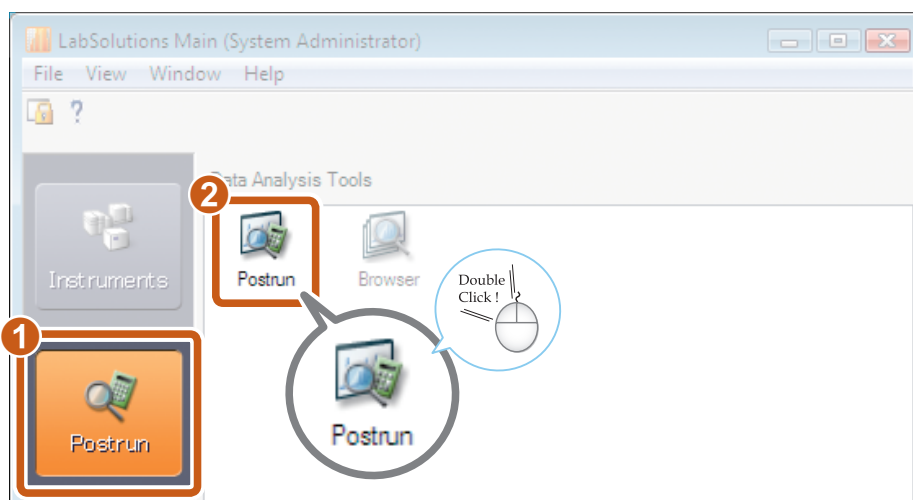


# Chapter 4

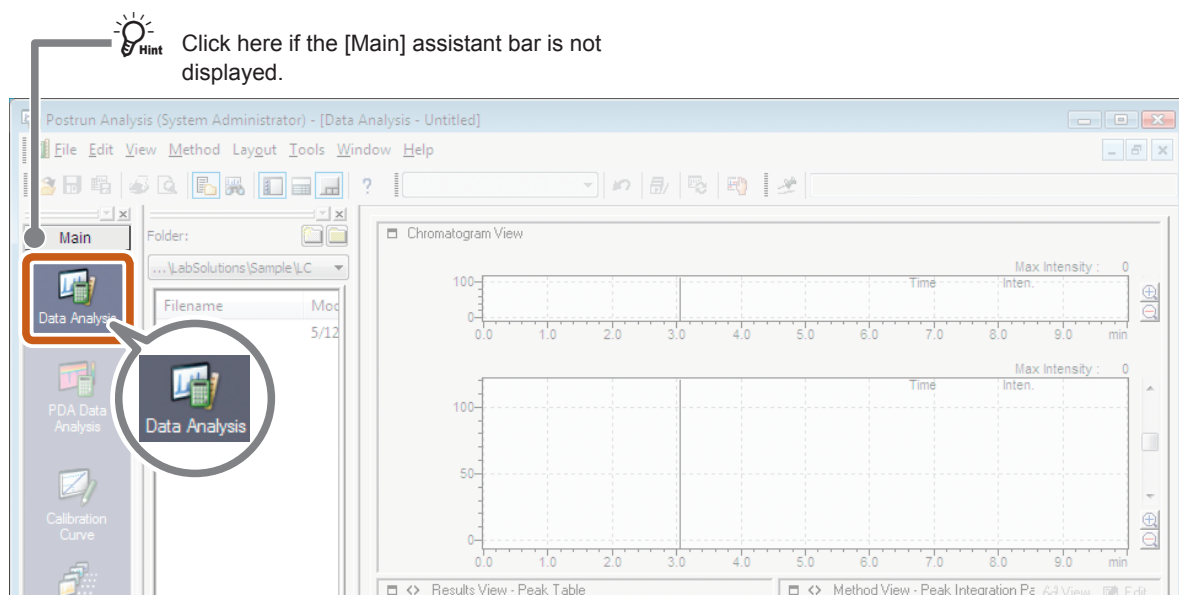
## Data Analysis

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".

The screenshot shows the Postrun Analysis software interface. The 'Data Explorer' sub-window is highlighted with an orange border and contains a callout bubble that says "Double Click!". The main window shows a 'Chromatogram View' with two plots and a 'Results View - Peak Table' with columns for Peak#, Ret. Time, Area, and Height. A 'Method View - Peak Integration' panel is also visible on the right.

Click  on the [Data Explorer] sub-window, and double-click "Test".



**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
1	1.657	4782	1
2	3.046	582518	1
3	3.924	524530	8
4	5.505	527123	8
5	8.267	494019	4
Total		2132972	2943

Integration parameters:  
 Channel: Detector A - Ch1 (254nm)  
 Width: 5 sec  
 Slope: 1000 uV/min  
 Drift: 0  
 Calculated by:  Area  Height



**Hint** 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.

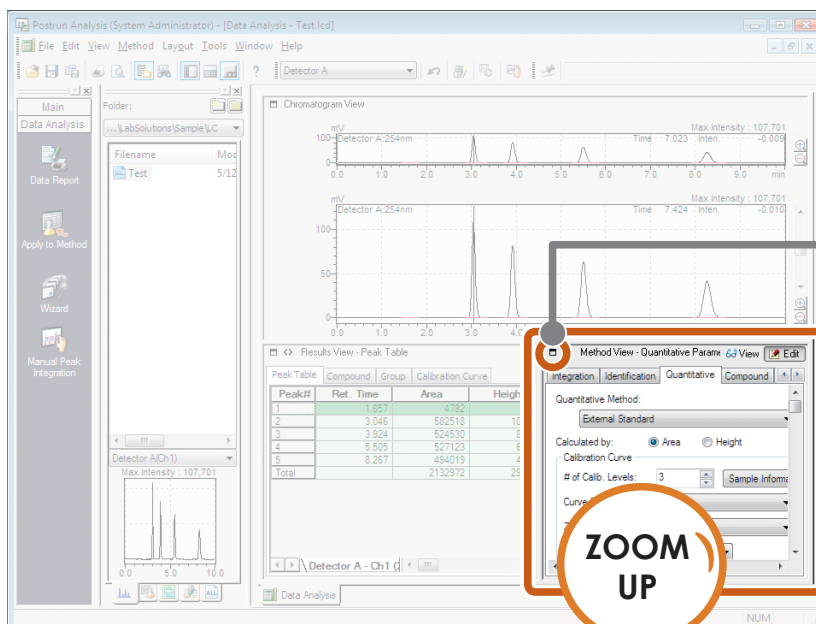
The positions where the absolute values of the baseline slope become these values are the start and end points of the peak.



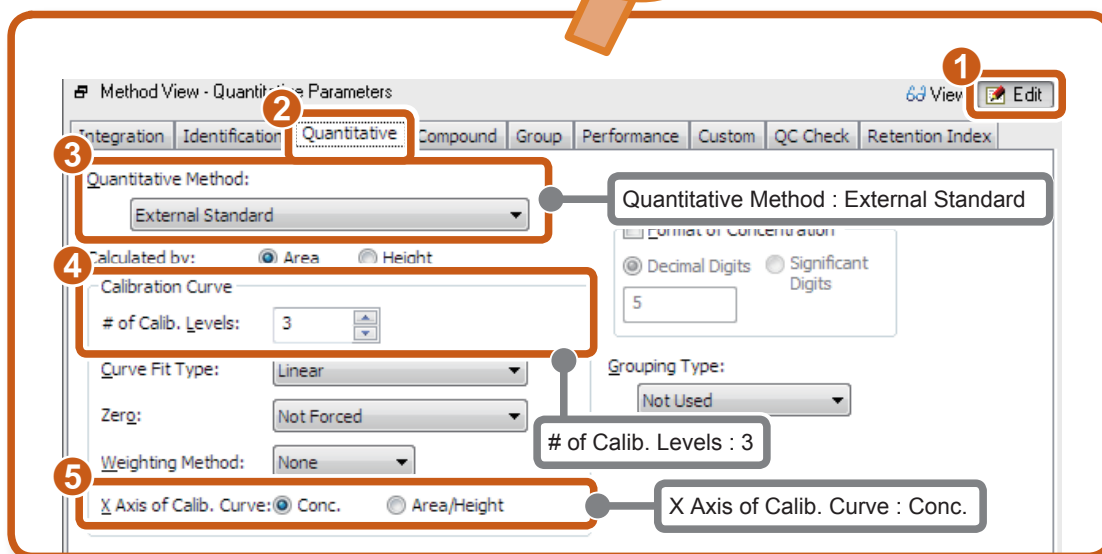
**Reference**

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.



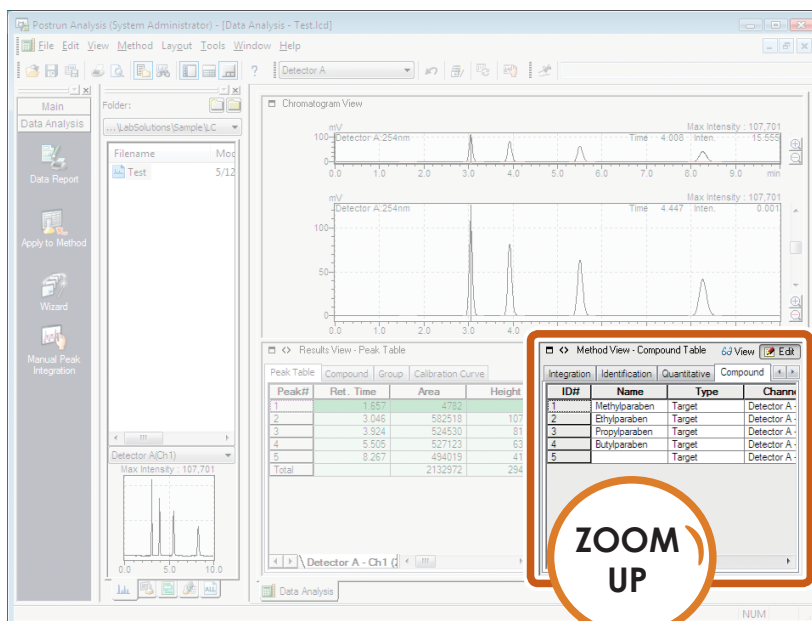
Hint Click to enlarge the window.



- 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.



Method View - Compound Table

1 Integration Identification Quantitative Compound

2

ID#	Name	Type	Channel	Ret. Time	Conc.(1)	Conc.(2)	Conc.(3)
1	Methylparaben	Target	Detector A - C	3.046	10	20	40
2	Ethylparaben	Target	Detector A - C	3.924	10	20	40
3	Propylparaben	Target	Detector A - C	5.505	10	20	40
4	Butylparaben	Target	Detector A - C	8.267	10	20	40

3 [View](#)

Name	Type	Ret. Time	Conc.(1)	Conc.(2)	Conc.(3)
Methylparaben	Target	3.046	10	20	40
Ethylparaben	Target	3.924	10	20	40
Propylparaben	Target	5.505	10	20	40
Butylparaben	Target	8.267	10	20	40

Click [View](#) to change the cell background color to yellow to fix the newly edited parameters.

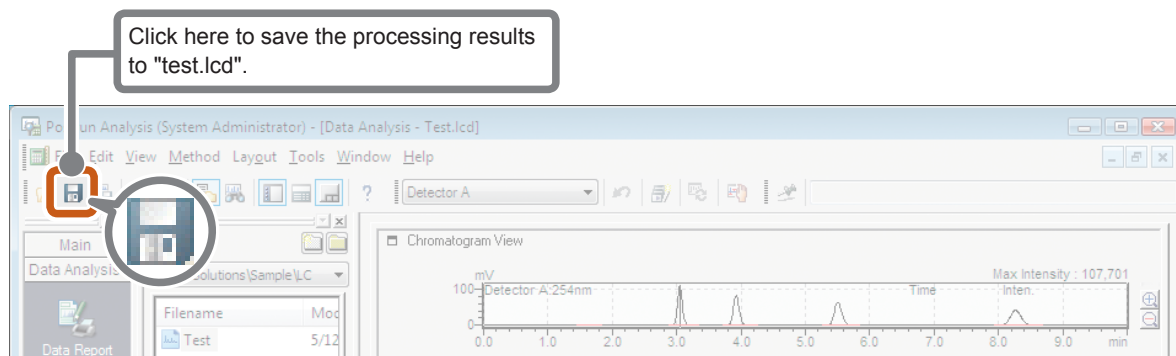


- The result obtained by performing data acquisition is used for [Ret. Time].
- Selecting the [Ret. Time] cell, and clicking the peak in [Chromatogram View] automatically enters the retention time of that peak to the currently selected [Ret. Time] cell. The retention time can be set by simply clicking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

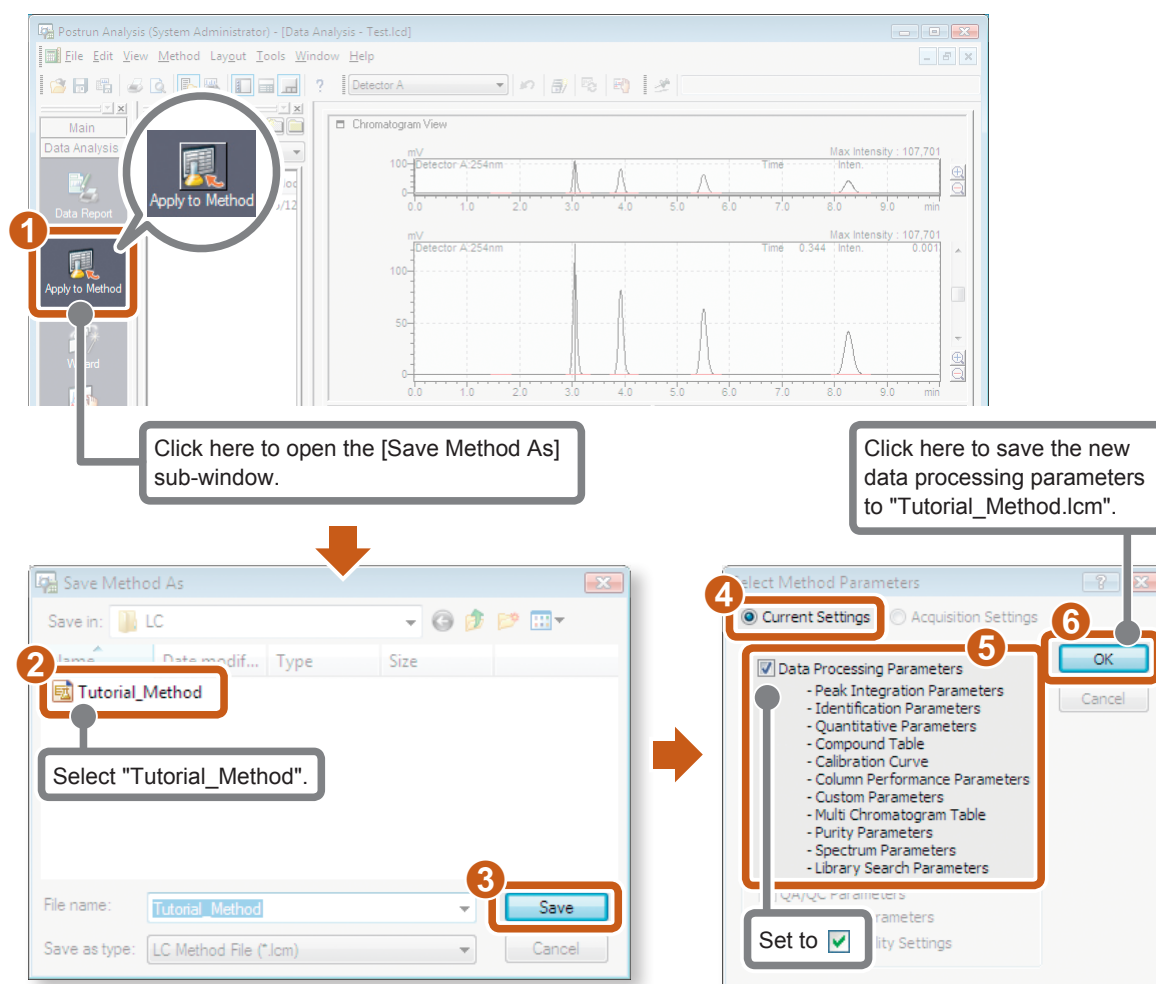


Refer to "Compound Table Retention Times Using the Mouse" of the "Data Analysis" chapter in the *Operators Guide* for details on setting retention times.


# 7 Save the processing results to a data file.



# 8 Save the method file.



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

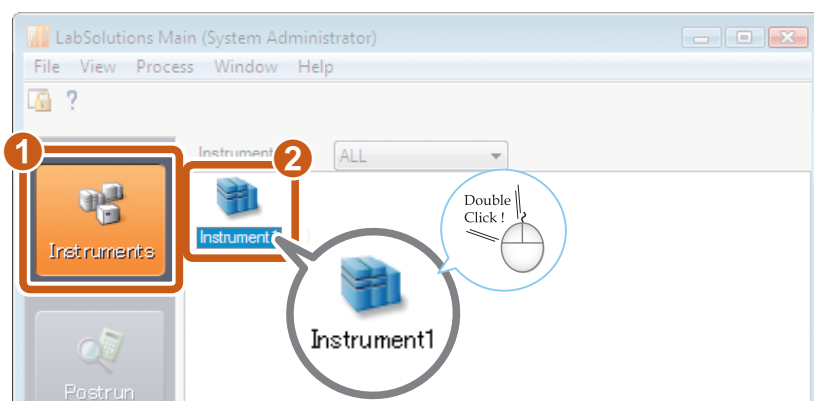
## Realtime Batch

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.

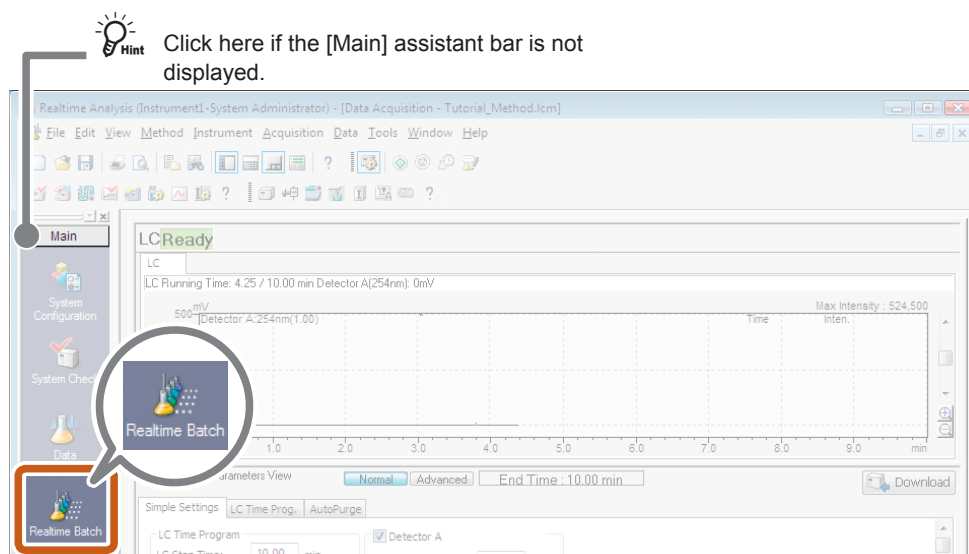
### 5.1 Create a Batch Table

In the following example, create a Batch Table with standard samples set to 1st to 3rd rows, and unknown samples set to the 4th and 5th 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  $\mu$ L  
 Repetitions : 3  
 Data File : Tutorial\_Std

4 **Set [Unknown] to .**  
 Vial# : 4 to 5  
 Injection Volume : 10  $\mu$ L  
 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#
1	1	1			1:Standard (I)	Tutorial_Method.lcm	Tutorial_Std001.lcd	1
2	1	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std002.lcd	1
3	1	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std003.lcd	1
4	2	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std004.lcd	2
5	2	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std005.lcd	2
6	2	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std006.lcd	2
7	3	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std007.lcd	3
8	3	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std008.lcd	3
9	3	1			1:Standard	Tutorial_Method.lcm	Tutorial_Std009.lcd	3
10	4	1			0:Unknown	Tutorial_Method.lcm	Tutorial_Unk001.lcd	0
11	5	1			0:Unknown	Tutorial_Method.lcm	Tutorial_Unk002.lcd	0



- In Batch Tables, you can set the sample information of each sample and output of reports.



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.

Folder: C:\LabSolutions\Sample\LC

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1	1	1				Tutorial_Method.lcm	Tutorial_Std001.lcd	1
2	1	1				Tutorial_Method.lcm	Tutorial_Std002.lcd	1
3	1	1				Tutorial_Method.lcm	Tutorial_Std003.lcd	1
4	2	1				Tutorial_Method.lcm	Tutorial_Std004.lcd	2
5	2	1				Tutorial_Method.lcm	Tutorial_Std005.lcd	2
6	2	1				Tutorial_Method.lcm	Tutorial_Std006.lcd	2
7	3	1				Tutorial_Method.lcm	Tutorial_Std007.lcd	3

1 Select here. 2 Fill Down

Sample Name

Row #: 1 9

Sample Name: Paraben Mixture

Auto-increment Repetitions: 1

OK Cancel Help

3 4 5

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		1:Standard.()	Tutorial_Method.lcm	Tutorial_Std001.lcd	1
2	1	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std002.lcd	1
3	1	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std003.lcd	1
4	2	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std004.lcd	2
5	2	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std005.lcd	2
6	2	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std006.lcd	2
7	3	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std007.lcd	3
8	3	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std008.lcd	3
9	3	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std009.lcd	3
10	4	1			0:Unknown	Tutorial_Method.lcm	Tutorial_Unk001.lcd	0

Sample Name

# 5 Enter a numbered series.

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		1:Standard.()	Tutorial_Method.lcm	Tutorial_Std001.lcd	1
2	1	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std002.lcd	1
3	1	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std003.lcd	1
4	2	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std004.lcd	2
5	2	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std005.lcd	2
6	2	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std006.lcd	2
7	3	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std007.lcd	3
8	3	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std008.lcd	3
9	3	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std009.lcd	3
10	4	1			0:Unknown	Tutorial_Method.lcm	Tutorial_Unk001.lcd	0
11	5	1			0:Unknown	Tutorial_Method.lcm	Tutorial_Unk002.lcd	0

Select here. 1 2 Fill Series

Sample ID

Row #: 10 11

Sample ID: Unknown01

Auto-increment Repetitions: 1

OK Cancel Help

3 4 5

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		1:Standard.()	Tutorial_Method.lcm	Tutorial_Std001.lcd	1
2	1	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std002.lcd	1
3	1	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std003.lcd	1
4	2	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std004.lcd	2
5	2	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std005.lcd	2
6	2	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std006.lcd	2
7	3	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std007.lcd	3
8	3	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std008.lcd	3
9	3	1	Paraben Mixture		1:Standard	Tutorial_Method.lcm	Tutorial_Std009.lcd	3
10	4	1			Unknown	Tutorial_Method.lcm	Tutorial_Unk001.lcd	0
11	5	1			Unknown	Tutorial_Method.lcm	Tutorial_Unk002.lcd	0

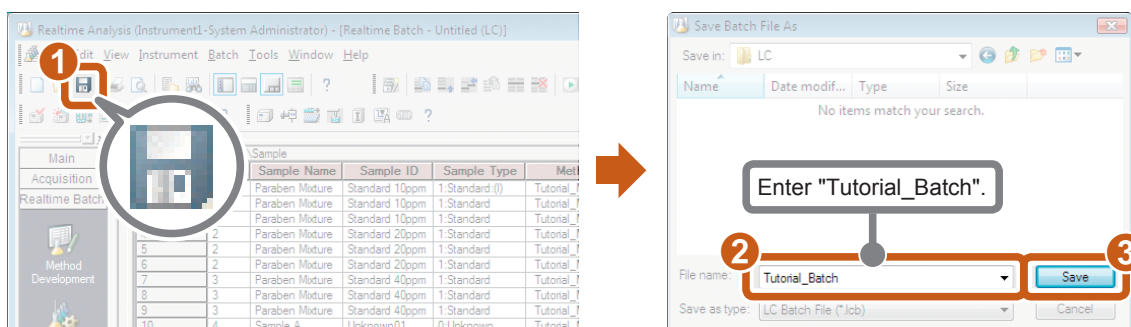
Unknown01  
Unknown02

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

Folder: C:\Lab Solutions\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:(I)	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.



# 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.

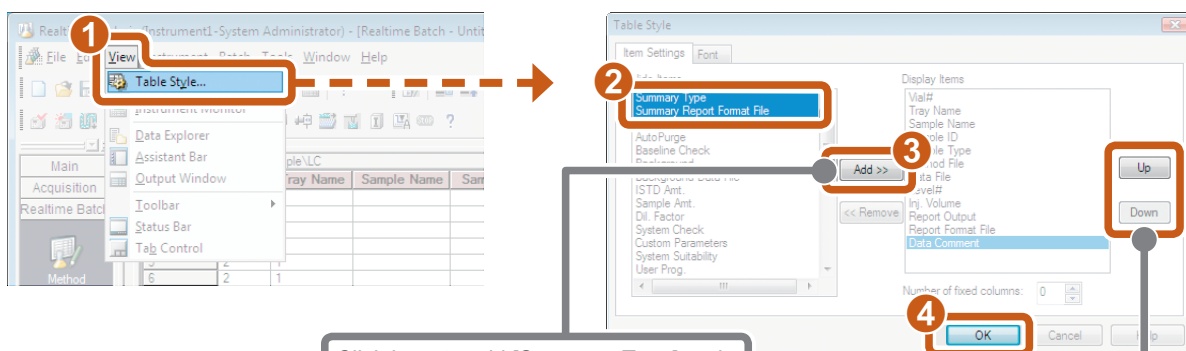
Click here to cancel data acquisition midway. To edit the content of the Batch Table during realtime batch, click to pause realtime batch.

LabSolutions



# Print a Summary Report

## 1 Add items to display in the Batch Table.

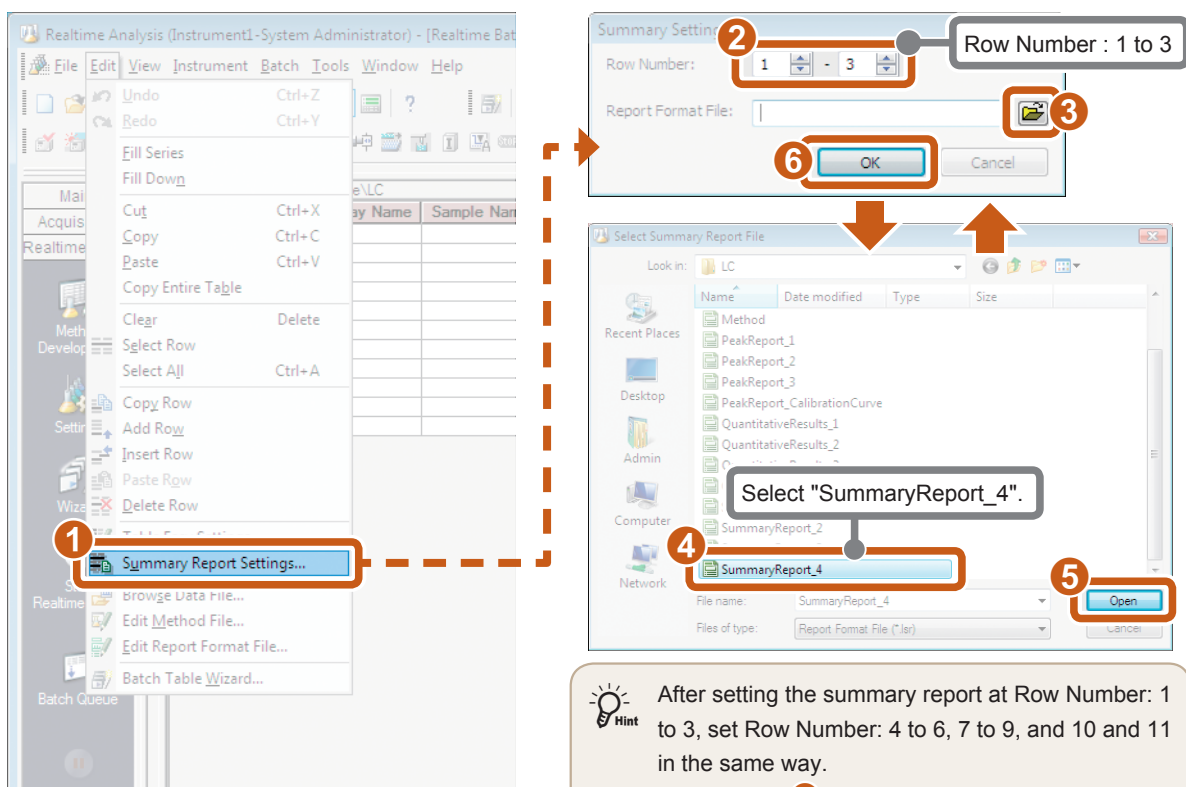


Click here to add [Summary Type] and [Summary Report Format File] to the items to display in the Batch Table.



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	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Inj. Volume	Report Format F	Summary Type	Summary Report Format File
1	Paraben Mixture	Standard 10ppm	1:Standard (I)	Tutorial_Method.lcm	Tutorial_Std001.lcd	1	10	Peak-Report_1.lsr	Summary Start	SummaryReport_4.lsr
2	Paraben Mixture	Standard 10ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std002.lcd	1	10	Peak-Report_1.lsr	Summary Run	
3	Paraben Mixture	Standard 10ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std003.lcd	1	10	Peak-Report_1.lsr	Summary End	
4	Paraben Mixture	Standard 20ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std004.lcd	2	10	Peak-Report_1.lsr	Summary Start	SummaryReport_4.lsr
5	Paraben Mixture	Standard 20ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std005.lcd	2	10	Peak-Report_1.lsr	Summary Run	
6	Paraben Mixture	Standard 20ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std006.lcd	2	10	Peak-Report_1.lsr	Summary End	
7	Paraben Mixture	Standard 40ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std007.lcd	3	10	Peak-Report_1.lsr	Summary Start	SummaryReport_4.lsr
8	Paraben Mixture	Standard 40ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std008.lcd	3	10	Peak-Report_1.lsr	Summary Run	
9	Paraben Mixture	Standard 40ppm	1:Standard	Tutorial_Method.lcm	Tutorial_Std009.lcd	3	10	Peak-Report_1.lsr	Summary End	
10	Sample A	Unknown01	0:Unknown	Tutorial_Method.lcm	Tutorial_Unk001.lcd	0	10	Peak-Report_1.lsr	Summary Start	SummaryReport_1.lsr
11	Sample B	Unknown02	0:Unknown	Tutorial_Method.lcm	Tutorial_Unk002.lcd	0	10	Peak-Report_1.lsr	Summary End	

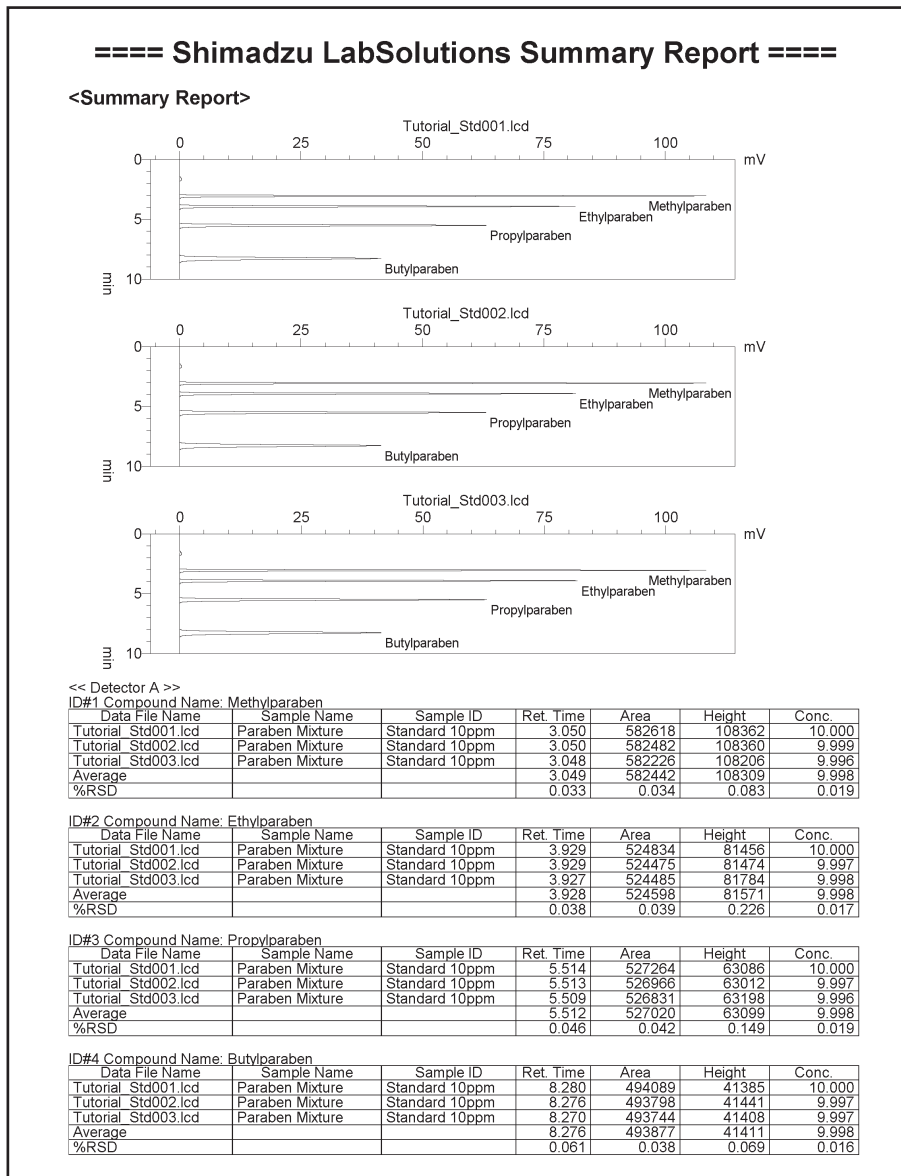
When you have finished the output configuration of the summary report, execute realtime batch to print the summary report.



Refer to "5.2 Realtime Batch Processing" P.32 for details on executing realtime batch.

## [Printout Example]

Standard samples

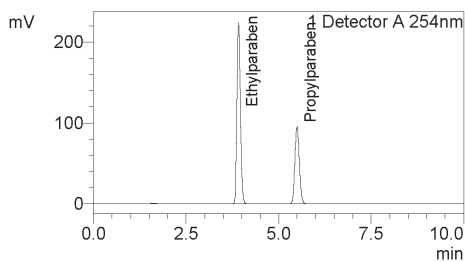


## Unknown samples

## ==== 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



Detector A 254nm

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	

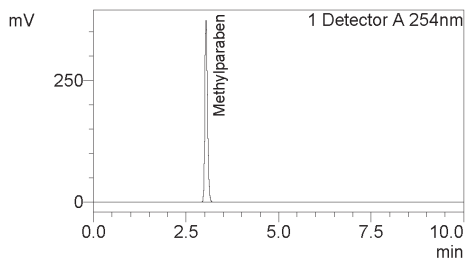
Detector A

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



Detector A 254nm

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	

Detector A

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

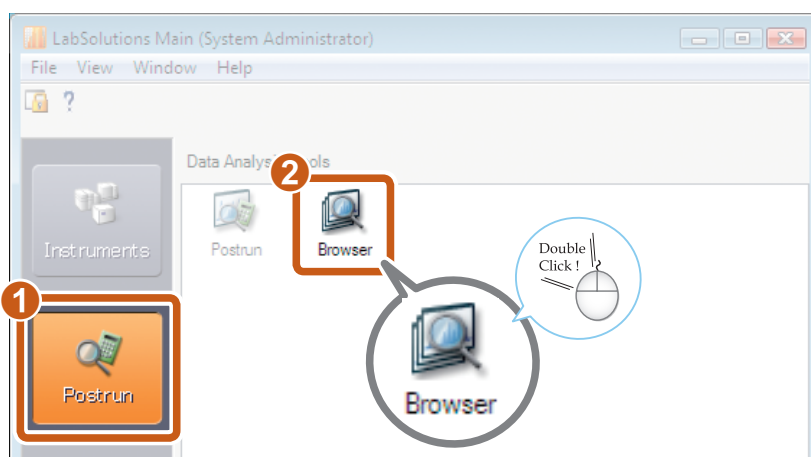
The LabSolutions [Browser] program is handy for checking the quantitative calculation results and chromatograms of multiple data.

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.

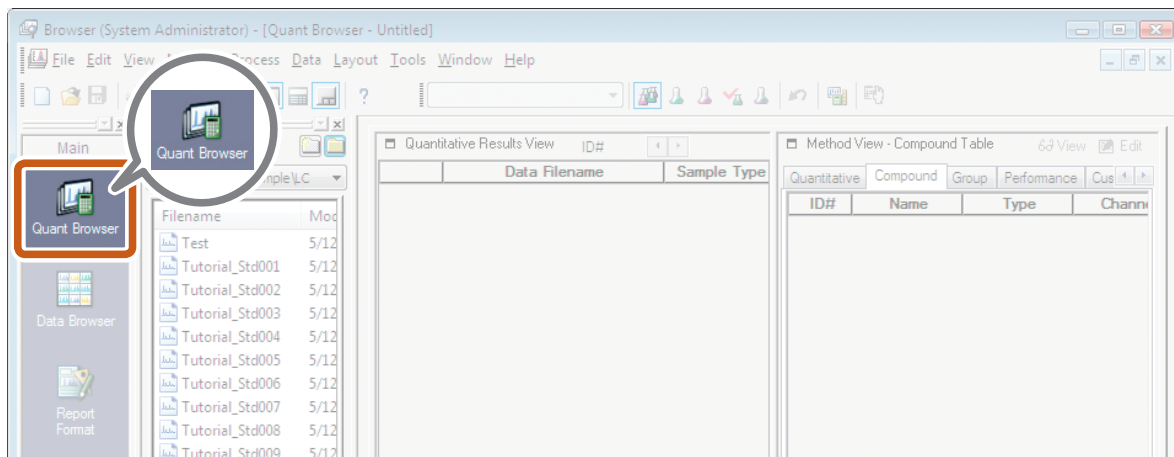


**Reference** Refer to "Quant Browser" chapter in *Operators Guide* for details on the "Quant Browser" window.

### 1 Open the [Browser] program.



### 2 Open the [Quant Browser] window.



Open the [Quant Browser] window.

# 3 Load the batch file.

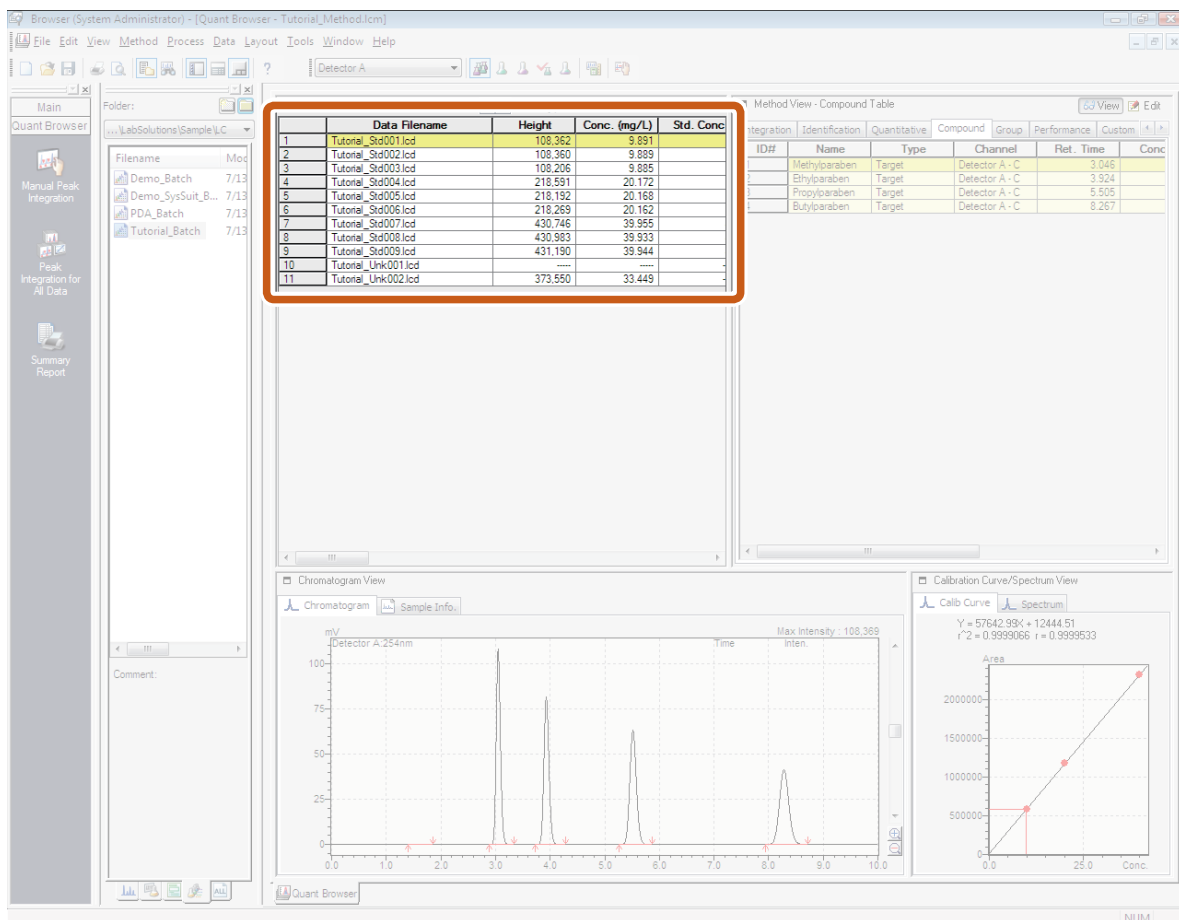
The screenshot displays the Quant Browser software interface. The main window is titled "Browser (System Administrator) - [Quant Browser - Untitled]". The interface includes a menu bar (File, Edit, View, Method, Process, Data, Layout, Tools, Window, Help), a toolbar, and several panels:

- Left Panel:** Contains a "Main" section with "Quant Browser" and a "Manual Peak Integration" button. Below this is a "Peak Integration for All Data" button and a "Summary Report" button.
- Folder Panel:** Shows the current folder as "...\LabSolutions\Sample\C". A file named "Tutorial\_Batch" with a date of "6/19" is highlighted. A red box with the number "2" and an arrow points to this file, with a callout box stating: "Drag and drop this file to display the quantitative results data."
- Quantitative Results View:** A table with columns "Data Filename" and "Sample Type".
- Method View - Compound Table:** A table with columns "Integration", "Identification", "Quantitative", and "Compound". Below this is a table with columns "ID#", "Name", "Type", and "Chann".
- Chromatogram View:** A plot showing "Chromatogram" and "Sample Info.". The y-axis is labeled "Max Intensity : 0" and the x-axis is labeled "Time : 0.000 Inten.". The plot area is currently empty.
- Calibration Curve/Spectrum View:** A plot showing "Calib Curve" and "Spectrum". The y-axis ranges from 0 to 100, and the x-axis ranges from 0 to 100. The plot area is currently empty.

A red box with the number "1" is located in the bottom-left corner of the interface, near the "Comment:" field and the "Quant Browser" button.

Continued on the following page 

# 4 Confirm the quantitative results.



LabSolutions



# Modify Calibration Curves

1

## Confirm peak integration parameters.

Confirm the peak integration parameters when peak detection is inappropriate.

**ZOOM UP**

Click here to perform postrun batch on all data.

Make sure that these values are appropriate.

Data	Filename	Height	Conc. (mg/L)	Std. Cor
1	Tutorial_Sst001.lcd	108.360	9.889	
2	Tutorial_Sst002.lcd	108.206	9.885	
3	Tutorial_Sst003.lcd	218.891	20.172	
4	Tutorial_Sst004.lcd	218.192	20.168	
5	Tutorial_Sst005.lcd	218.269	20.162	
6	Tutorial_Sst006.lcd	430.746	39.955	
7	Tutorial_Sst007.lcd	430.983	39.933	
8	Tutorial_Sst008.lcd	431.190	39.944	
9	Tutorial_Sst009.lcd	373.950	33.449	
10	Tutorial_Unk001.lcd			
11	Tutorial_Unk002.lcd			

Method View - Peak Integration Parameters

Channel: Detector A - Ch1(254nm)

Width: 5 sec

Slope: 1000 uV/min

Drift: 0 uV/min

T. DBL: 1000 min

Min. Area/Height: 1000 counts

Calculated by:  Area  Height

Calib Curve

Y = 57642.99X + 12444.51  
 $r^2 = 0.9999066$   $r = 0.9999533$

Continued on the following page



# 2

## Confirm identification parameters.

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

**ZOOM UP**

**Make sure that these values are appropriate.**

Method View - Identification Parameters

Window/Band:  Window  Band

Window: 5 %

Default Bandwidth: 0.01 min

Identification Method: Absolute Rt

Peak Selection: Closest Peak

Display not identified peaks as peaks with zero area(height)

Add the peaks with zero area(height) to calibration level

Retention Time Update:  None  Replace  Average

Calibration Curve/Spectrum View

Y = 57642.98x + 12444.51  
r<sup>2</sup> = 0.9999066 t = 0.9999533

# 3

## Confirm the Compound Table.

**ZOOM UP**

**Make sure that these time settings are appropriate.**

Method View - Compound Table

ID#	Name	Type	Channel	Ret. Time	Conc. (1)	Conc. (2)	Conc. (3)
1	Methylparaben	Target	Detector A - C	3.046	10	20	40
2	Ethylparaben	Target	Detector A - C	3.924	10	20	40
3	Propylparaben	Target	Detector A - C	5.505	10	20	40
4	Butylparaben	Target	Detector A - C	8.267	10	20	40
5				0.001	10	20	40

Calibration Curve/Spectrum View

Y = 57642.98x + 12444.51  
r<sup>2</sup> = 0.9999066 t = 0.9999533

# 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 .

Y = 57642.996 \* X - 44.51  
R<sup>2</sup> = 0.9999666

Data Filename	Height	Conc. (mg/L)	Std. Conc.
Tutorial_Std001.lcd	108.362	9.831	10
Tutorial_Std002.lcd	108.360	9.889	10
Tutorial_Std003.lcd	108.206	9.885	10
Tutorial_Std004.lcd	218.591	20.172	20
Tutorial_Std005.lcd	218.192	20.168	20
Tutorial_Std006.lcd	218.269	20.152	20
Tutorial_Std007.lcd	430.746	39.955	40
Tutorial_Std008.lcd	430.983	39.933	40
Tutorial_Std009.lcd	431.190	39.944	40
Tutorial_Unk001.lcd	---	---	---
Tutorial_Unk002.lcd	373.550	33.449	---

ID#	Name	Type	Channel
1	Methylparaben	Target	Detector A - C
2	Ethylparaben	Target	Detector A - C
3	Propylparaben	Target	Detector A - C
4	Butylparaben	Target	Detector A - C

# 5 Save the method file and data file.

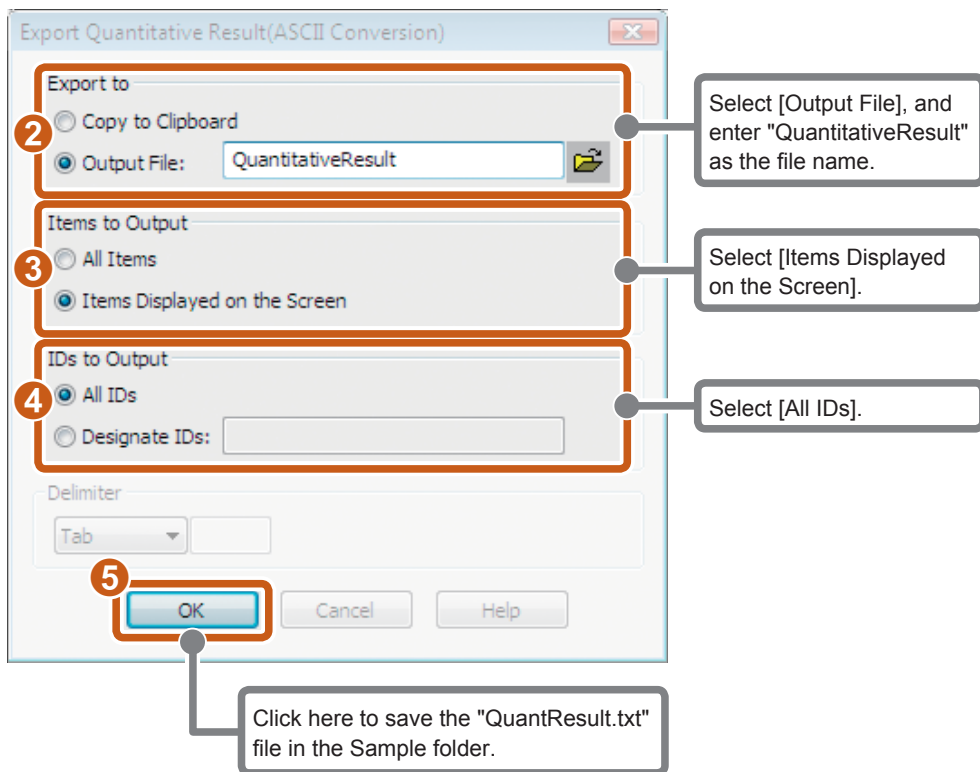
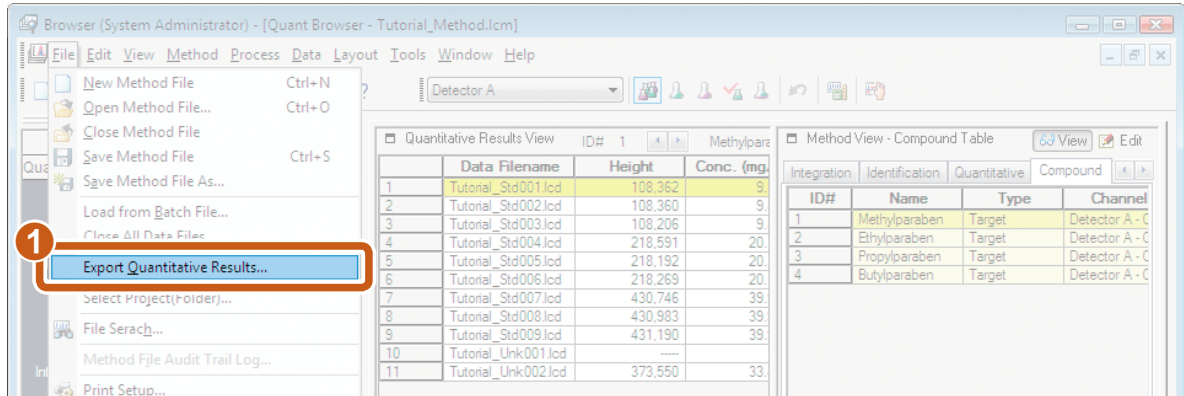
Save the method file and data file.

Data Filename	Sample Type
Tutorial_Std001.lcd	Standard(Calc. Pd)
Tutorial_Std002.lcd	Standard(Calc. Pd)
Tutorial_Std003.lcd	Standard(Calc. Pd)
Tutorial_Std004.lcd	Standard(Calc. Pd)
Tutorial_Std005.lcd	Standard(Calc. Pd)
Tutorial_Std006.lcd	Standard(Calc. Pd)
Tutorial_Std007.lcd	Standard(Calc. Pd)
Tutorial_Std008.lcd	Standard(Calc. Pd)
Tutorial_Std009.lcd	Standard(Calc. Pd)
Tutorial_Unk001.lcd	Unknown
Tutorial_Unk002.lcd	Unknown

ID#	Name	Type	Channel
1	Methylparaben	Target	Detector A.
2	Ethylparaben	Target	Detector A.
3	Propylparaben	Target	Detector A.
4	Butylparaben	Target	Detector A.

# Export Quantitative Calculation Results

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



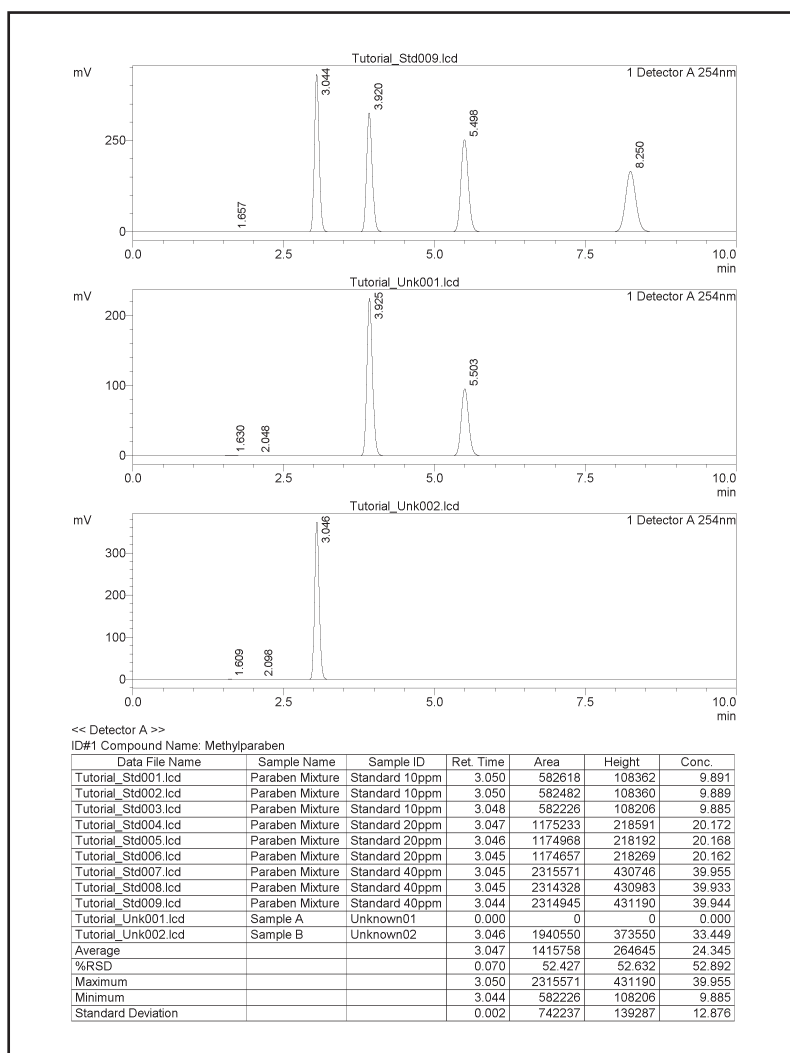
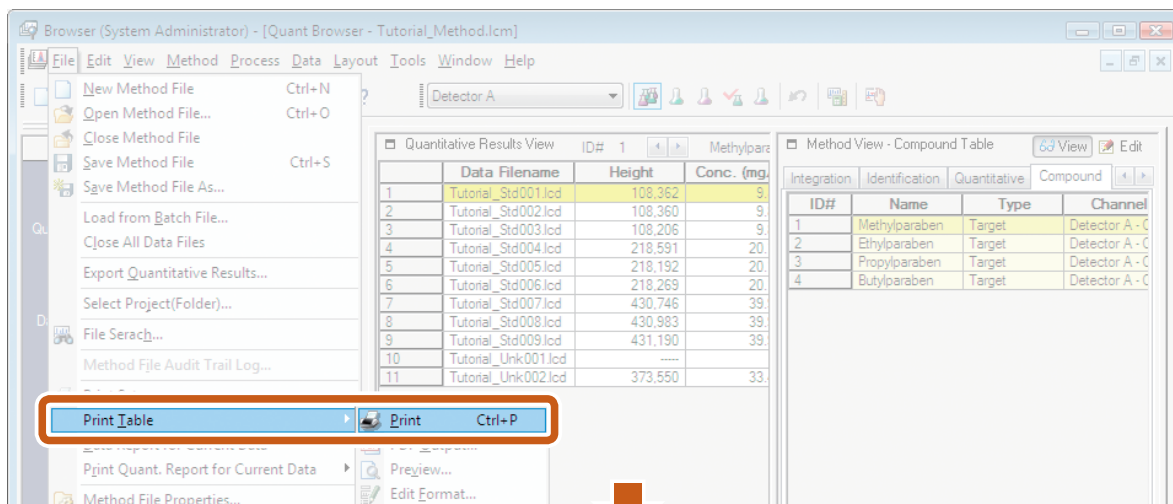
Refer to "Export the Quantitative Results" of the "Quant Browser" chapter in *Operators Guide* for details on exporting quantitative results.

LabSolutions



# Print the Quantitative Results Table

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



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

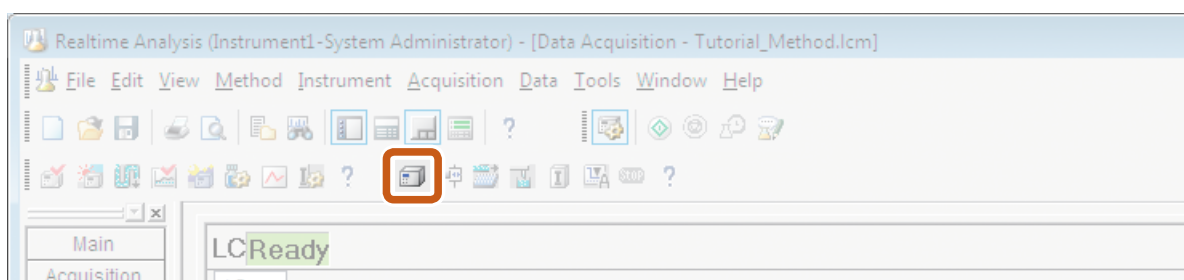
# Chapter 7 ShutDown

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

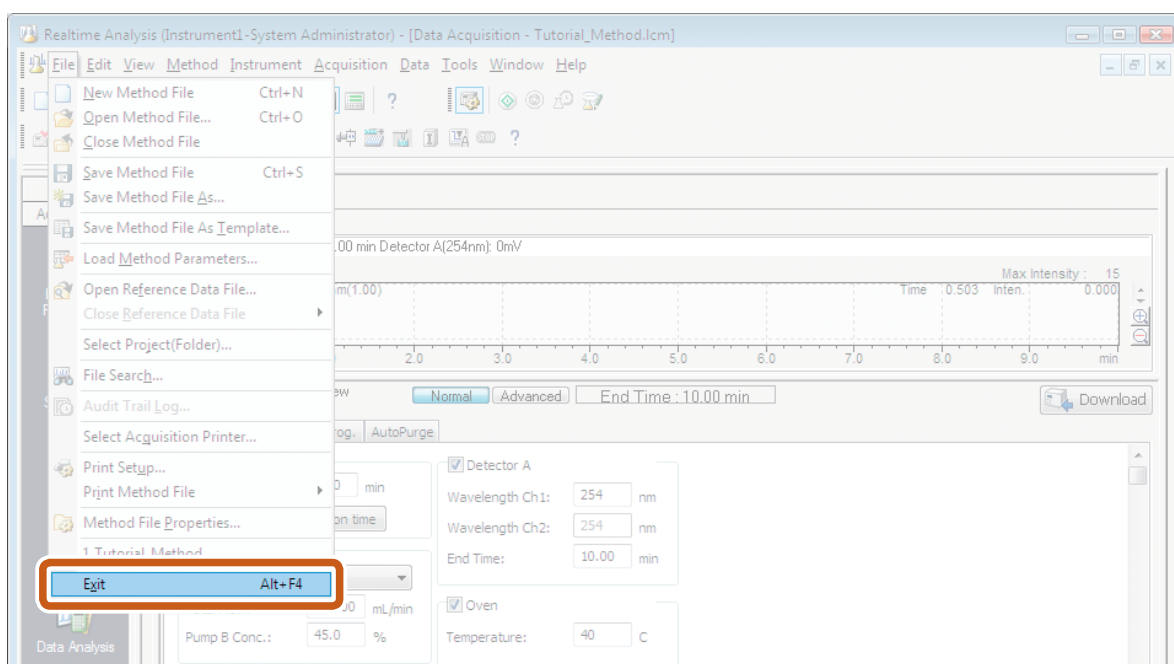
## 1 Stop instrument operation.

Stop pump solvent delivery and heating of the column oven.

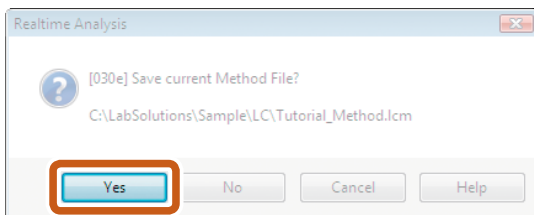
## 2 Set to OFF.



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



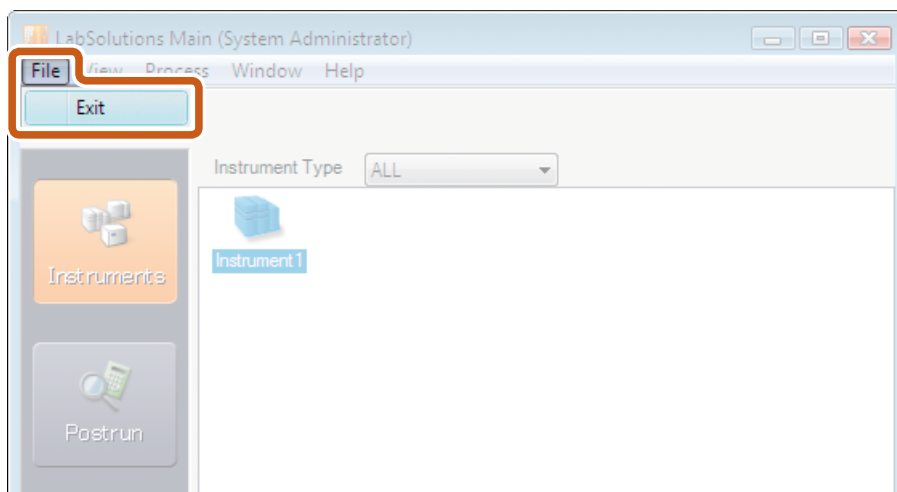
## 4 Click [Yes].



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.