SHIMADZU

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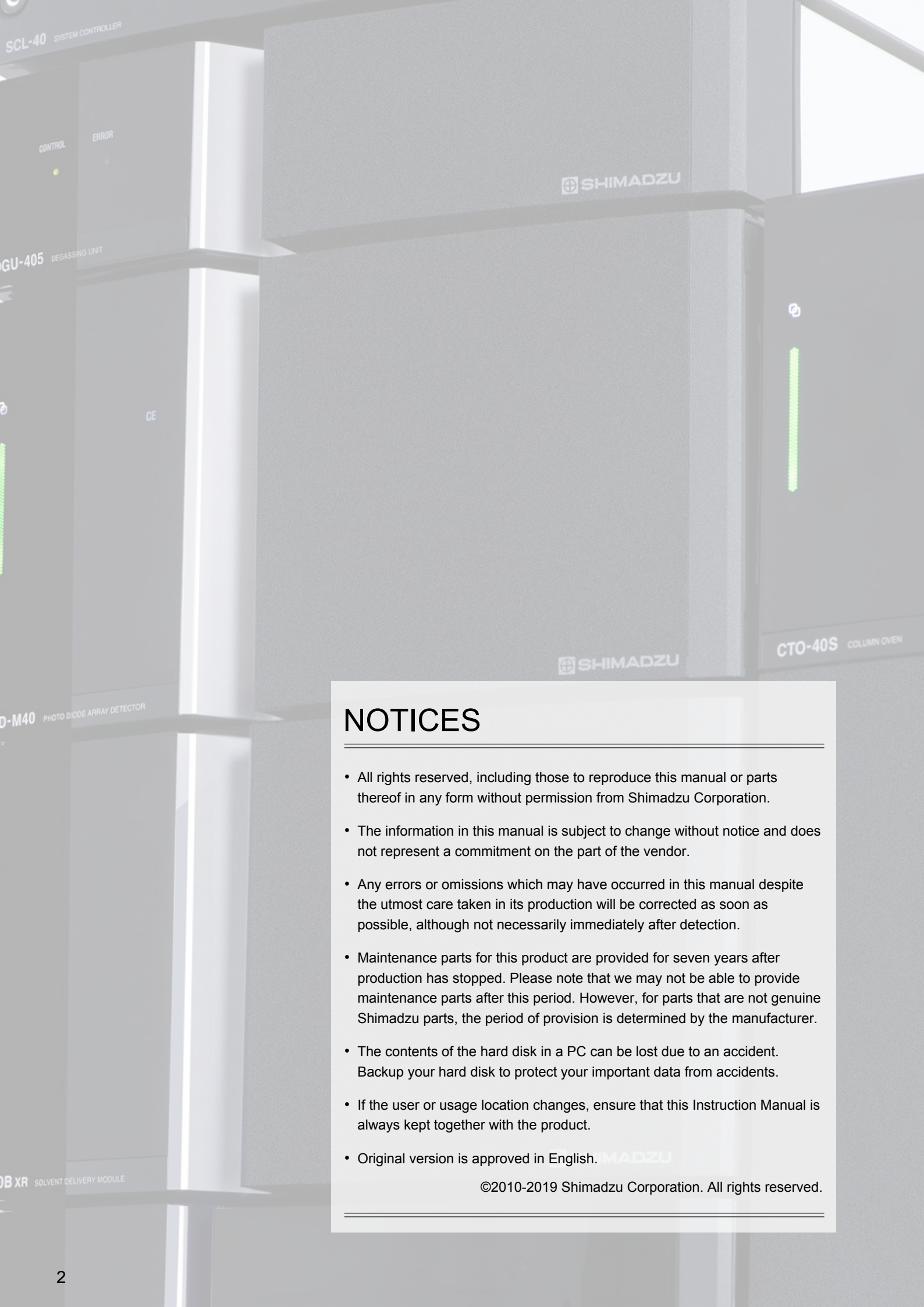
LabSolutions™

LC Getting Started Guide



NOTICES

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- 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.

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

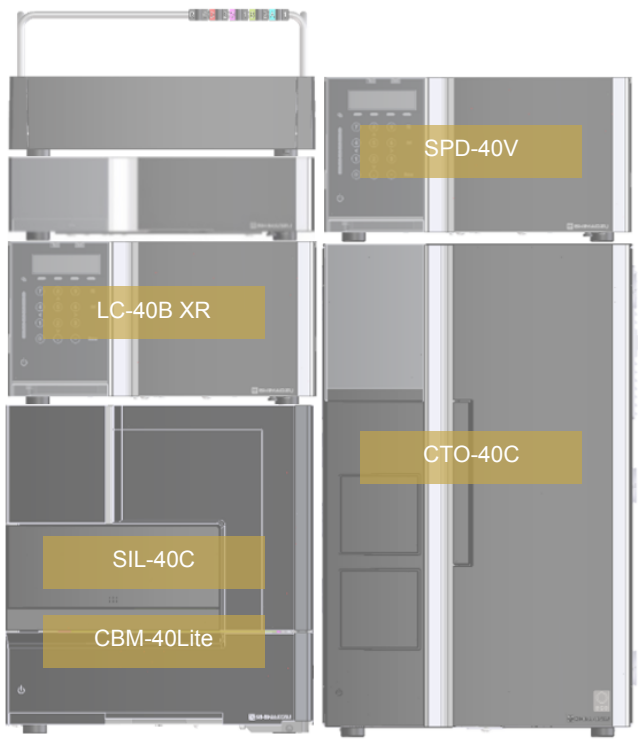
LabSolutions software is very easy to use, while incorporating high-grade functions. It provides powerful support for automating and improving the efficiency of sequential data acquisition and analysis operations.
Use LabSolutions to perform the following functions.

- 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 benzonic 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.

Reference *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.

Reference *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.

Reference *5* **Realtime Batch** P.31

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

STEP 5

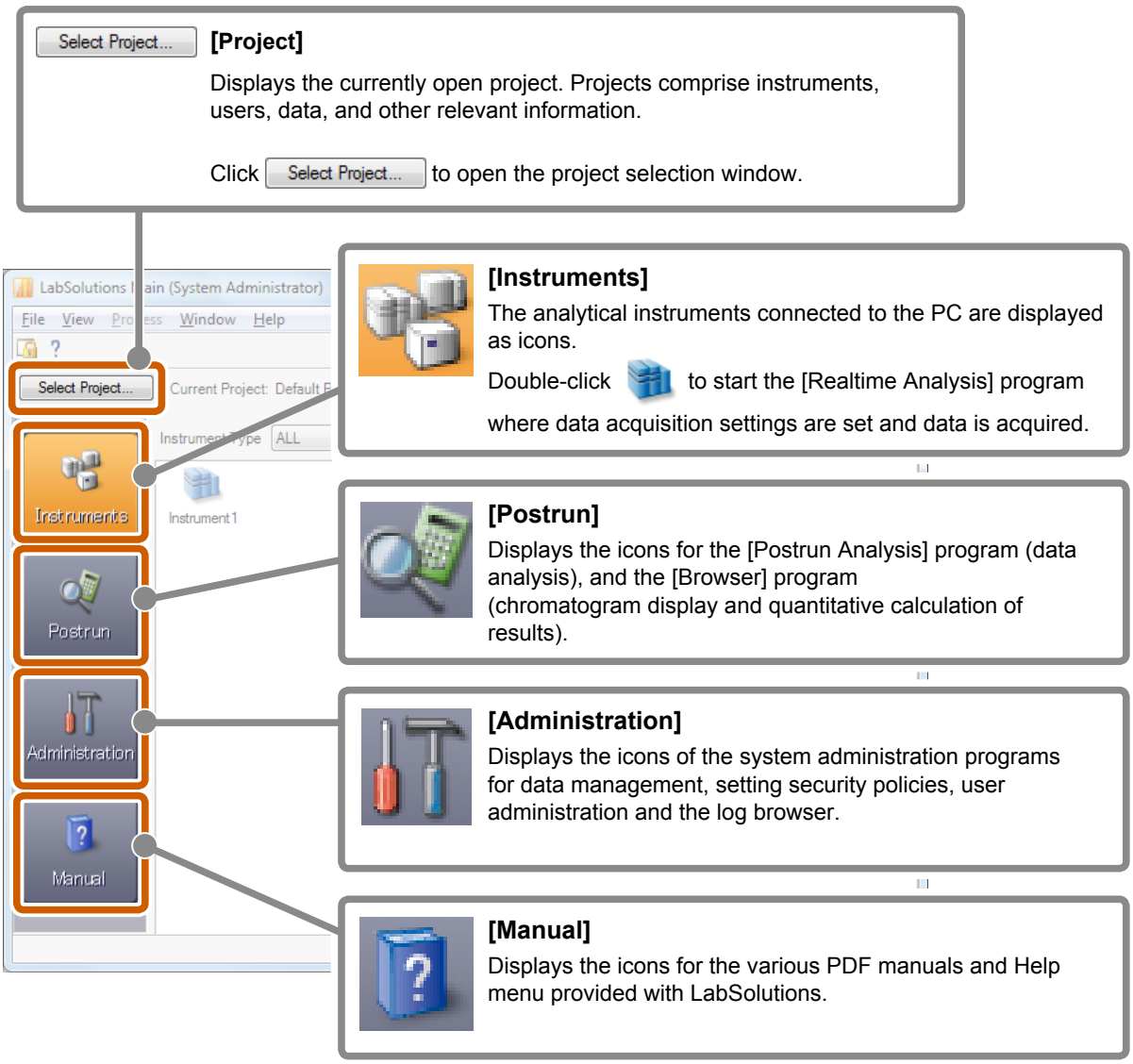
Data Management

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

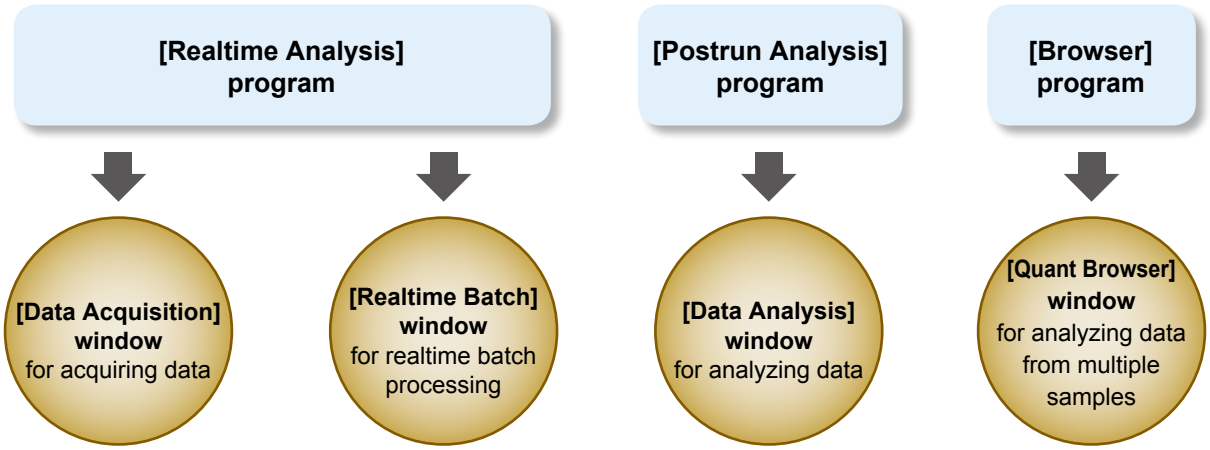
The Data Manager can display PDF files created during data acquisition.

Reference *7* **Data Management** P.48

LabSolutions Main Window

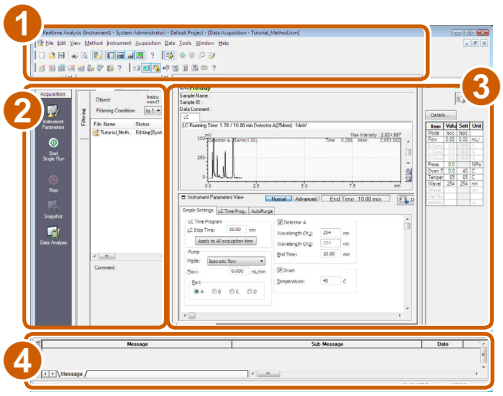


LabSolutions Main Programs and Main Windows



LabSolutions Windows

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

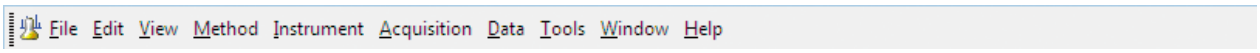


1 Title Bar

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

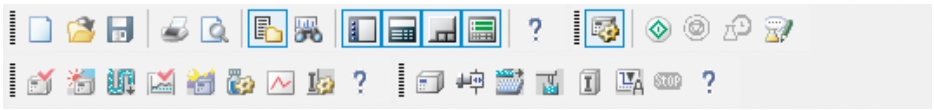
Menu Bar

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



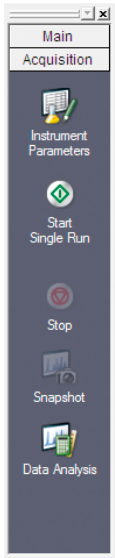
Toolbar

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

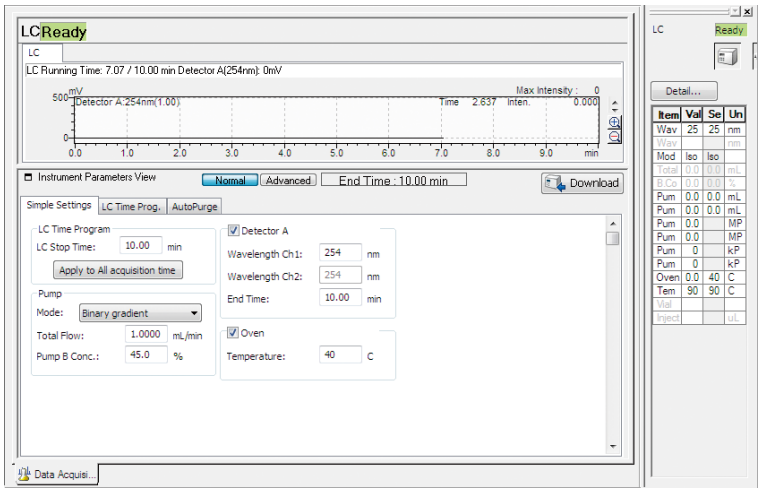
This sub-window displays files for the selected project and instruments.

3 Window

In the [Realtime Analysis] program, [Data Acquisition], [Realtime Batch] and other windows are displayed as icons on the assistant bar.

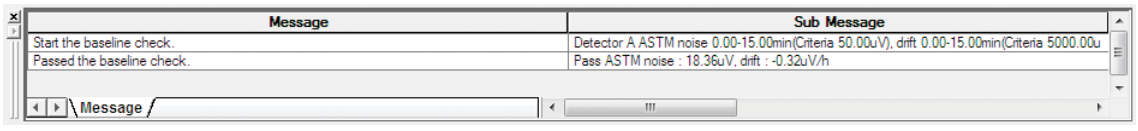
In the [Postrun Analysis] program, [Data Analysis], [PDA Data Analysis], [Calibration Curve], [Report Format] and other windows are displayed.

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.

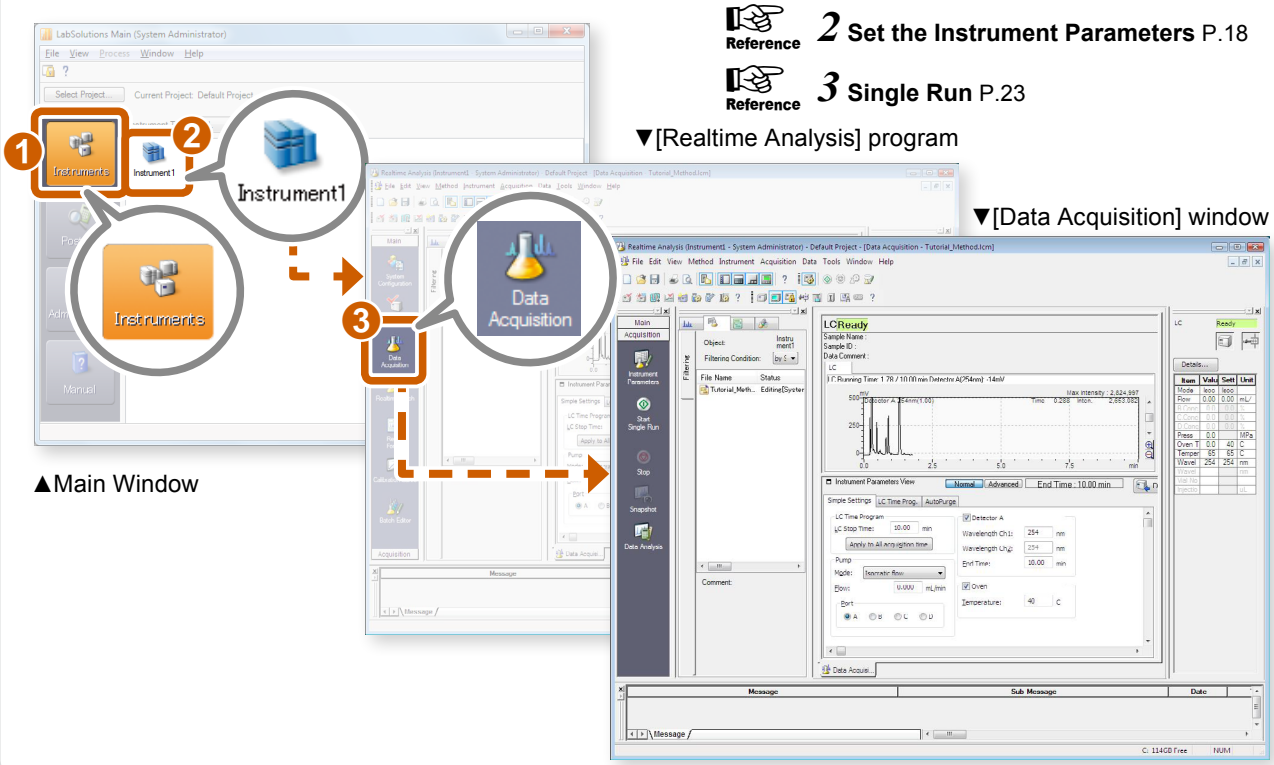
Reference *1* **Start Up** P.12

Set the Data Acquisition Parameters and Execute a Single Run:

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

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

Reference *3* **Single Run** P.23



▲Main Window

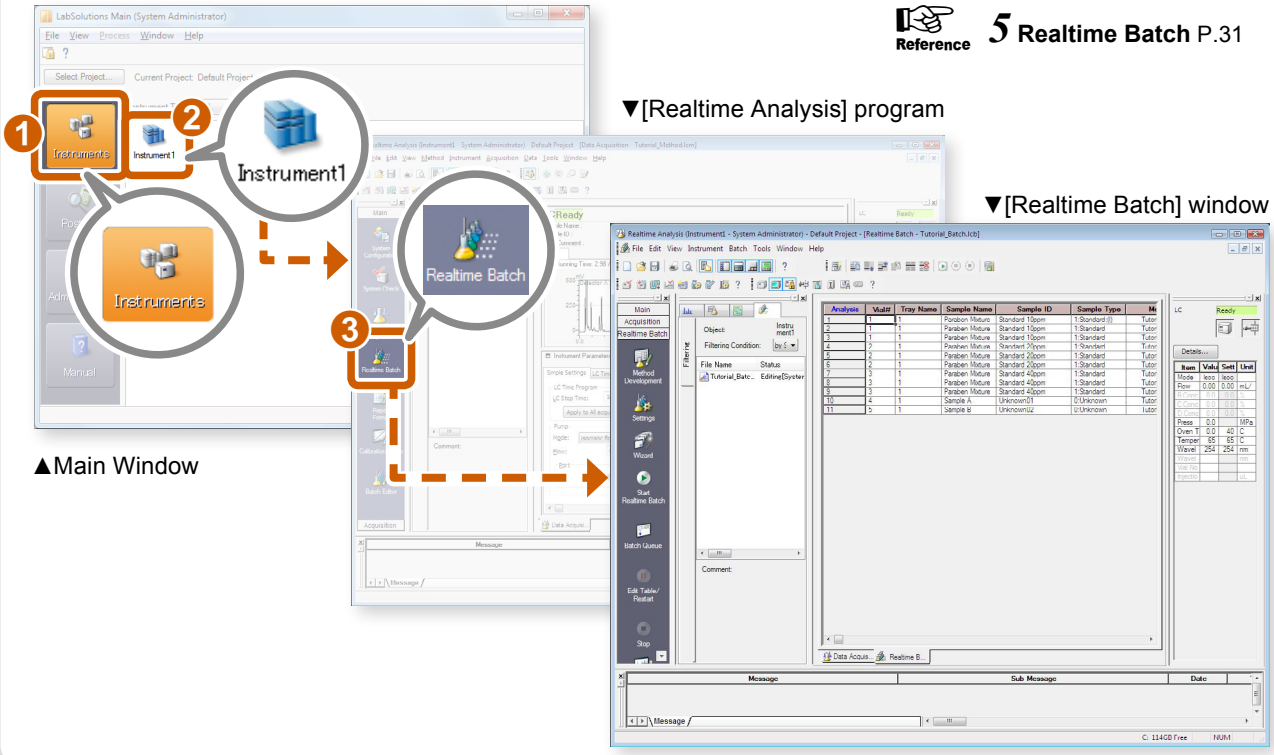
▼[Realtime Analysis] program

▼[Data Acquisition] window

Continuous Data Acquisition of Sequential Samples:

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

Reference *5* **Realtime Batch** P.31



▲Main Window

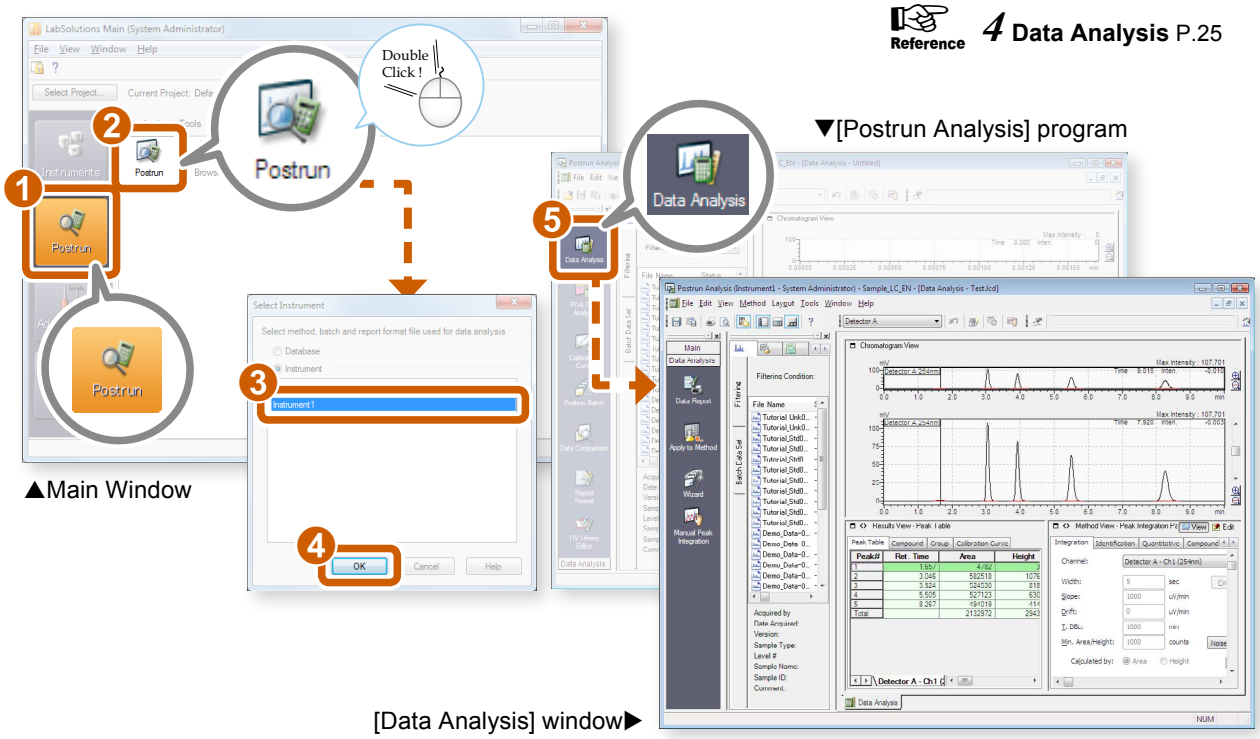
▼[Realtime Analysis] program

▼[Realtime Batch] window

Data Analysis and Quantitative Calculations:

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

Reference *4* **Data Analysis** P.25



▼[Postrun Analysis] program

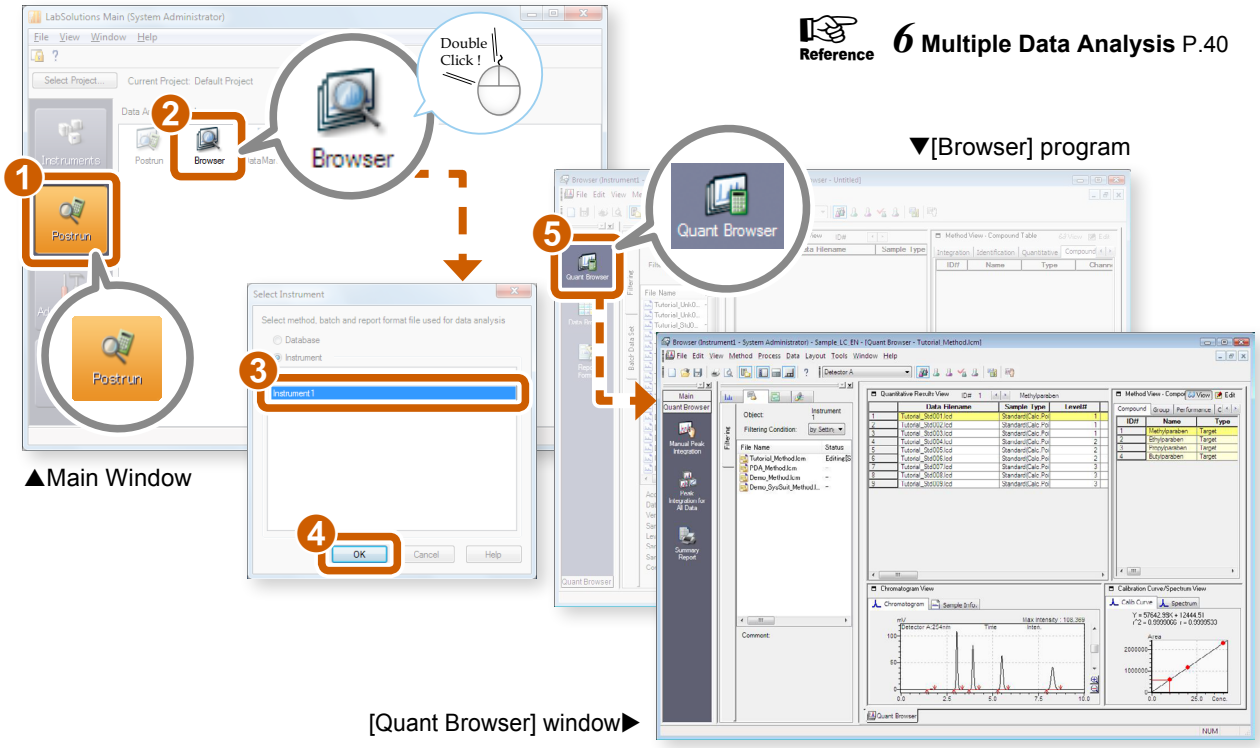
▲Main Window

[Data Analysis] window▶

Multiple Data Analysis and Quantitative Calculations:

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

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



▼[Browser] program

▲Main Window

[Quant Browser] window▶

Chapter 1

Start Up

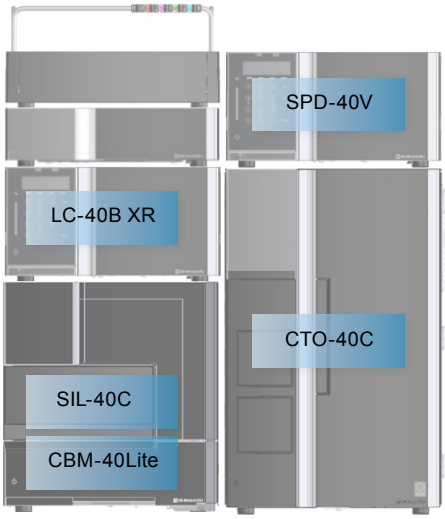
This chapter describes how to start up LabSolutions.

Reference 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.

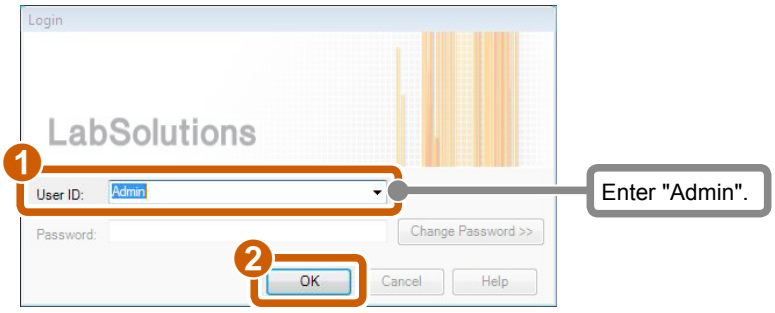


3 Turn the PC and printer on.

4 Double-click  on the desktop.

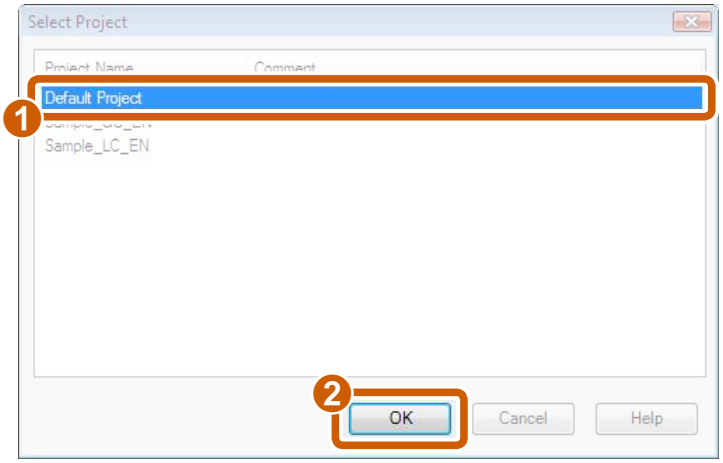
The [Login] sub-window opens.

5 Log in.



6 Select a project.

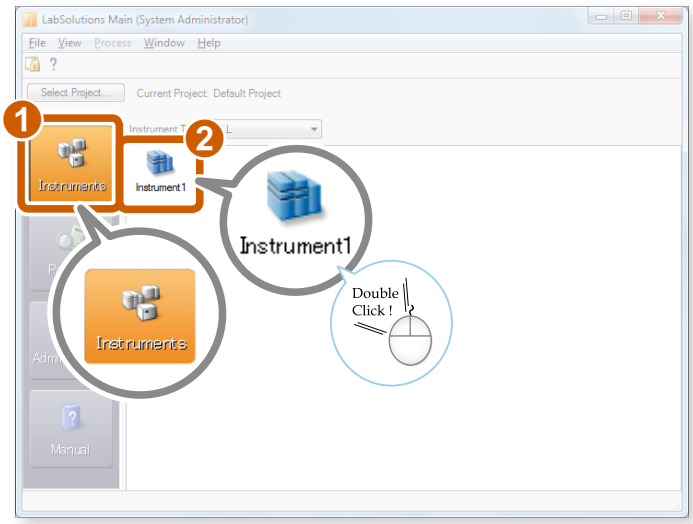
Upon initial startup, the project selection window is displayed after logging in. In this case, select the desired project. For subsequent startups, the [Realtime Analysis] program opens using the project selected when the previous session was closed.



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.

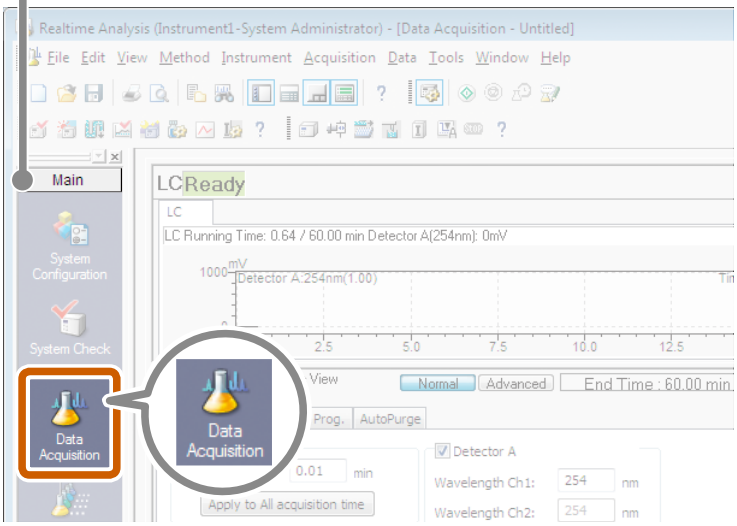
7 Open the [Realtime Analysis] program.



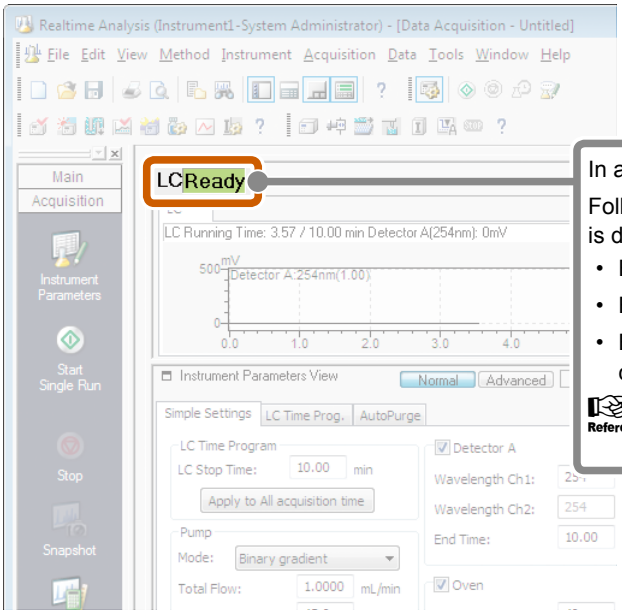
Continued on the following page

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

SUPPLEMENT

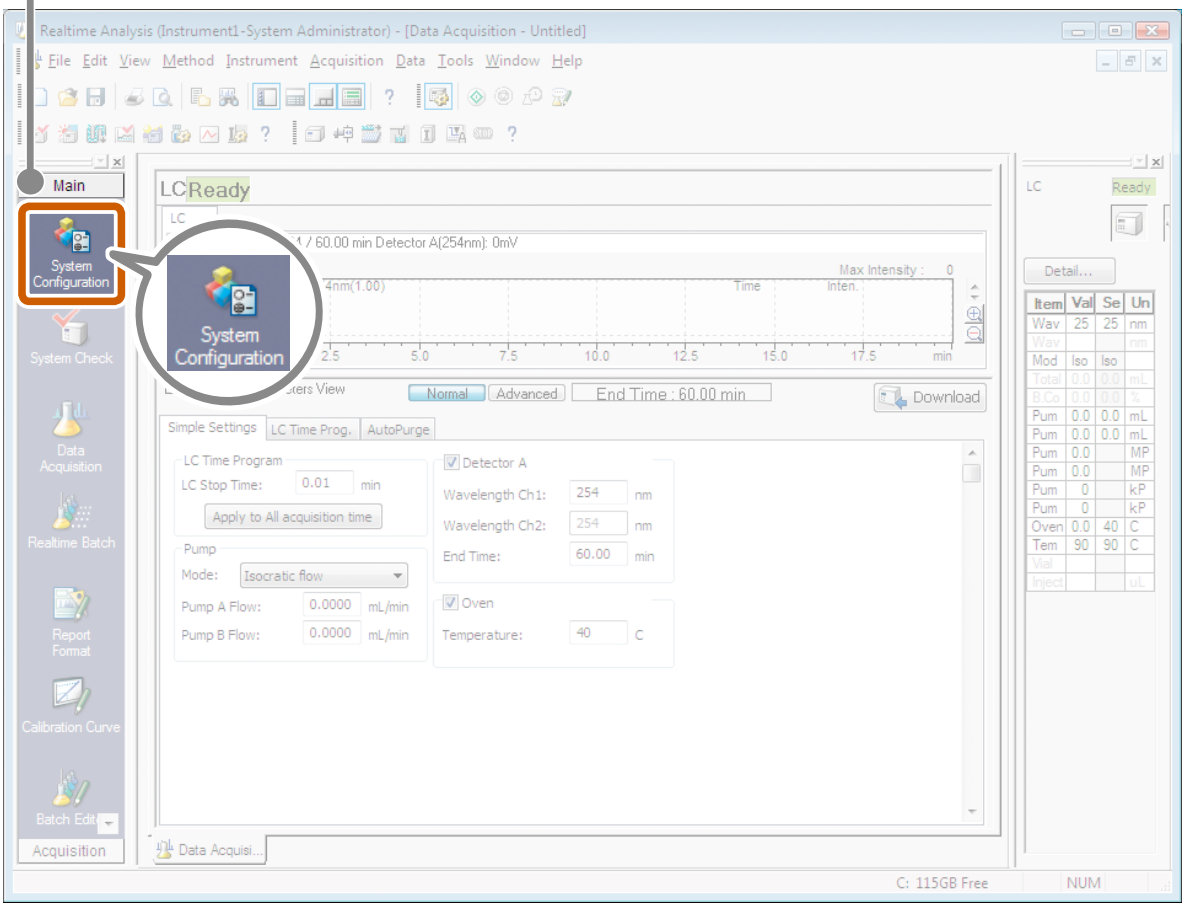
"I want to connect to the system."
"I want to change the system configuration."

In such cases

Re-Set the System Configuration.

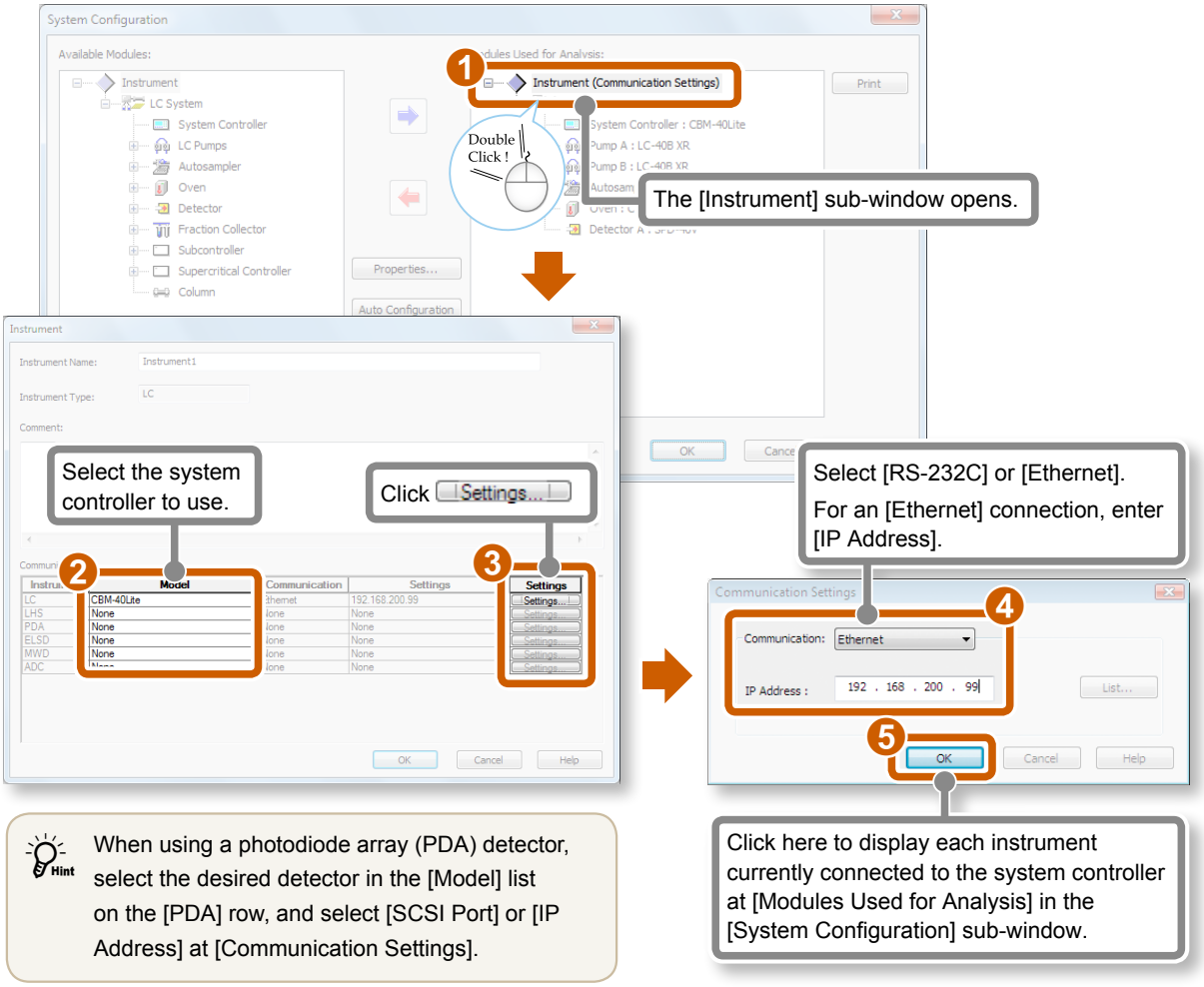
1 Open the [System Configuration] sub-window.

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



The [System Configuration] sub-window opens.

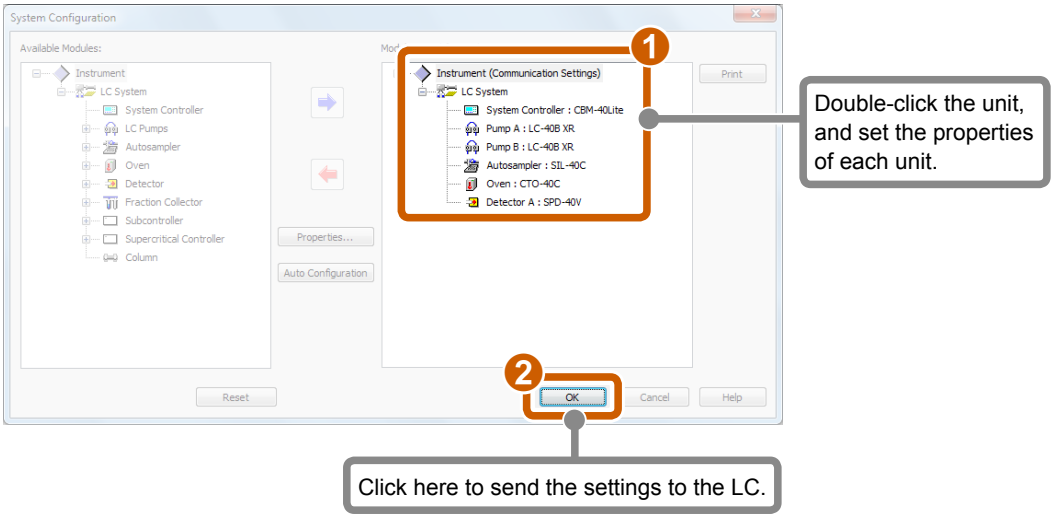
2 Open the [Data Acquisition] window.



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.



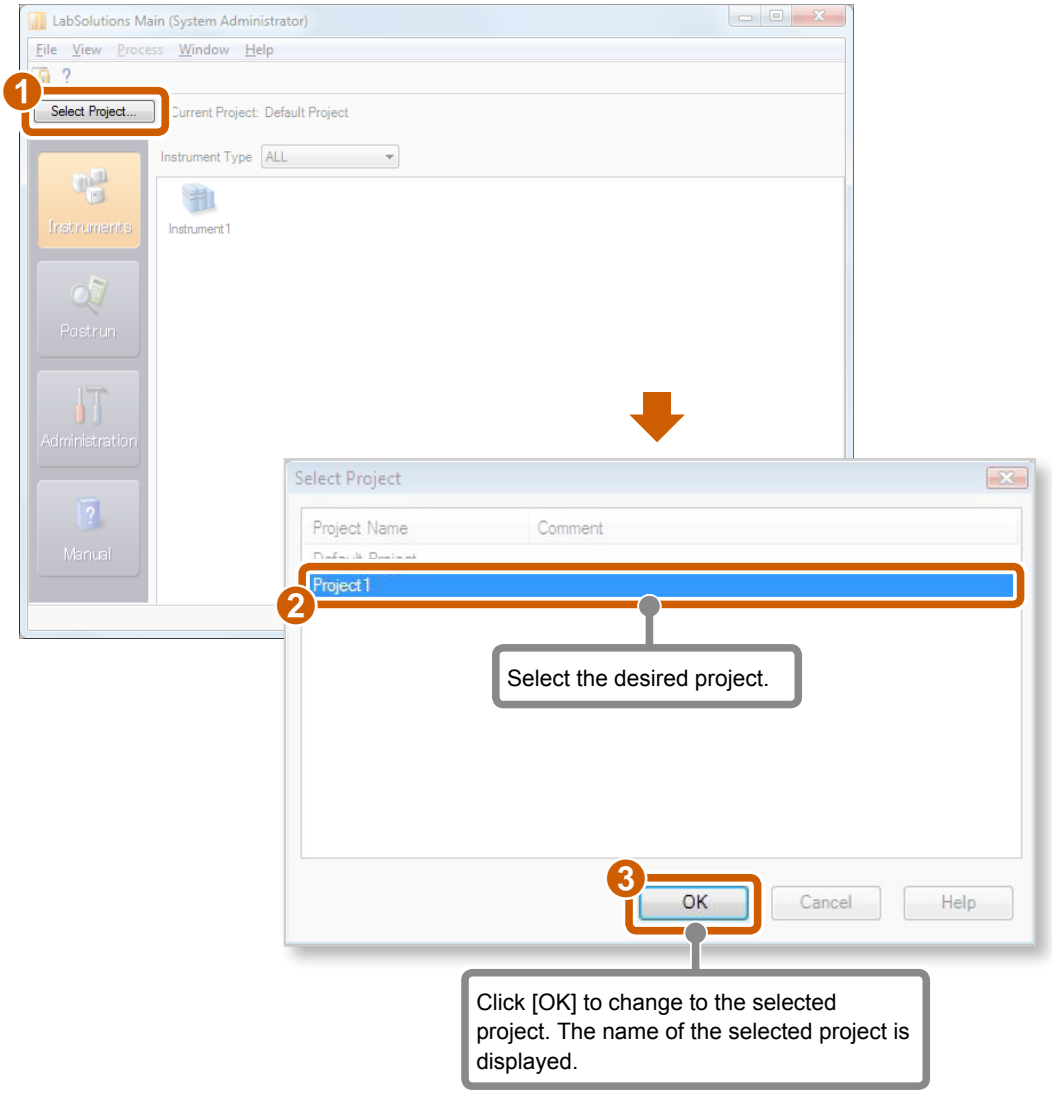
LabSolutions

SUPPLEMENT

"I want to change to another project."

In such cases

Click [Select Project].



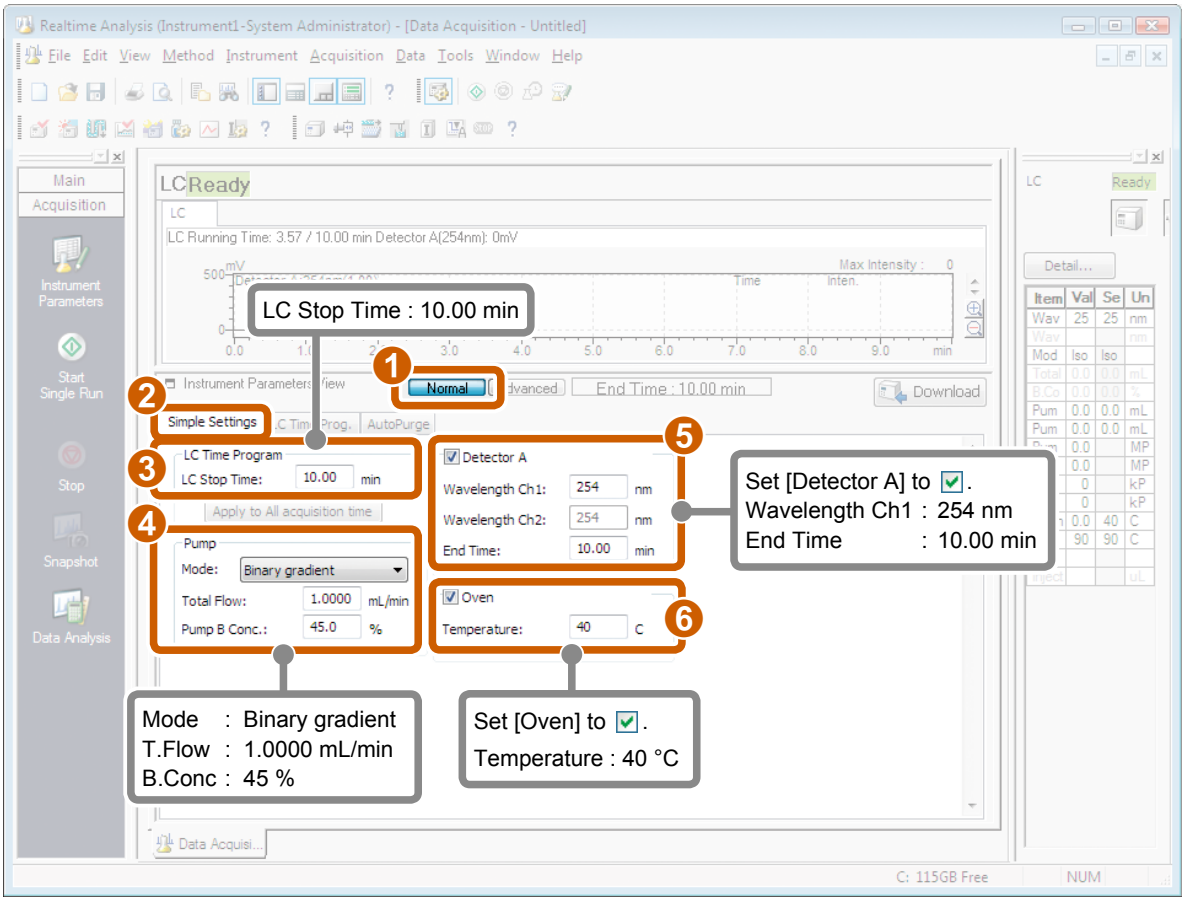
Chapter 2

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.

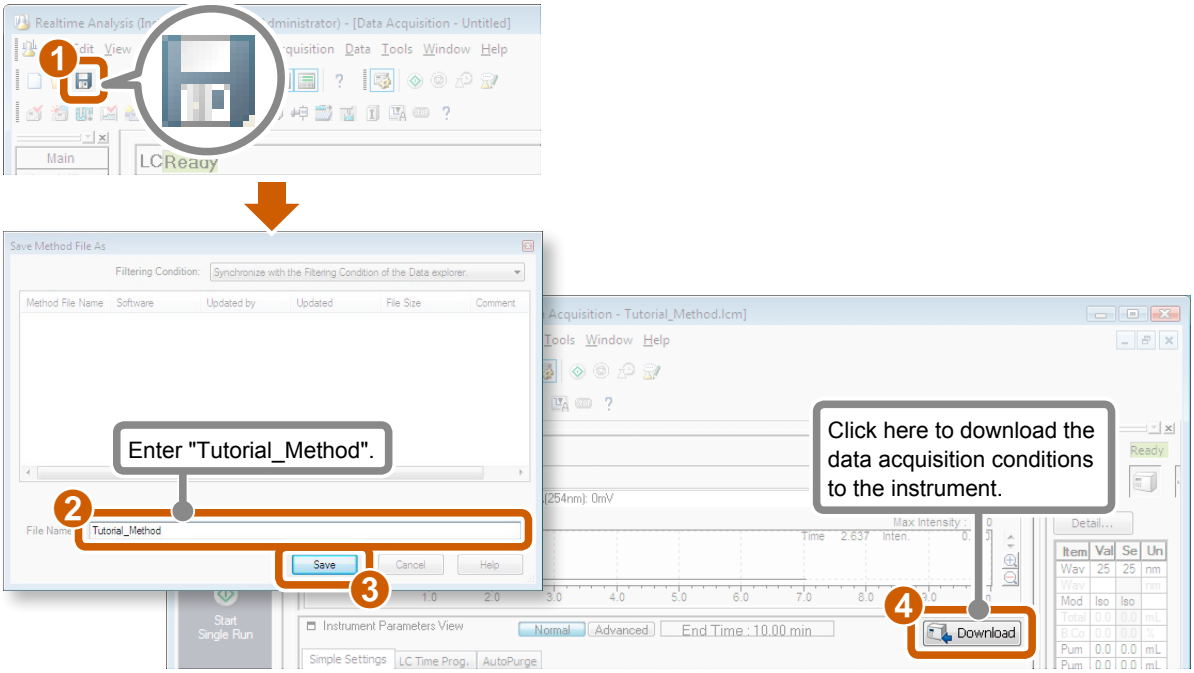
2 Set each of the parameters on the [Simple Settings] tab.



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.

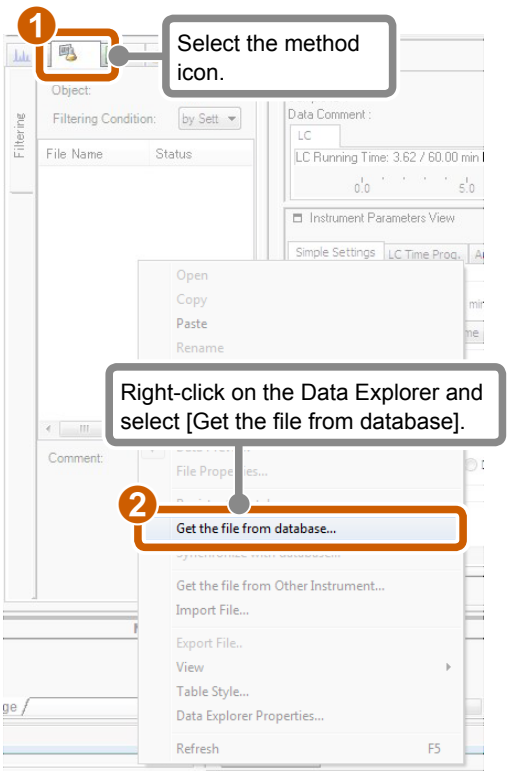
3 Save the data acquisition conditions.

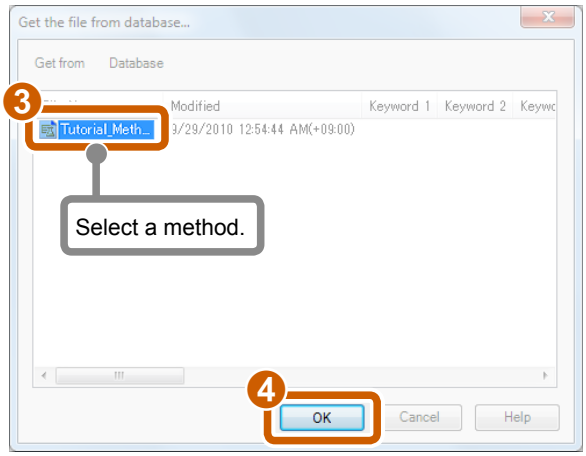


LabSolutions

SUPPLEMENT

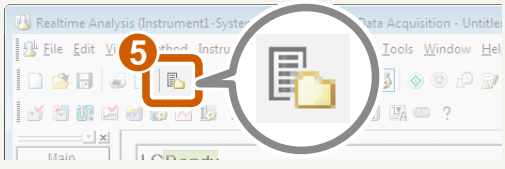
Retrieve a method from the database using the Data Explorer and perform analysis.





Hint

Click on the "Display Data Explorer" icon if the Data Explorer is hidden.

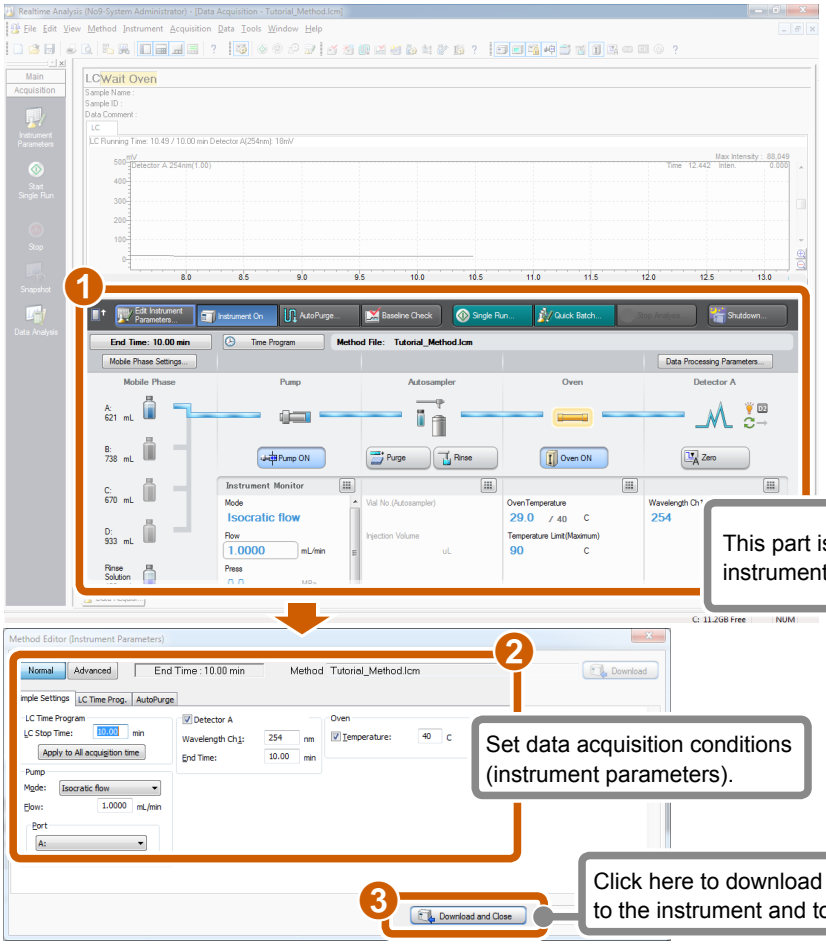


LabSolutions

SUPPLEMENT

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.



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

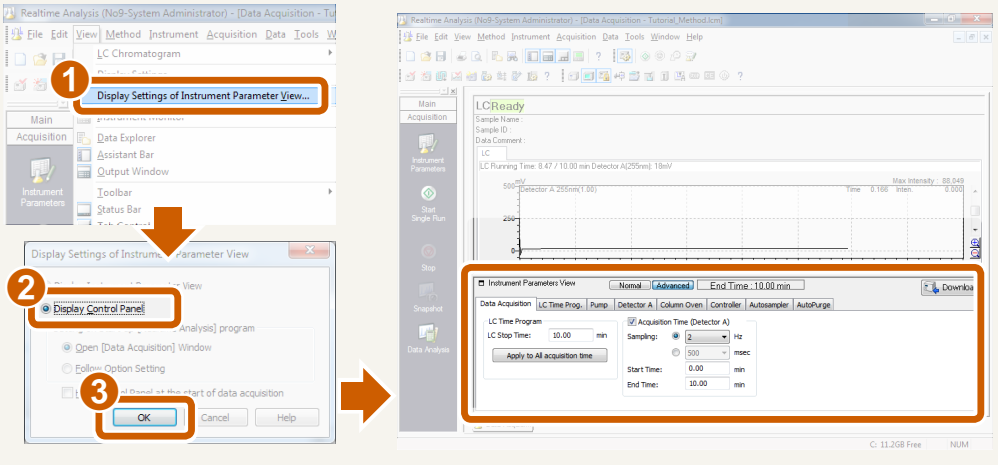
Set data acquisition conditions (instrument parameters).

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

Hint

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.



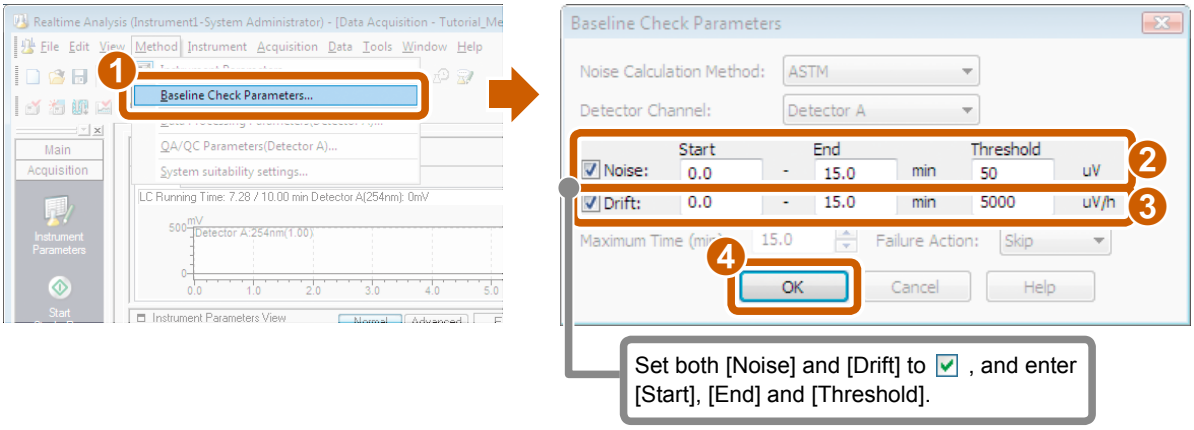
LabSolutions

SUPPLEMENT

Baseline Check

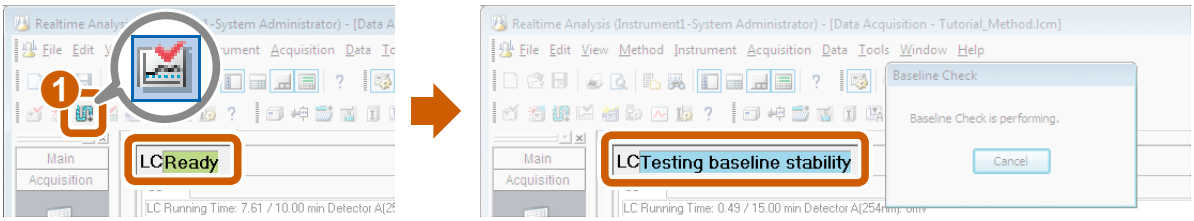
By the baseline check, you can check whether or not noise and drift values on the baseline are within the preset time and at the threshold or below.
Baseline check parameters are saved in the method file.

1 Set [Baseline Check Parameters].



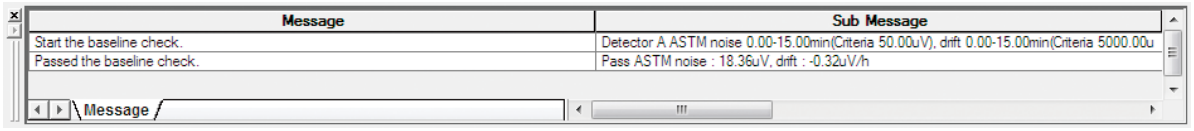
Hint In the [Baseline Check] sub-window, the noise calculation method can be changed, and the maximum delay time when the result of the baseline check is [Fail] within the preset time. Reference Help for details.

2 Perform the baseline check.



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

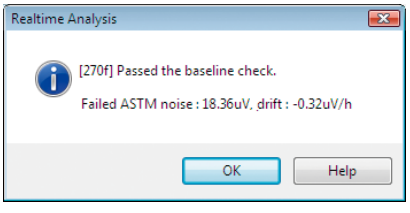
Output Window



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

Message

Baseline Check Results



LabSolutions

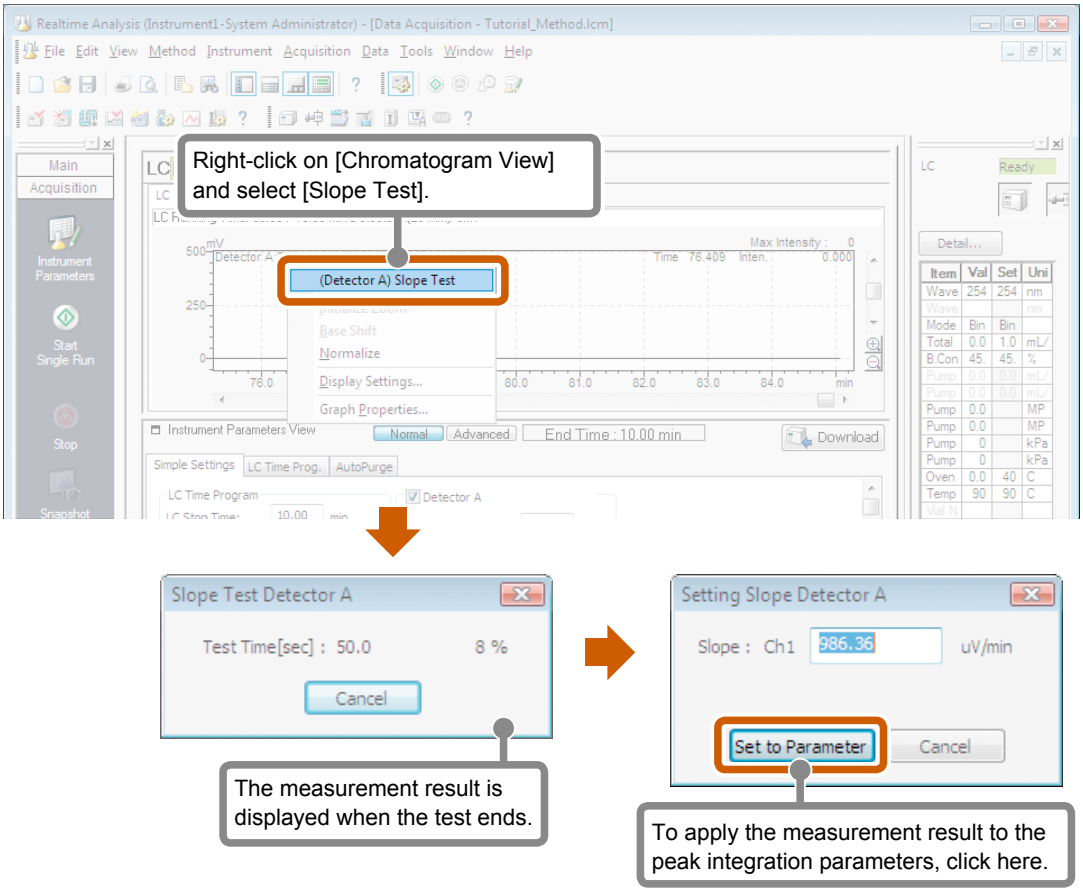
SUPPLEMENT

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.

Hint

- 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 a 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.



Hint

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".

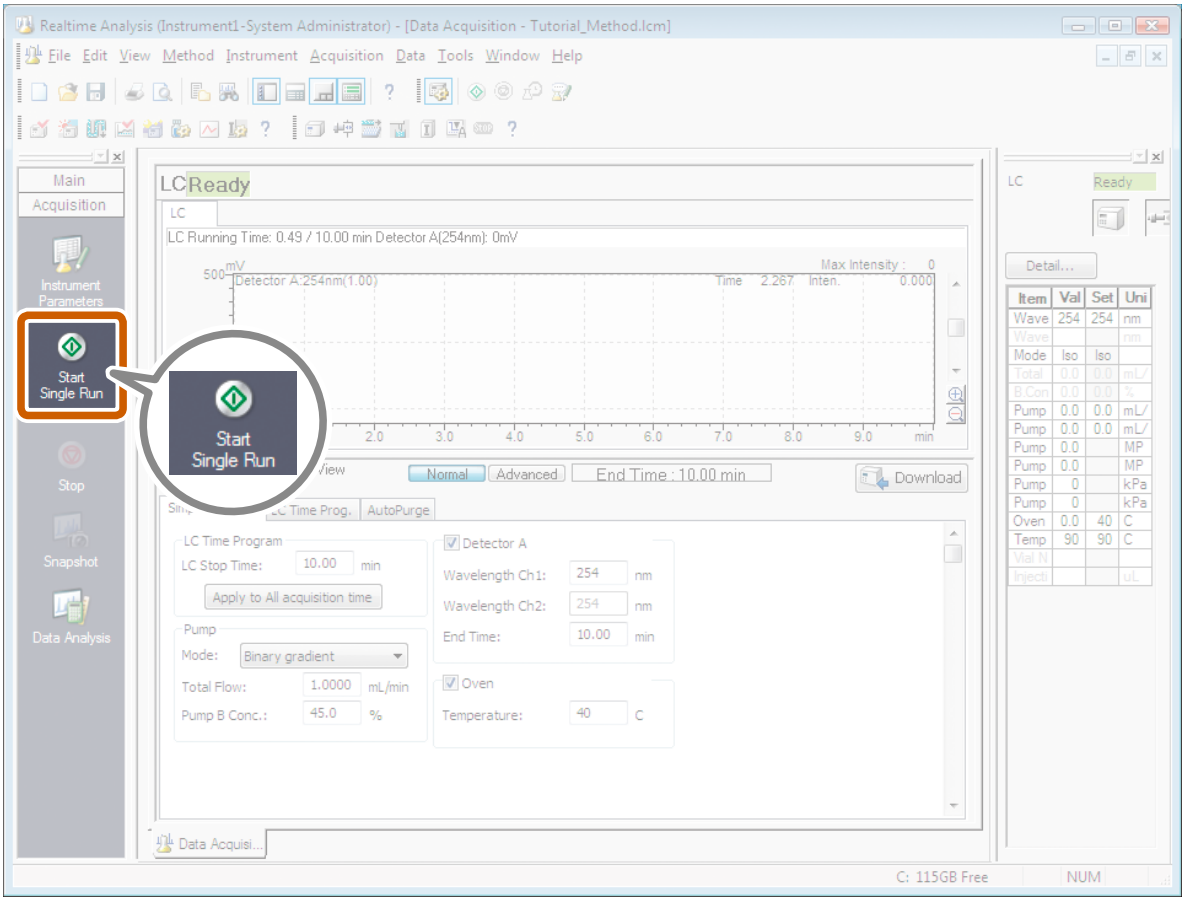
Chapter 3

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.

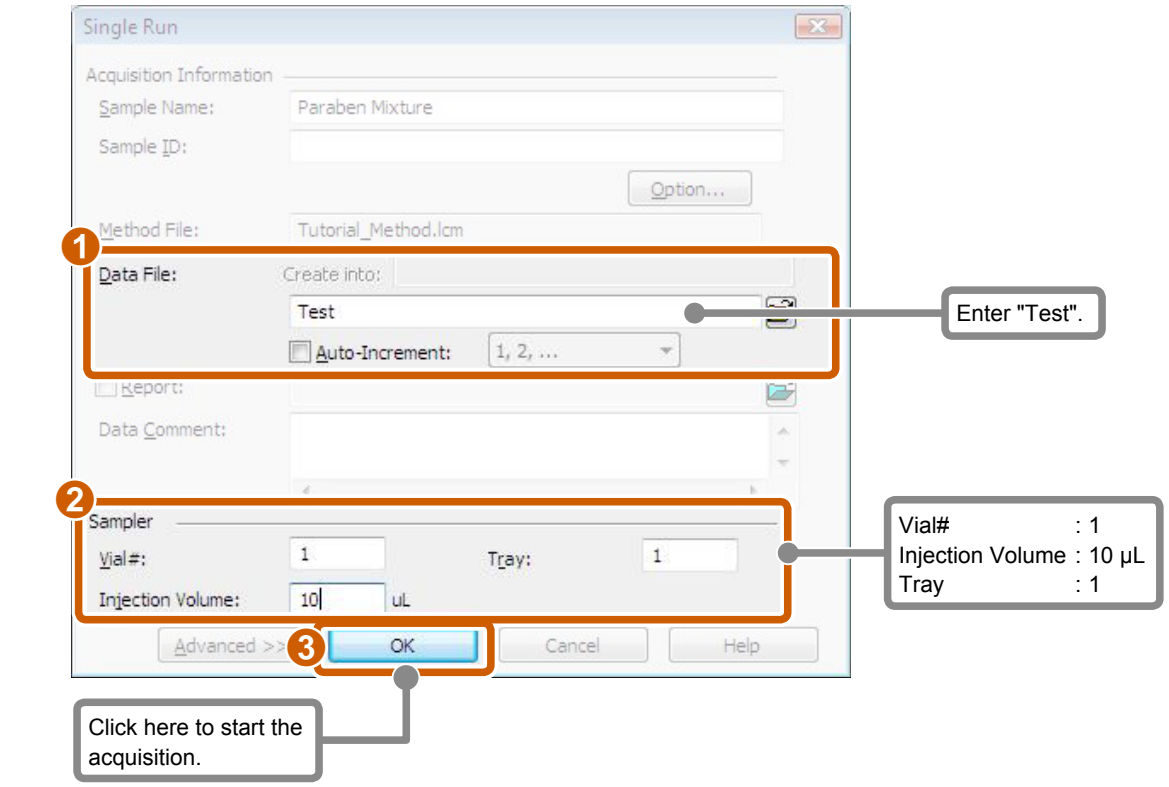
2 Open the [Single Run] sub-window.



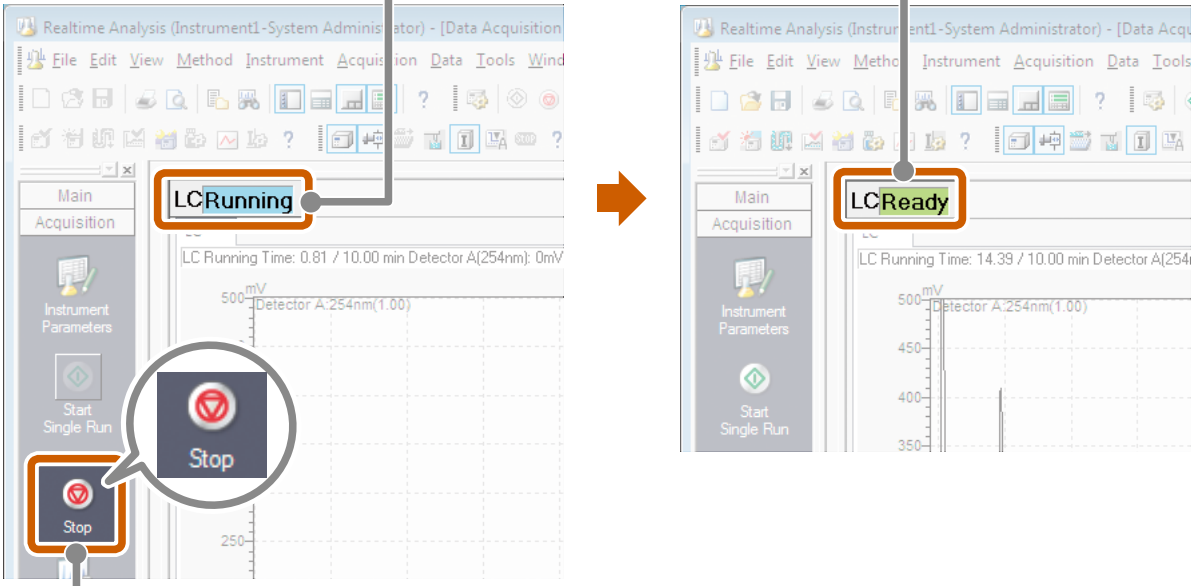
The [Single Run] sub-window opens.

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.



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



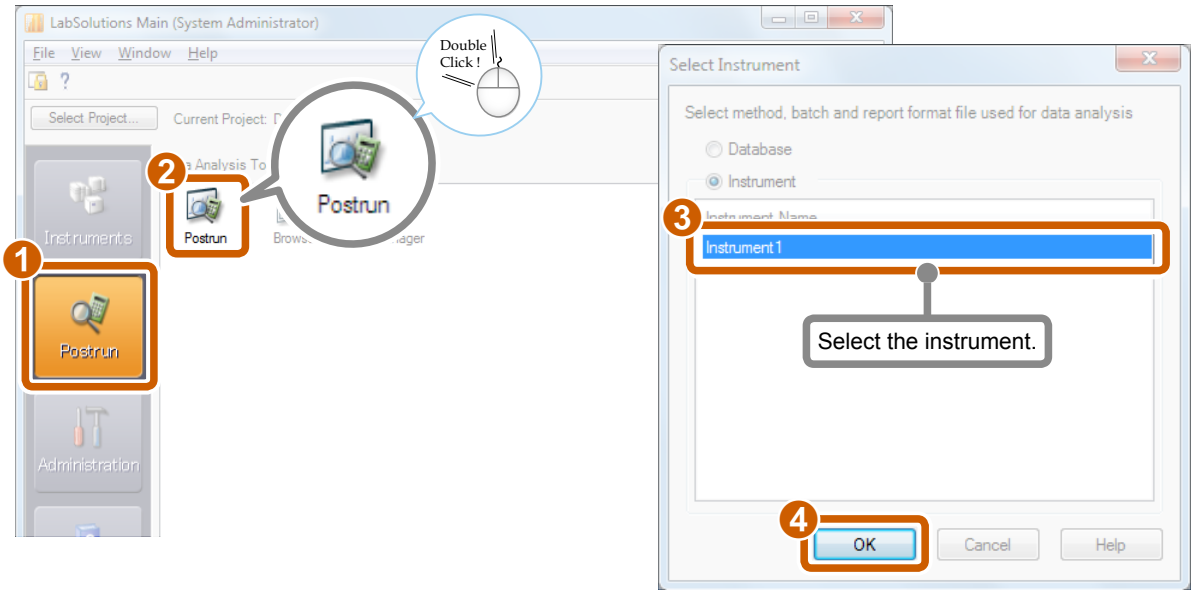
Hint Click here to cancel data acquisition midway.

Chapter 4

Data Analysis

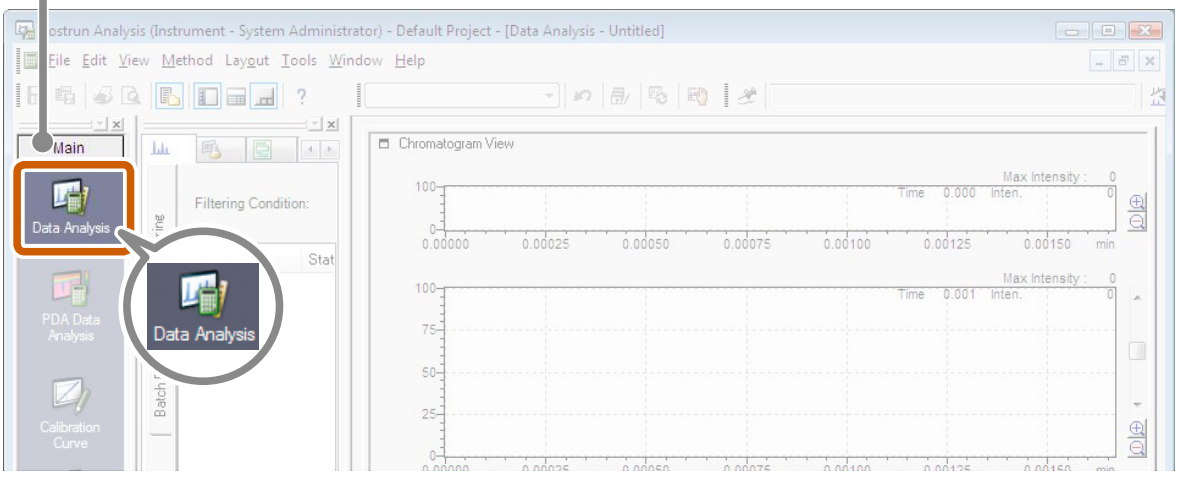
After single run ends, check the data to see if the peaks have been detected correctly. This chapter describes how to change the peak integration conditions of the data file "Test.lcd" obtained by performing single run to optimize the peak integration parameters.

1 Open the [Postrun Analysis] program.



2 Open the [Data Analysis] window.

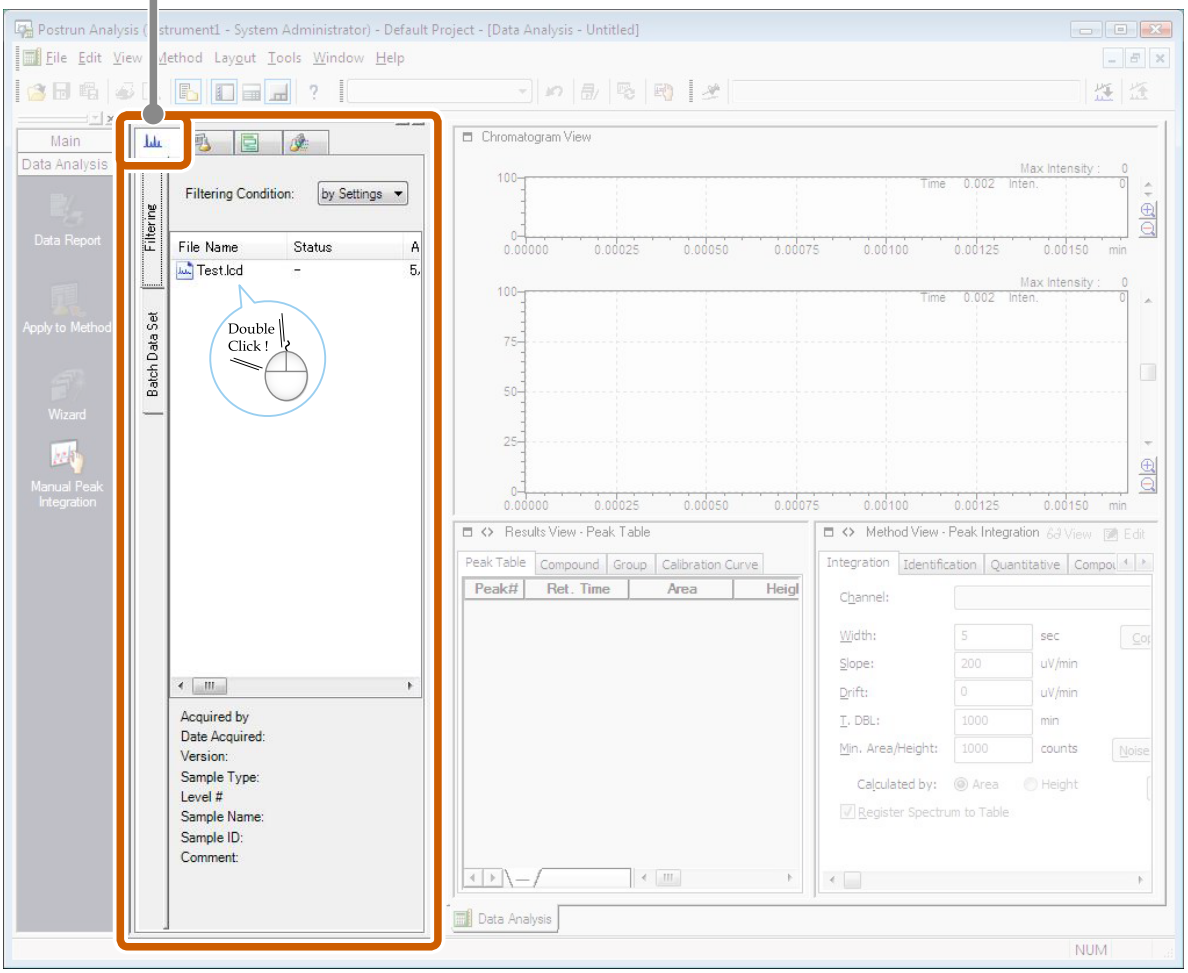
Hint Click here if the [Main] assistant bar is not displayed.



The [Data Analysis] window opens.

3 Display "Test.lcd".

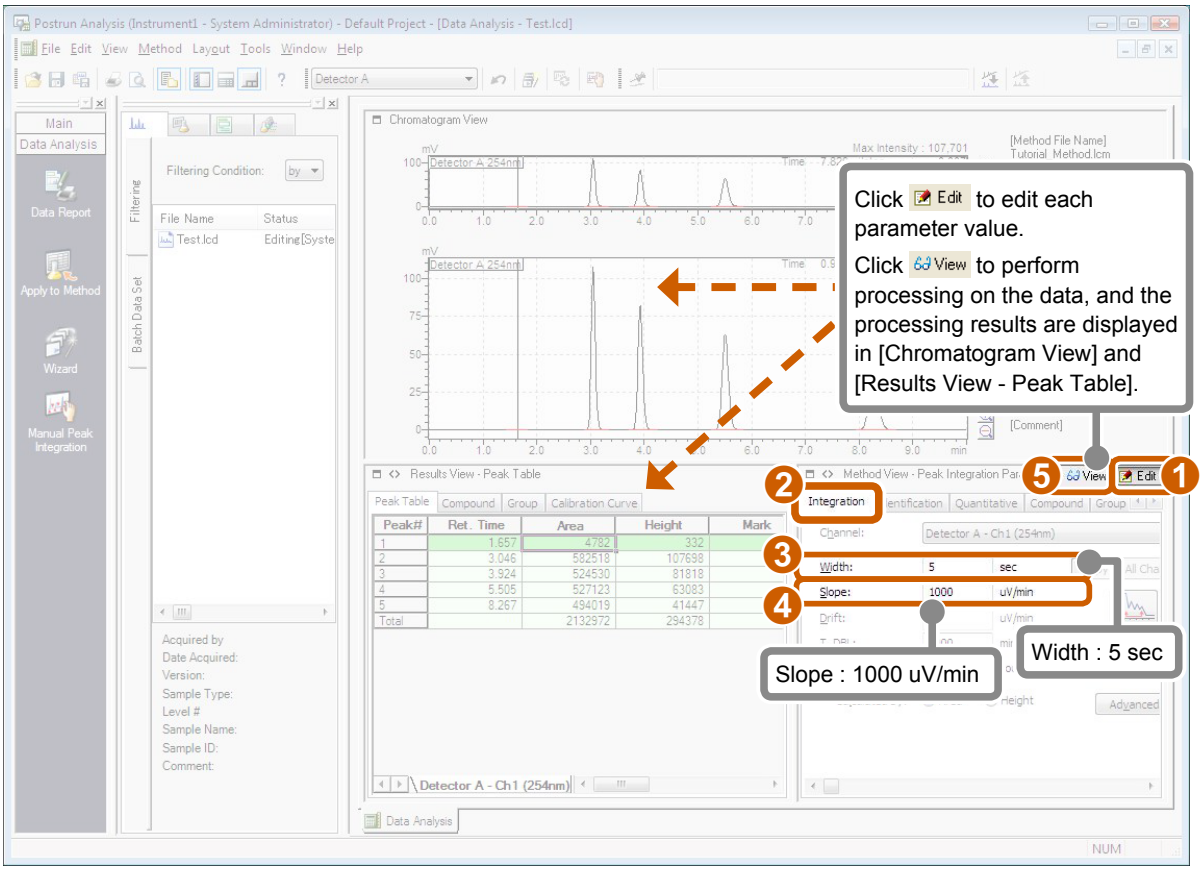
Click on the upper section of the Data Explorer and then double-click "Test.lcd".



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.



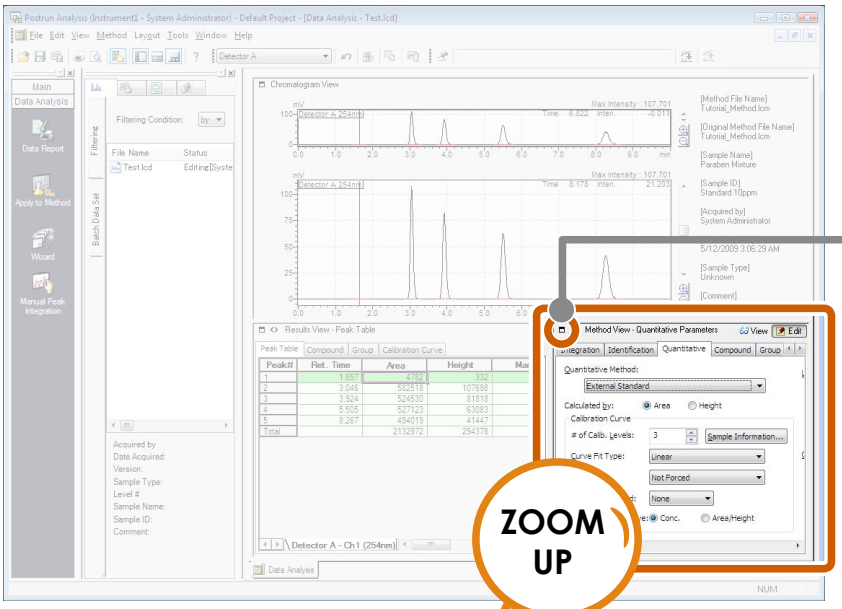
Hint

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.

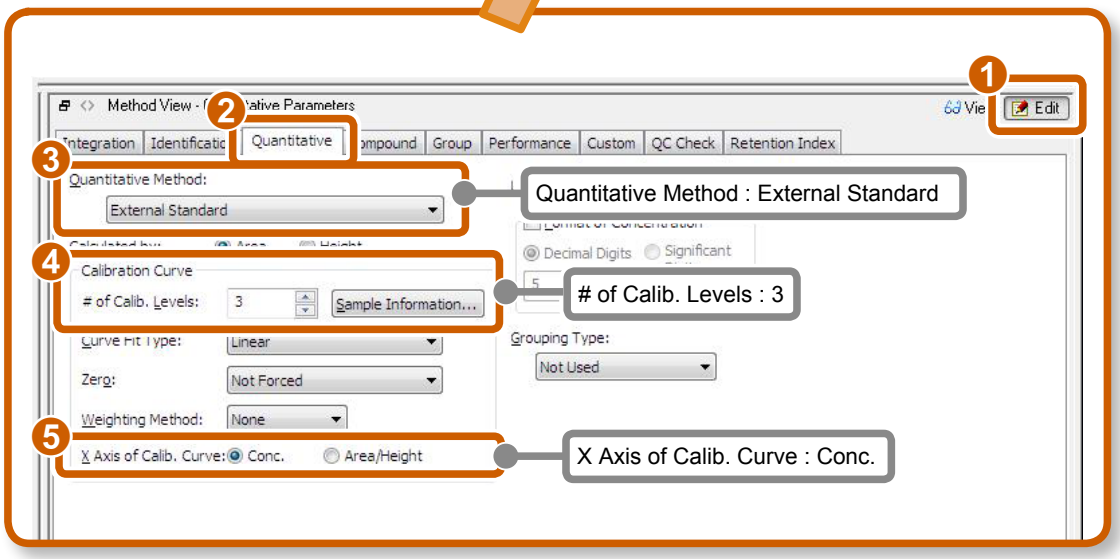
Reference

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.

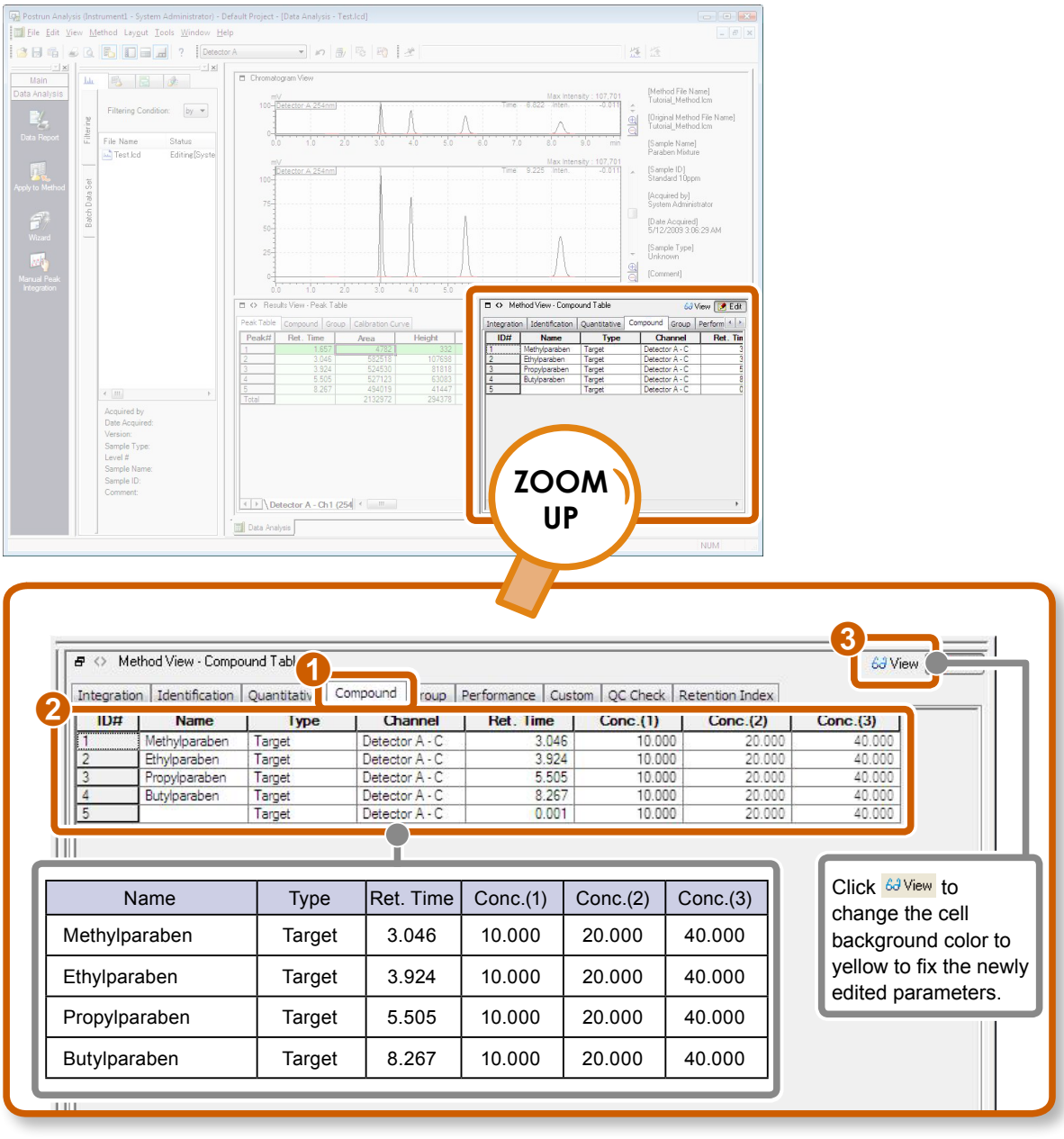


Hint

- 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.



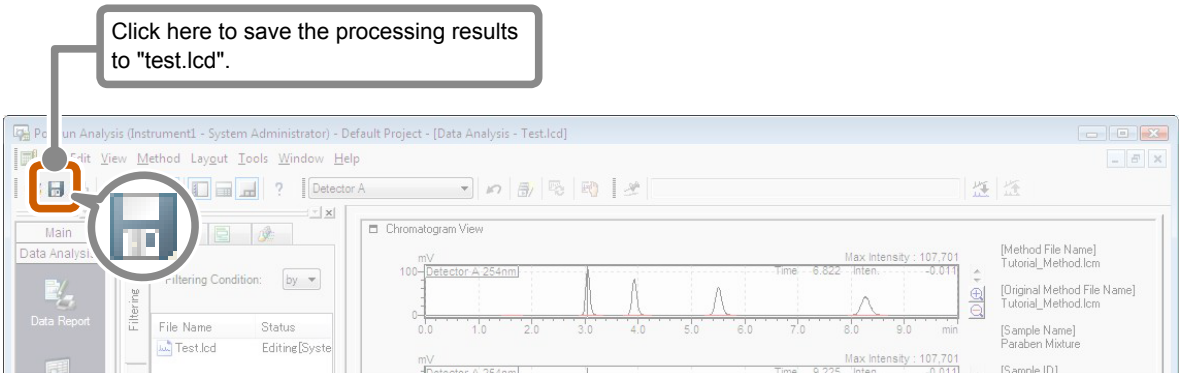
Name	Type	Ret. Time	Conc.(1)	Conc.(2)	Conc.(3)
Methylparaben	Target	3.046	10.000	20.000	40.000
Ethylparaben	Target	3.924	10.000	20.000	40.000
Propylparaben	Target	5.505	10.000	20.000	40.000
Butylparaben	Target	8.267	10.000	20.000	40.000

Hint

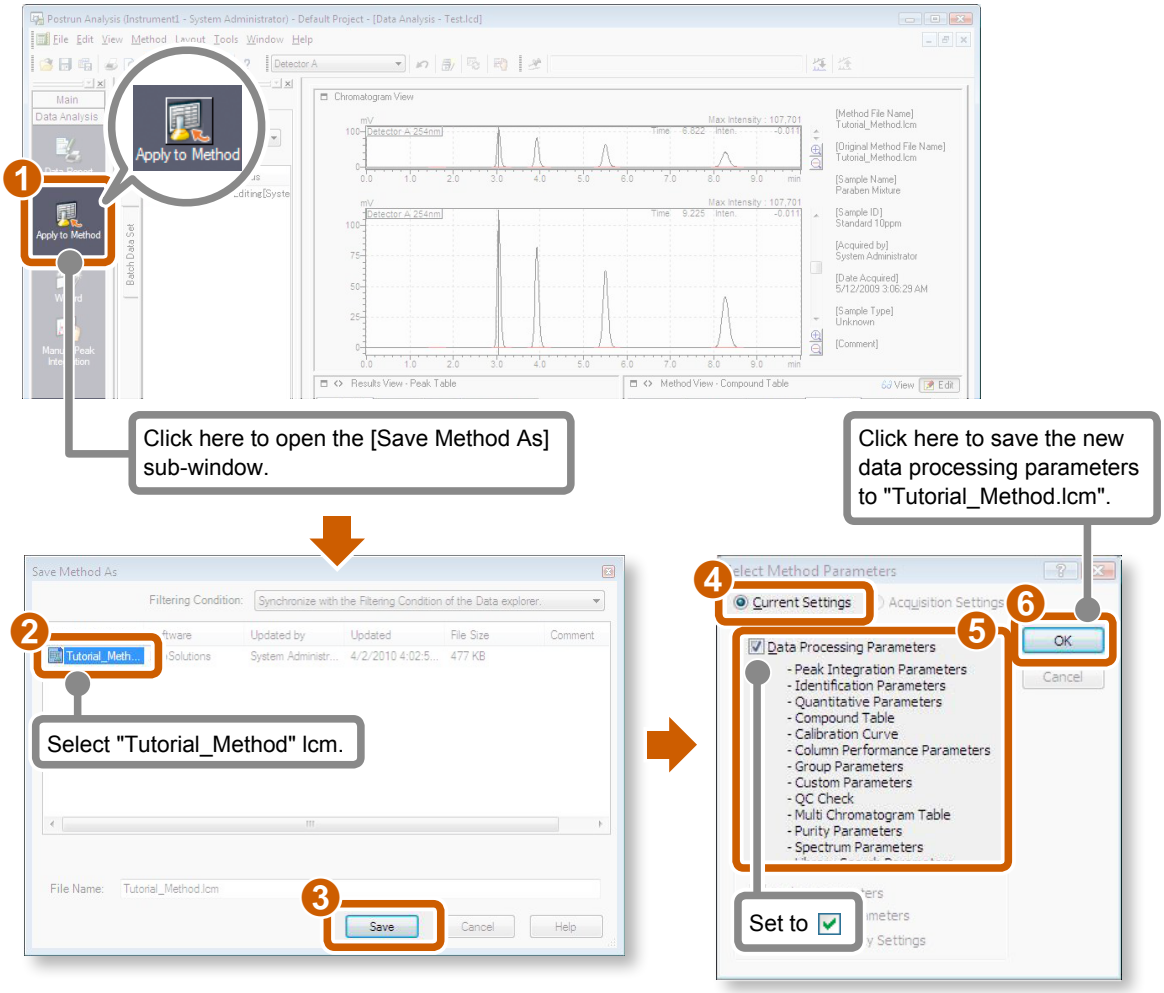
- The result obtained by performing data acquisition is used for [Ret. Time].
- Selecting the [Ret. Time] cell, and clicking the peak in [Chromatogram View] automatically enters the retention time of that peak to the currently selected [Ret. Time] cell. The retention time can be set by simply clicking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

Reference 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.



Hint

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).

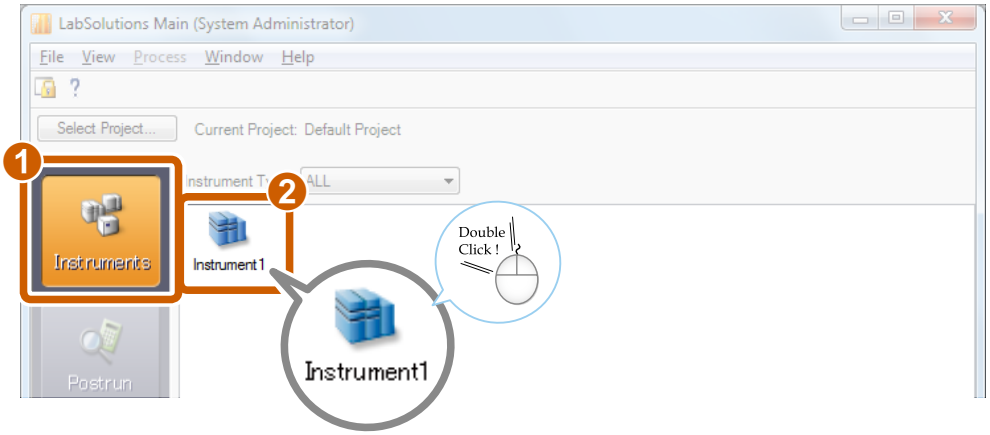
Chapter 5 Realtime Batch

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

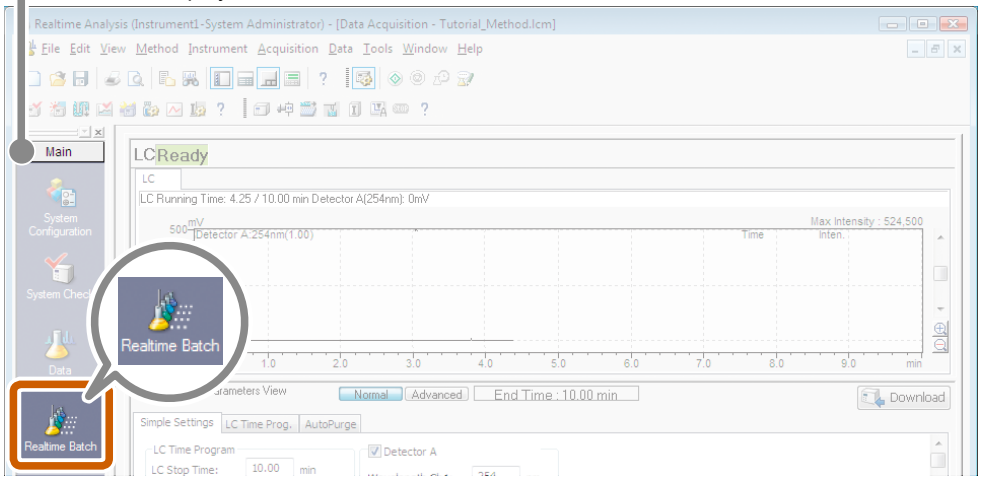
In the following example, create a Batch Table with standard samples set to 1st to 9th rows, and unknown samples set to the 10th and 11th rows.

1 Open the [Realtime Analysis] program.



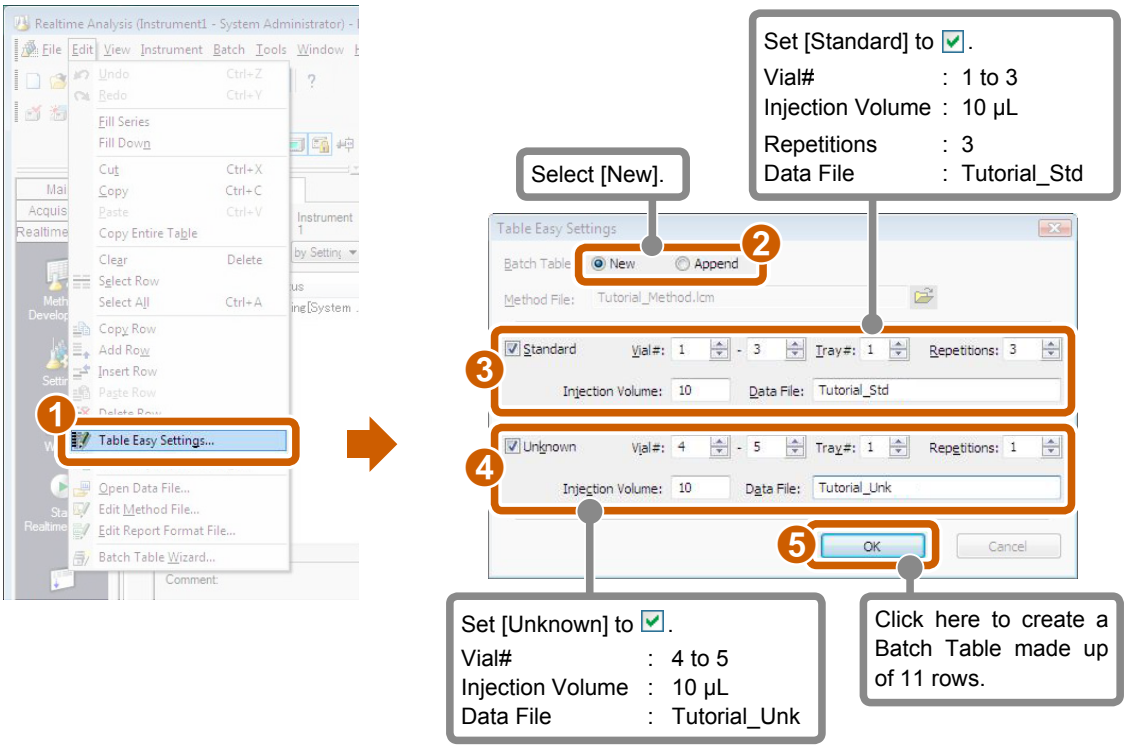
2 Open the [Realtime Batch] window.

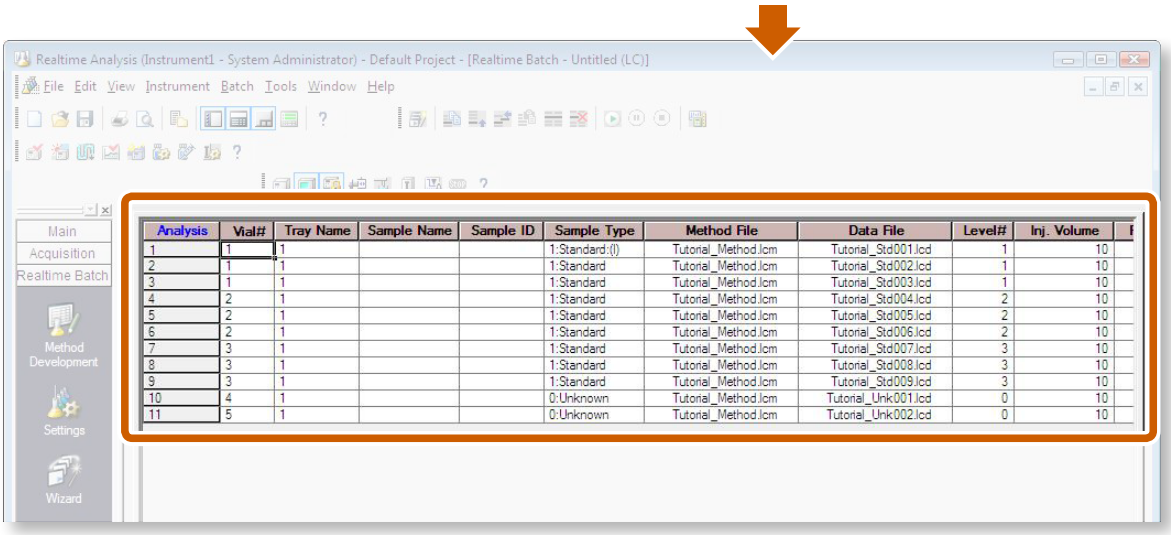
Hint Click here if the [Main] assistant bar is not displayed.



The [Realtime Batch] window opens.

3 Edit the Batch Table.





Hint

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

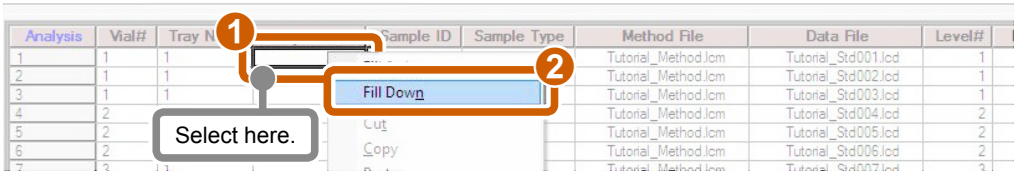
Reference

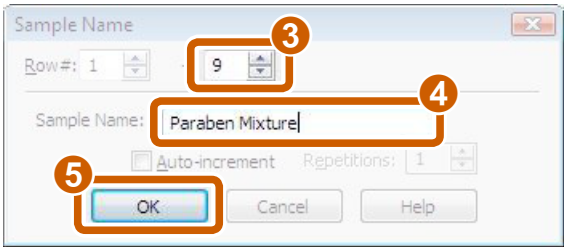
Refer to "Edit Batch Tables" of the "Realtime Batch" chapter, "Edit Batch Tables" of the "Calibration Curves" chapter in *Operators Guide* for details on the editing batch tables.

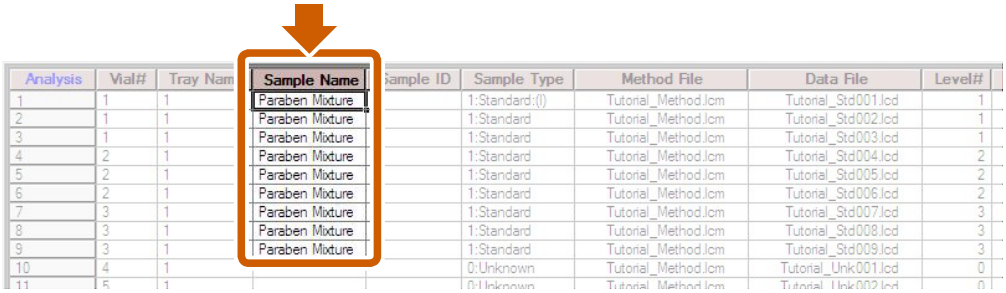
- Enter "-1" in [Vial#] to acquire data without injecting samples from the autosampler.

Continued on the following page

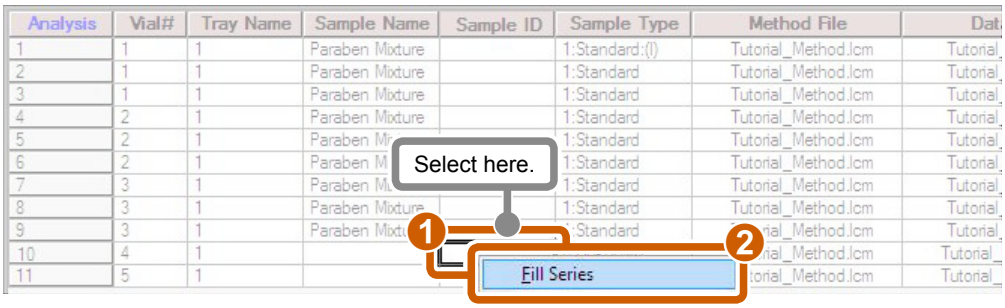
4 Copy a cell.

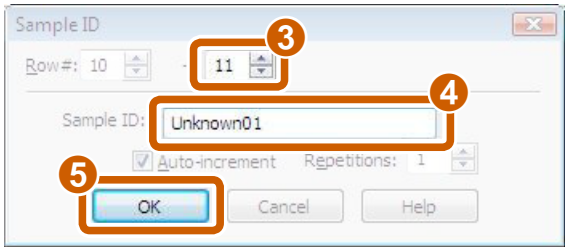


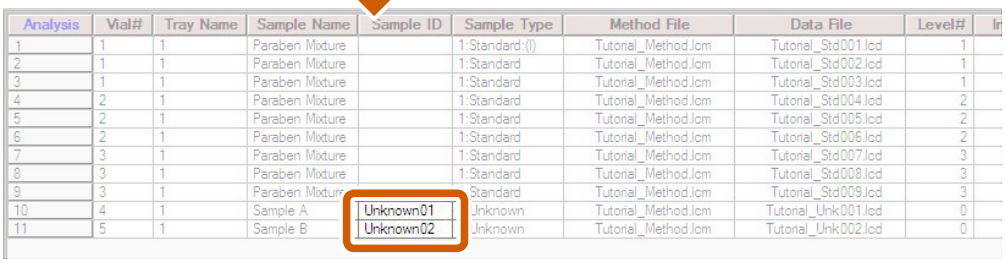




5 Enter a numbered series.





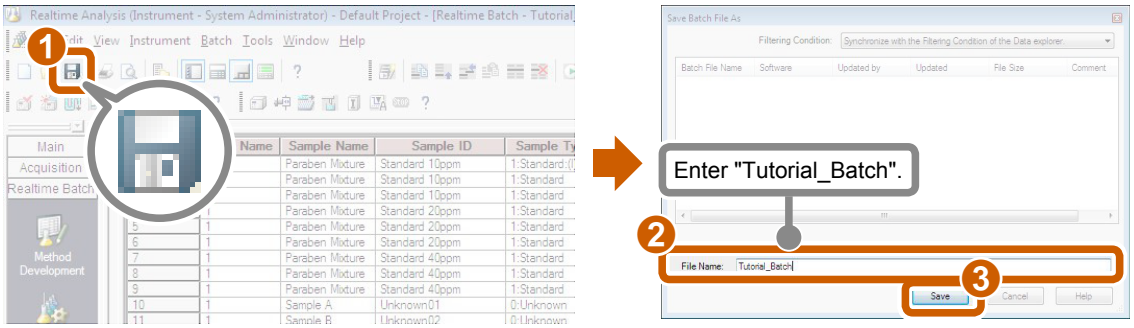


6 Directly enter remaining items to the Batch Table to create the Batch Table shown below.

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:(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

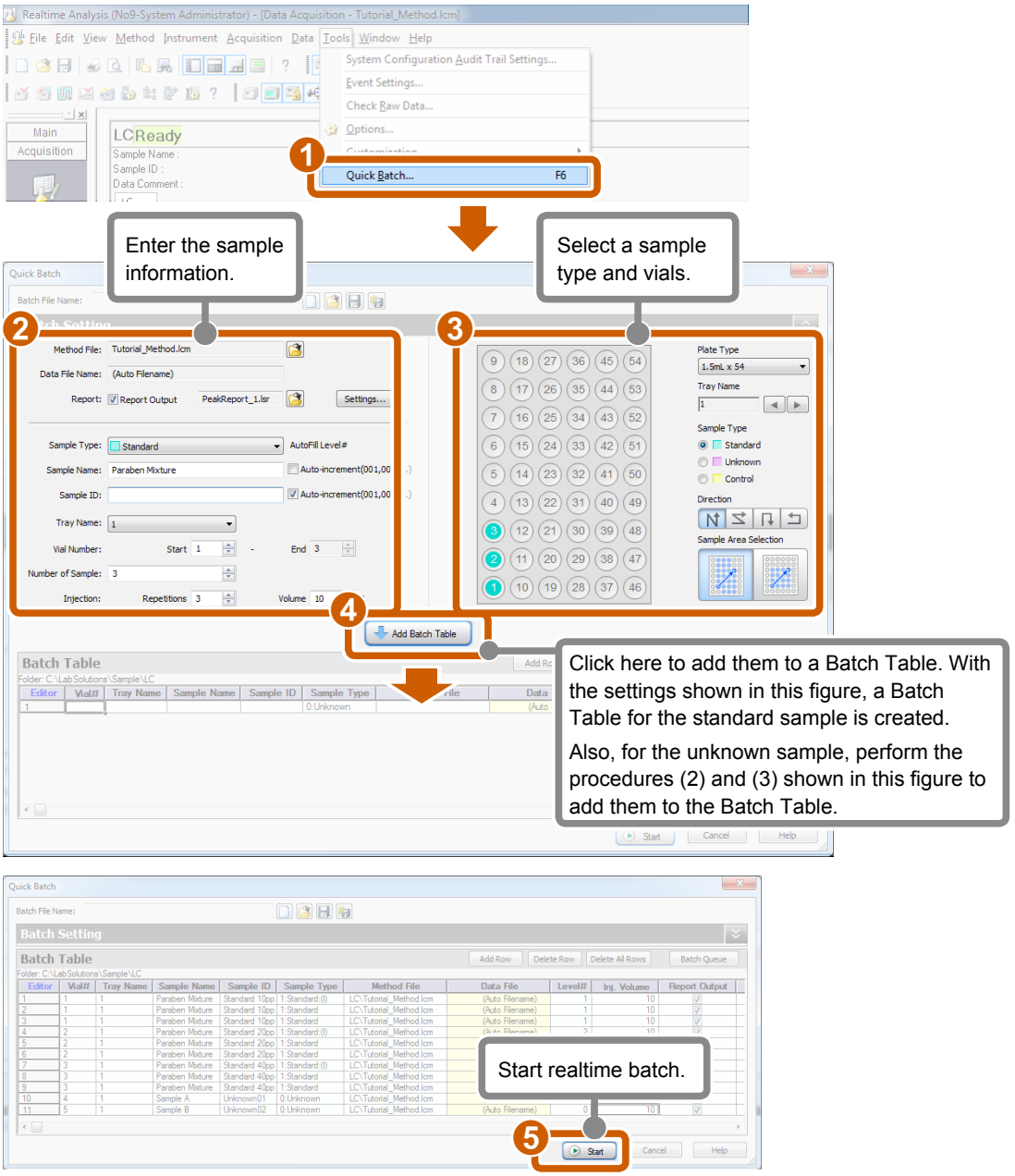
7 Save the batch file.



LabSolutions SUPPLEMENT

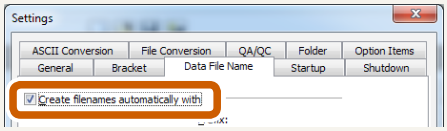
Create a Batch Table Using Quick Batch

You can also create a Batch Table using quick batch.



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 with] checkbox.



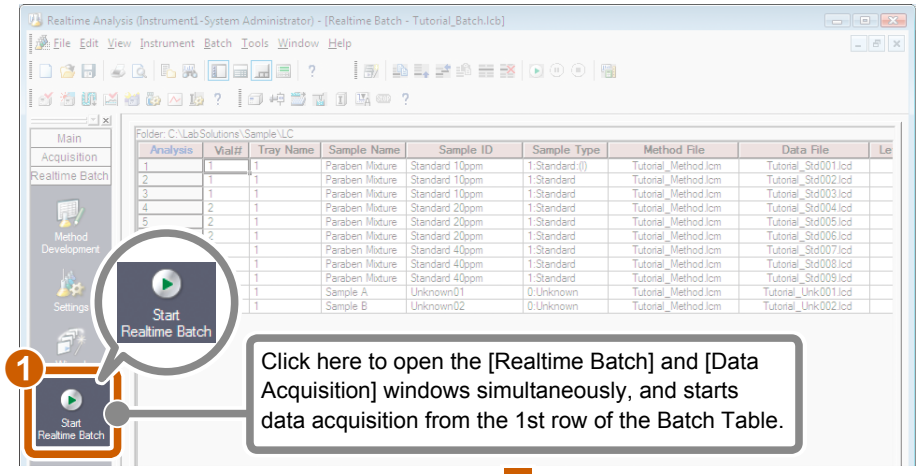
5.2 Realtime Batch Processing

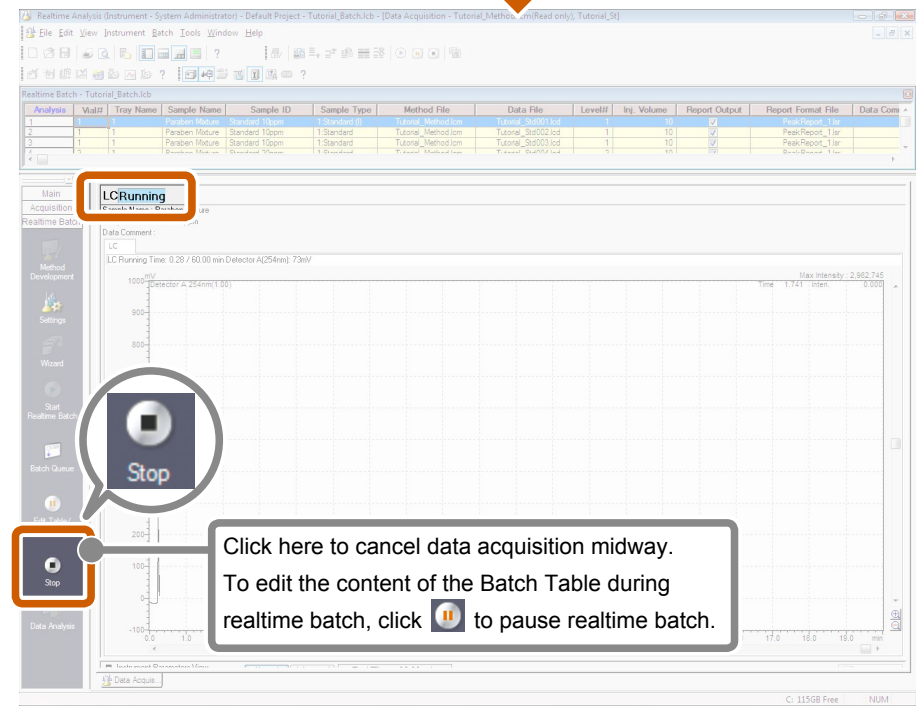
Execute realtime batch using the Batch Table you created.

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.

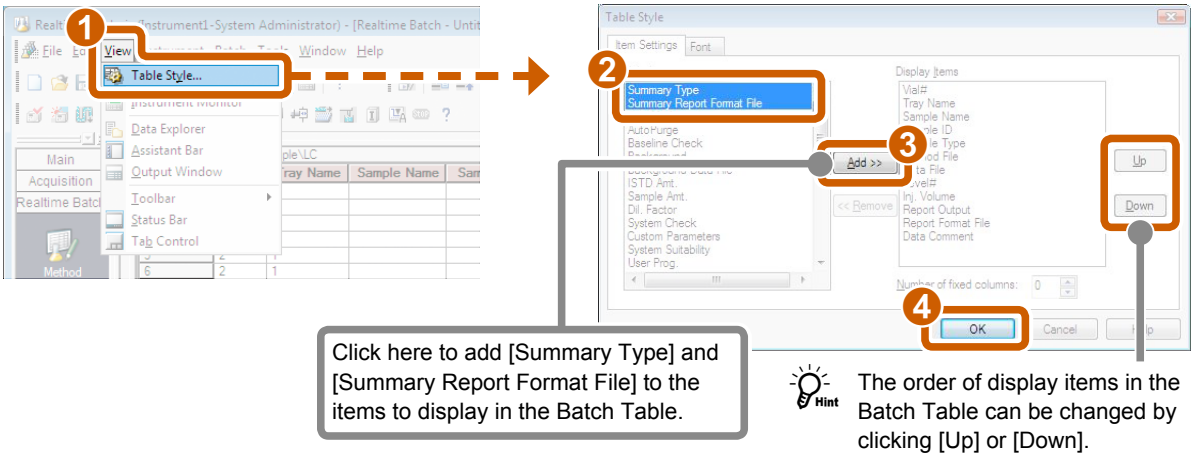




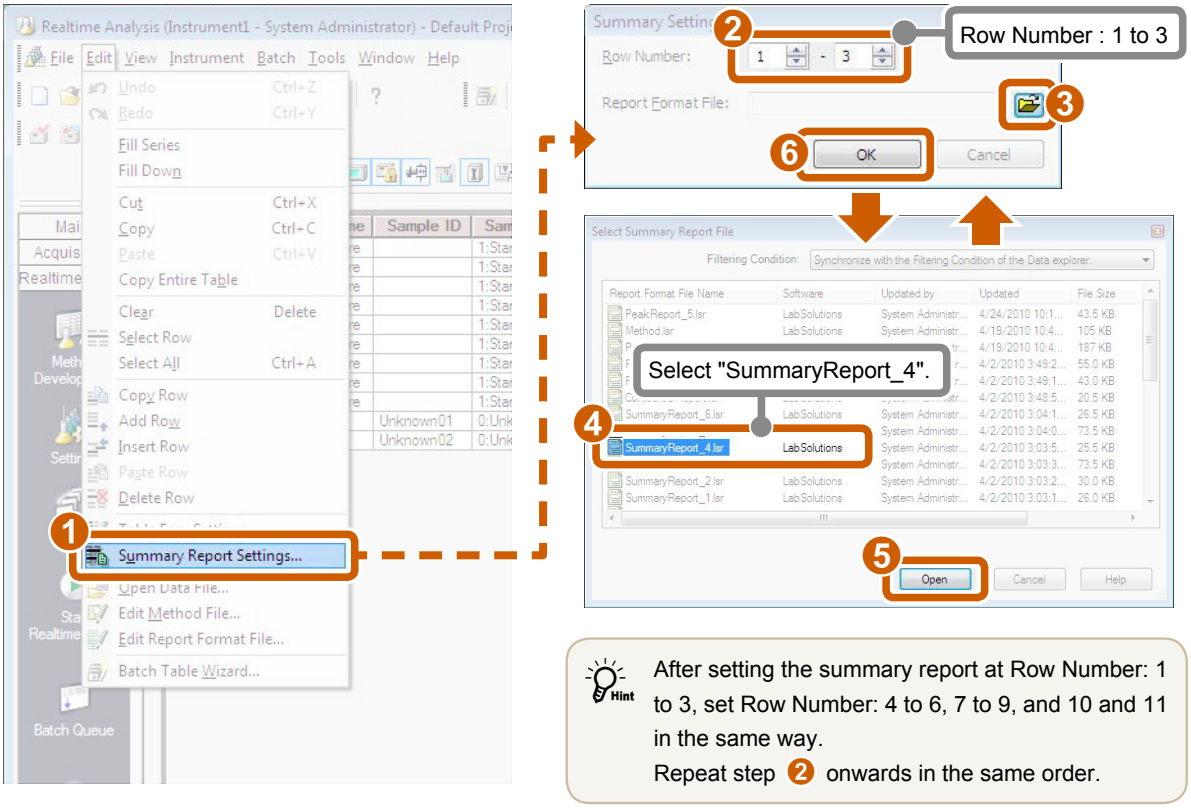
LabSolutions SUPPLEMENT

Print a Summary Report

1 Add items to display in the Batch Table.

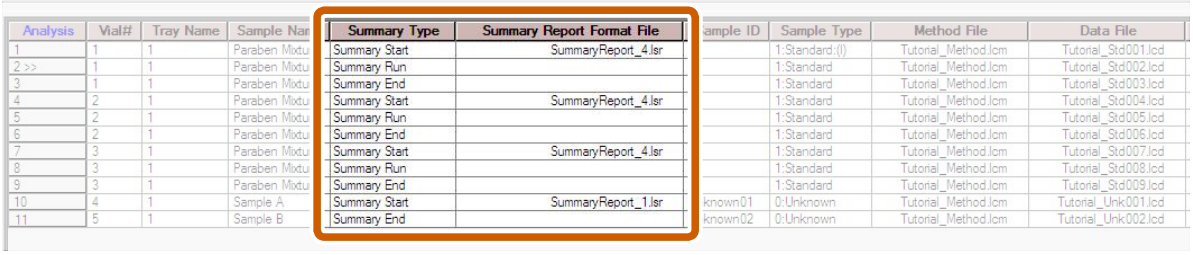


2 Set up the summary report.



Continued on the following page

3 Check the output configuration of the summary report.



Analysis	Vial#	Tray Name	Sample Nar	Summary Type	Summary Report Format File	ample 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.

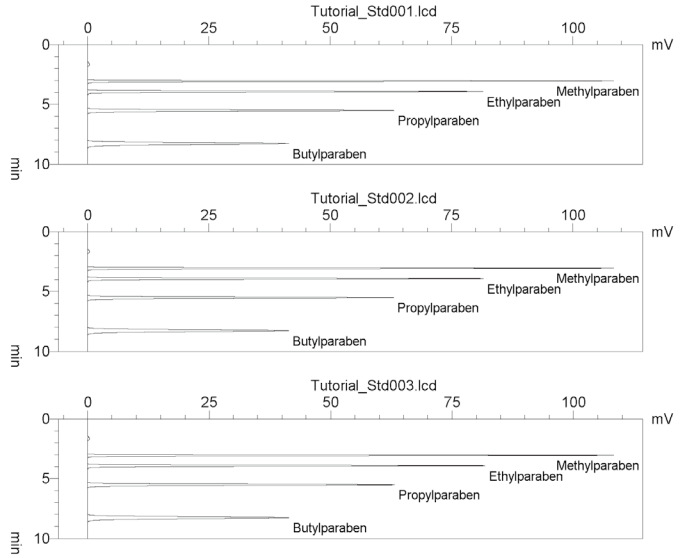
Reference Refer to "5.2 Realtime Batch Processing" P.36 for details on executing realtime batch.

[Printout Example]

Standard samples

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

<Summary Report>



<< Detector A >>

ID#1 Compound Name: Methylparaben

Data File Name	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Tutorial_Std001.lcd	Paraben Mixture	Standard 10ppm	3.050	582618	108362	10.000
Tutorial_Std002.lcd	Paraben Mixture	Standard 10ppm	3.050	582482	108360	9.999
Tutorial_Std003.lcd	Paraben Mixture	Standard 10ppm	3.048	582226	108206	9.996
Average			3.049	582442	108309	9.998
%RSD			0.033	0.034	0.083	0.019

ID#2 Compound Name: Ethylparaben

Data File Name	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Tutorial_Std001.lcd	Paraben Mixture	Standard 10ppm	3.929	524834	81456	10.000
Tutorial_Std002.lcd	Paraben Mixture	Standard 10ppm	3.929	524475	81474	9.997
Tutorial_Std003.lcd	Paraben Mixture	Standard 10ppm	3.927	524485	81784	9.998
Average			3.928	524598	81571	9.998
%RSD			0.038	0.039	0.226	0.017

ID#3 Compound Name: Propylparaben

Data File Name	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Tutorial_Std001.lcd	Paraben Mixture	Standard 10ppm	5.514	527264	63086	10.000
Tutorial_Std002.lcd	Paraben Mixture	Standard 10ppm	5.513	526966	63012	9.997
Tutorial_Std003.lcd	Paraben Mixture	Standard 10ppm	5.509	526831	63198	9.996
Average			5.512	527020	63099	9.998
%RSD			0.046	0.042	0.149	0.019

ID#4 Compound Name: Butylparaben

Data File Name	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Tutorial_Std001.lcd	Paraben Mixture	Standard 10ppm	8.280	494089	41385	10.000
Tutorial_Std002.lcd	Paraben Mixture	Standard 10ppm	8.276	493798	41441	9.997
Tutorial_Std003.lcd	Paraben Mixture	Standard 10ppm	8.270	493744	41408	9.997
Average			8.276	493877	41411	9.998
%RSD			0.061	0.038	0.069	0.016

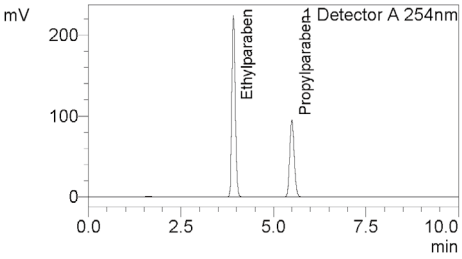
Unknown samples

==== 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	

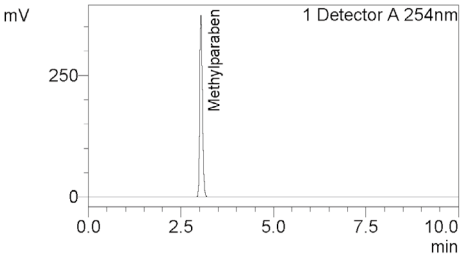
Detector A

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

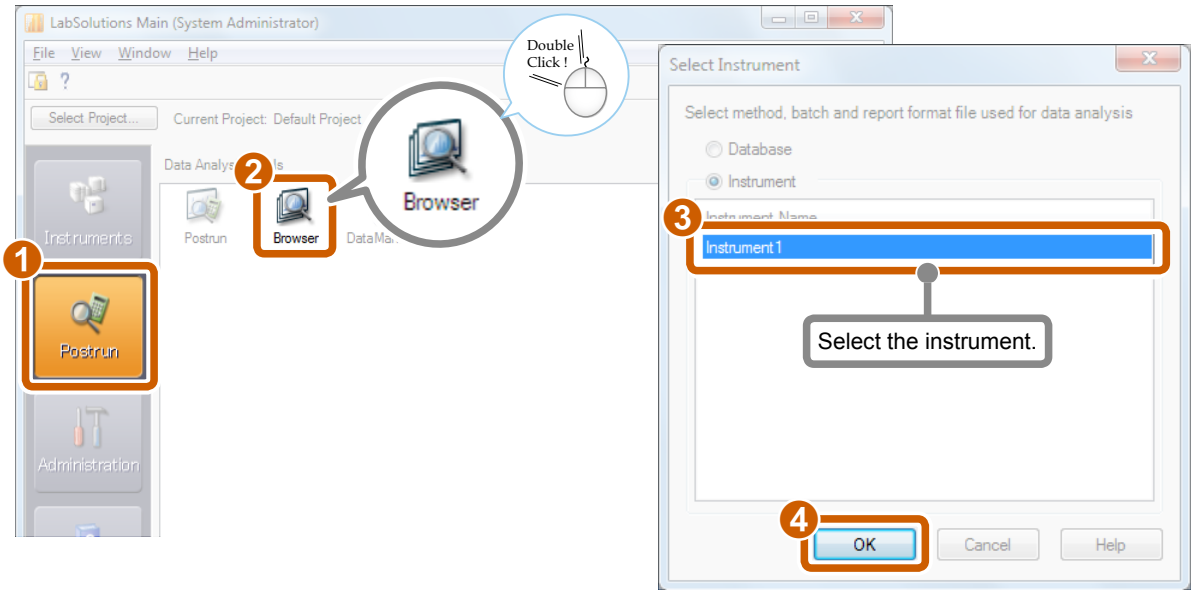
Chapter 6

Multiple Data Analysis

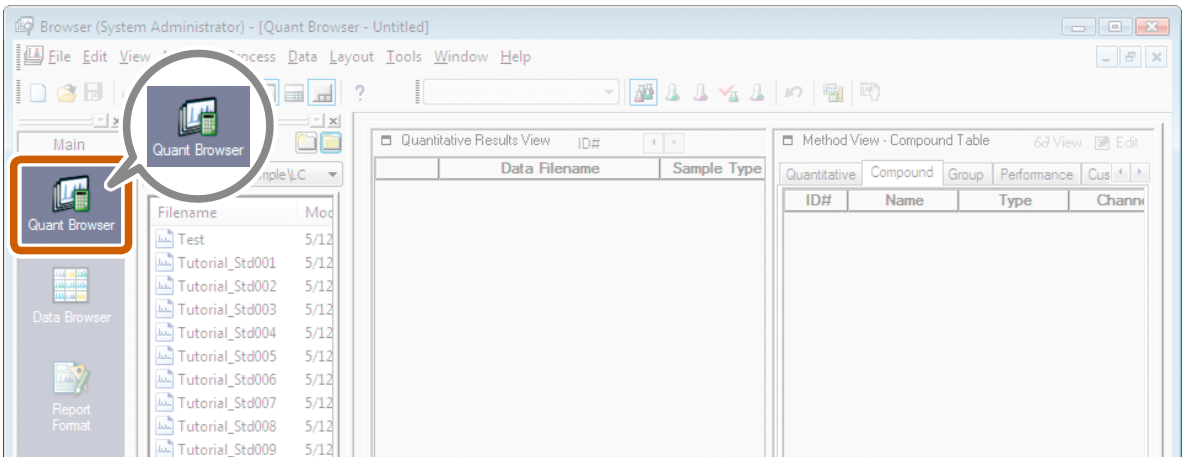
The LabSolutions [Browser] program is handy for checking the quantitative calculation results and chromatograms of multiple data.
In the [Quant Browser] window of the [Browser] program, you can check multiple data, and change the data processing parameters of the currently displayed method file to modify 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.

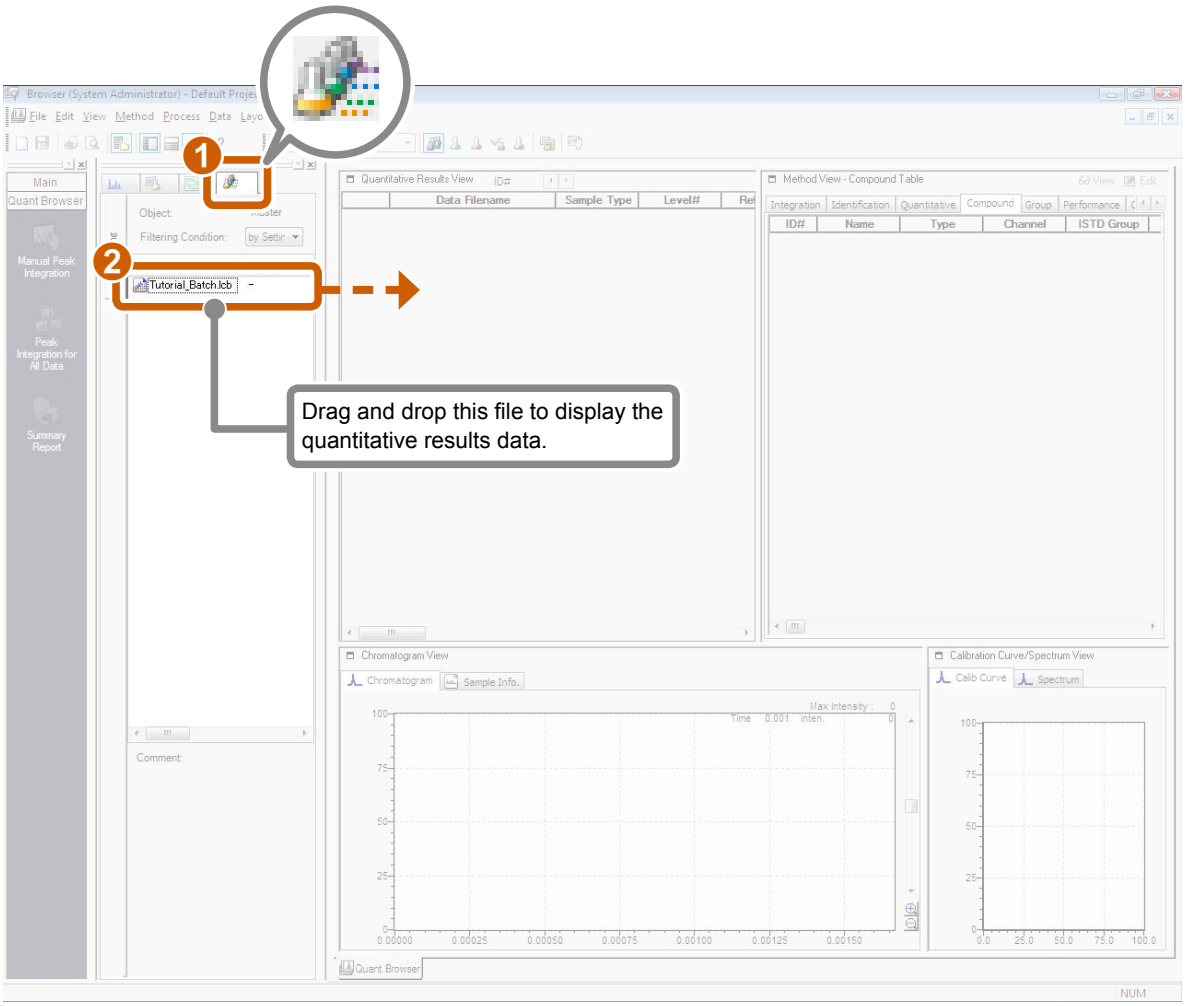


2 Open the [Quant Browser] window.



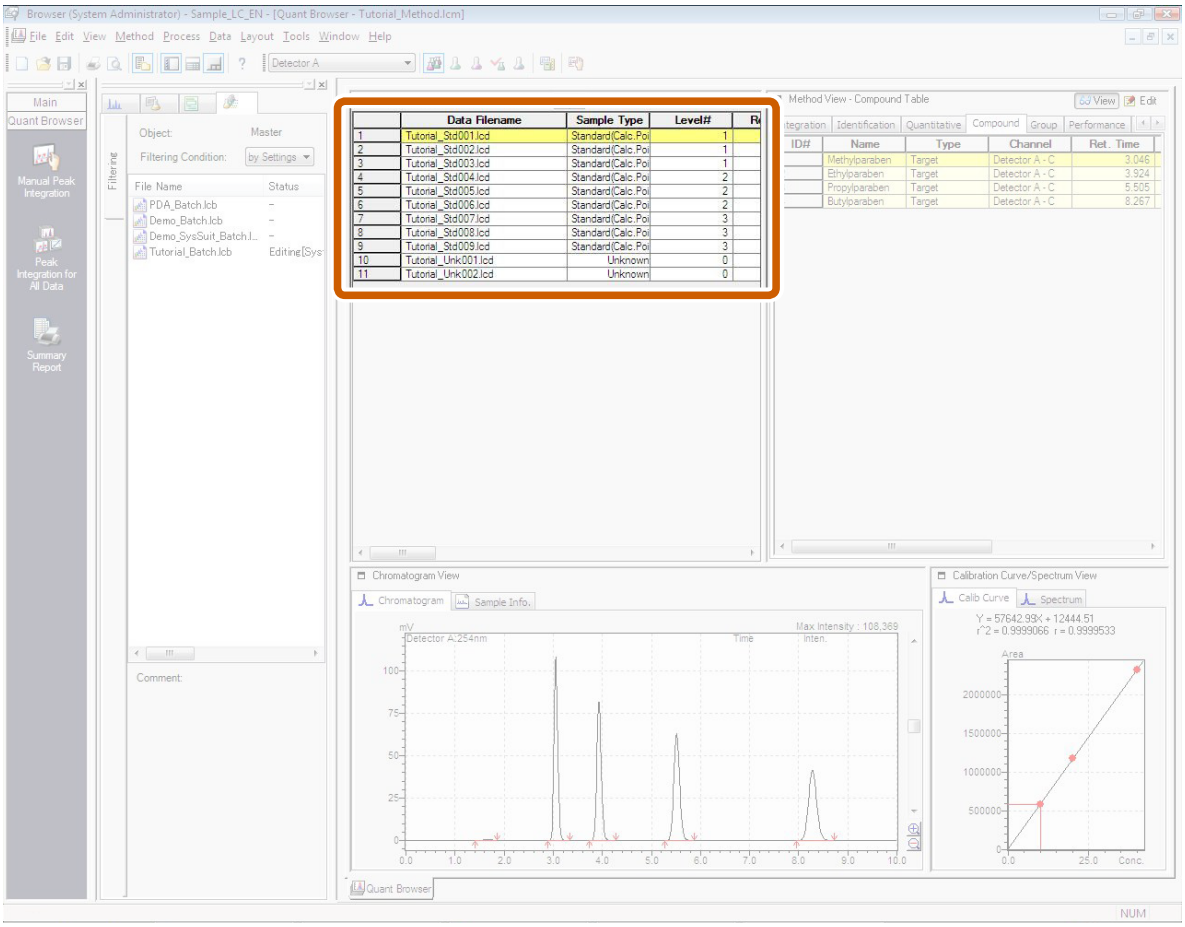
Open the [Quant Browser] window.

3 Load the batch file.



Continued on the following page

4 Confirm the quantitative results.

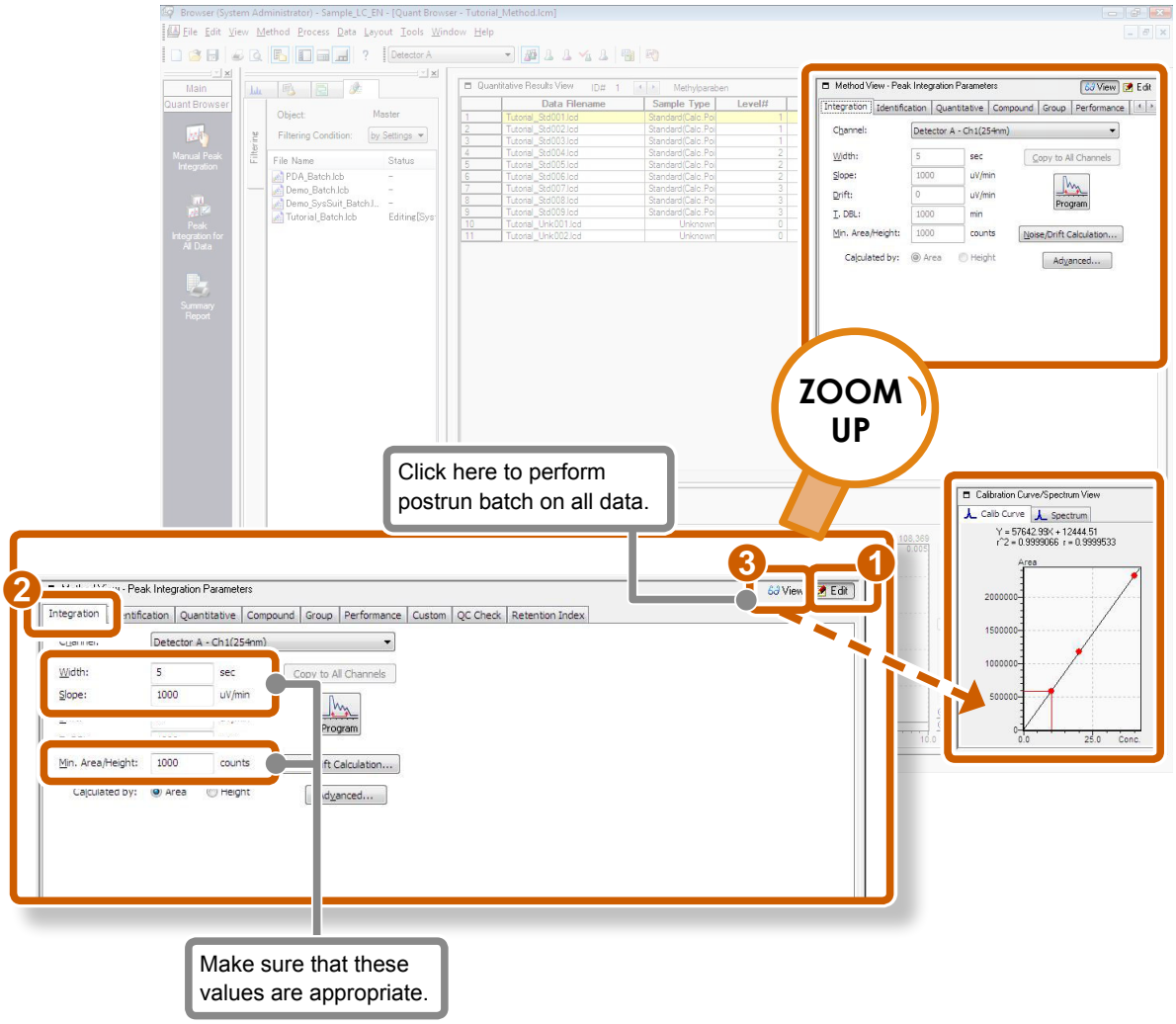


LabSolutions SUPPLEMENT

Modify Calibration Curves

1 Confirm peak integration parameters.

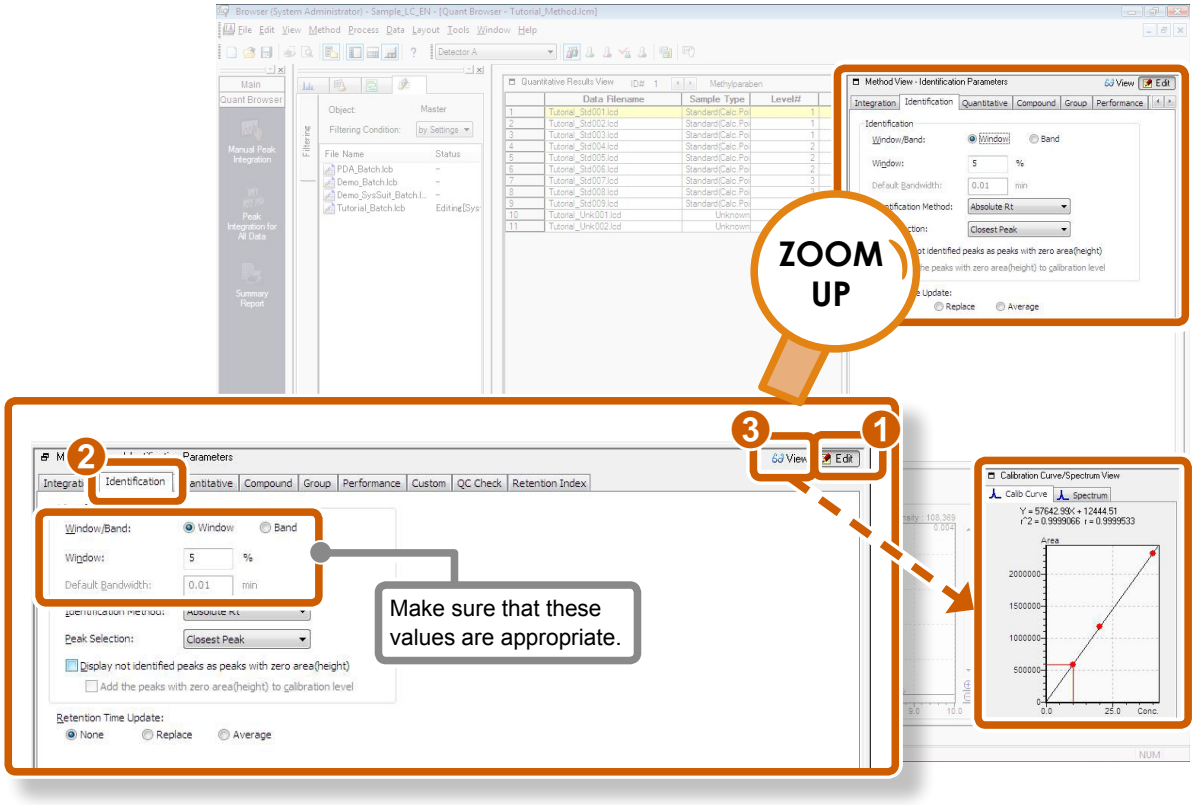
Confirm the peak integration parameters when peak detection is inappropriate.



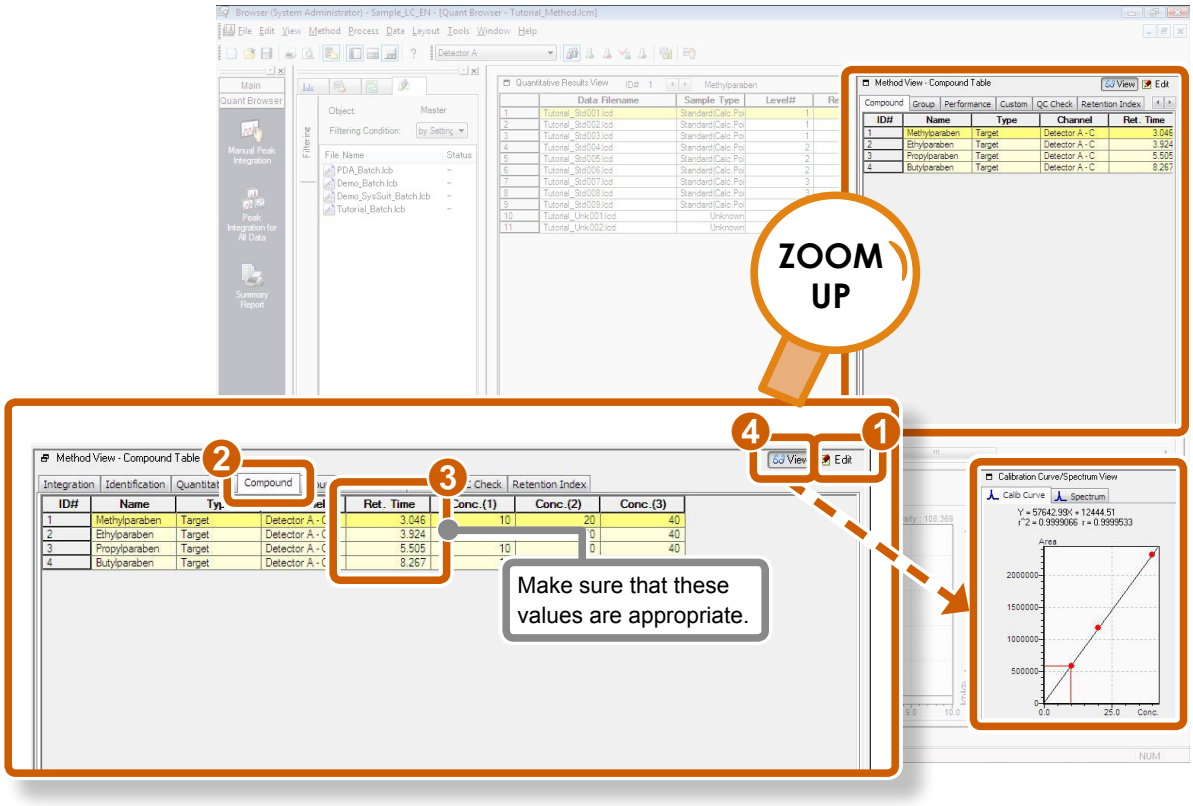
Continued on the following page

2 Confirm identification parameters.

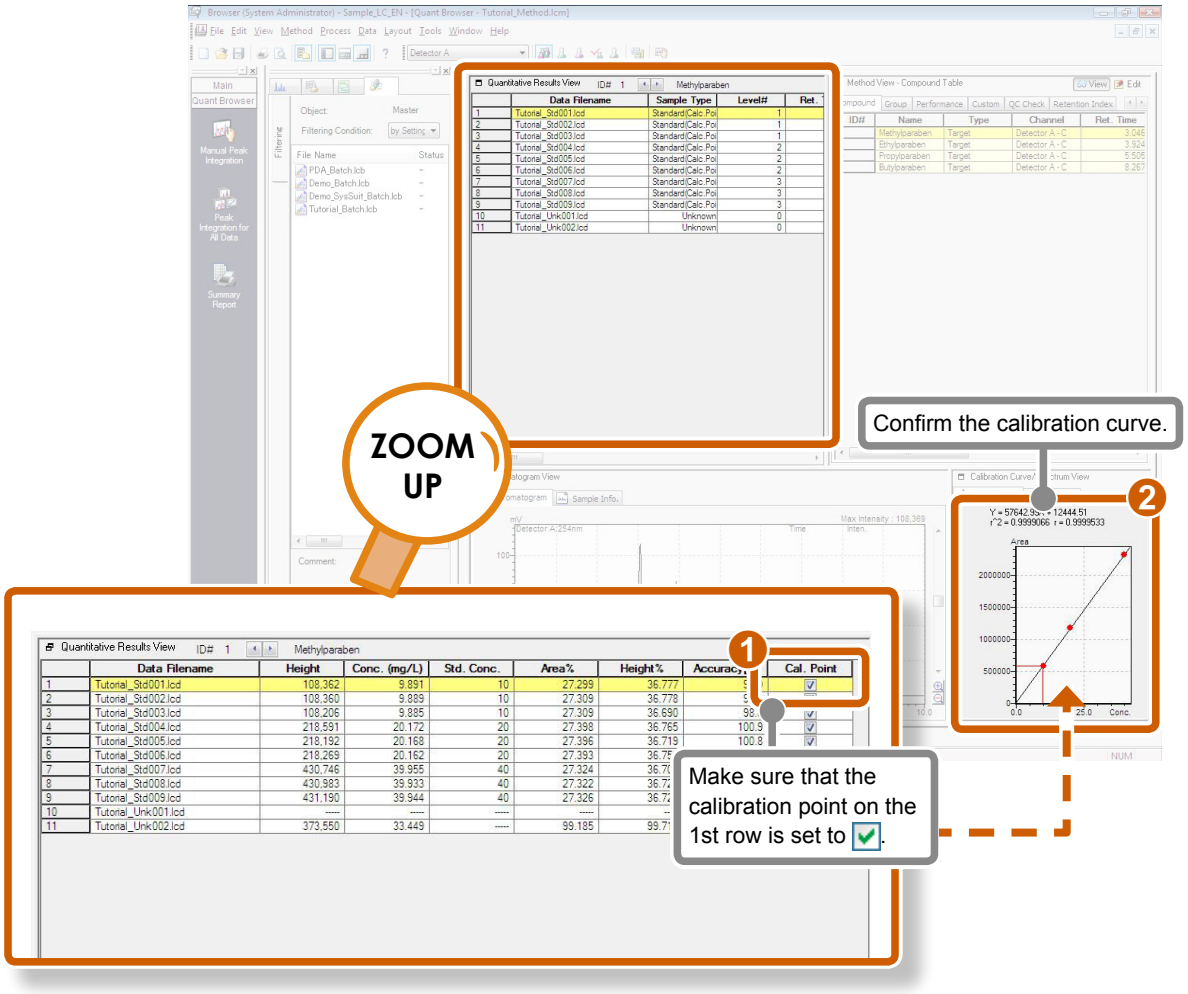
Confirm the identification parameters and Compound Table when peaks are not identified correctly.



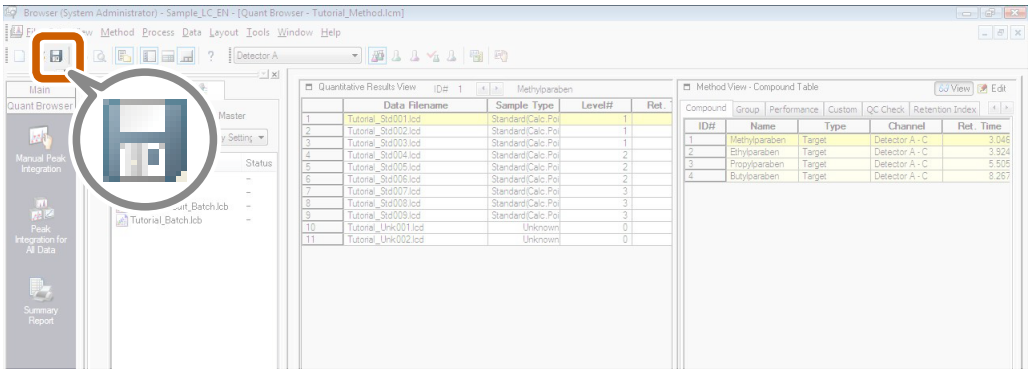
3 Confirm the Compound Table.



4 Confirm calibration points.



5 Save the method file and data file.

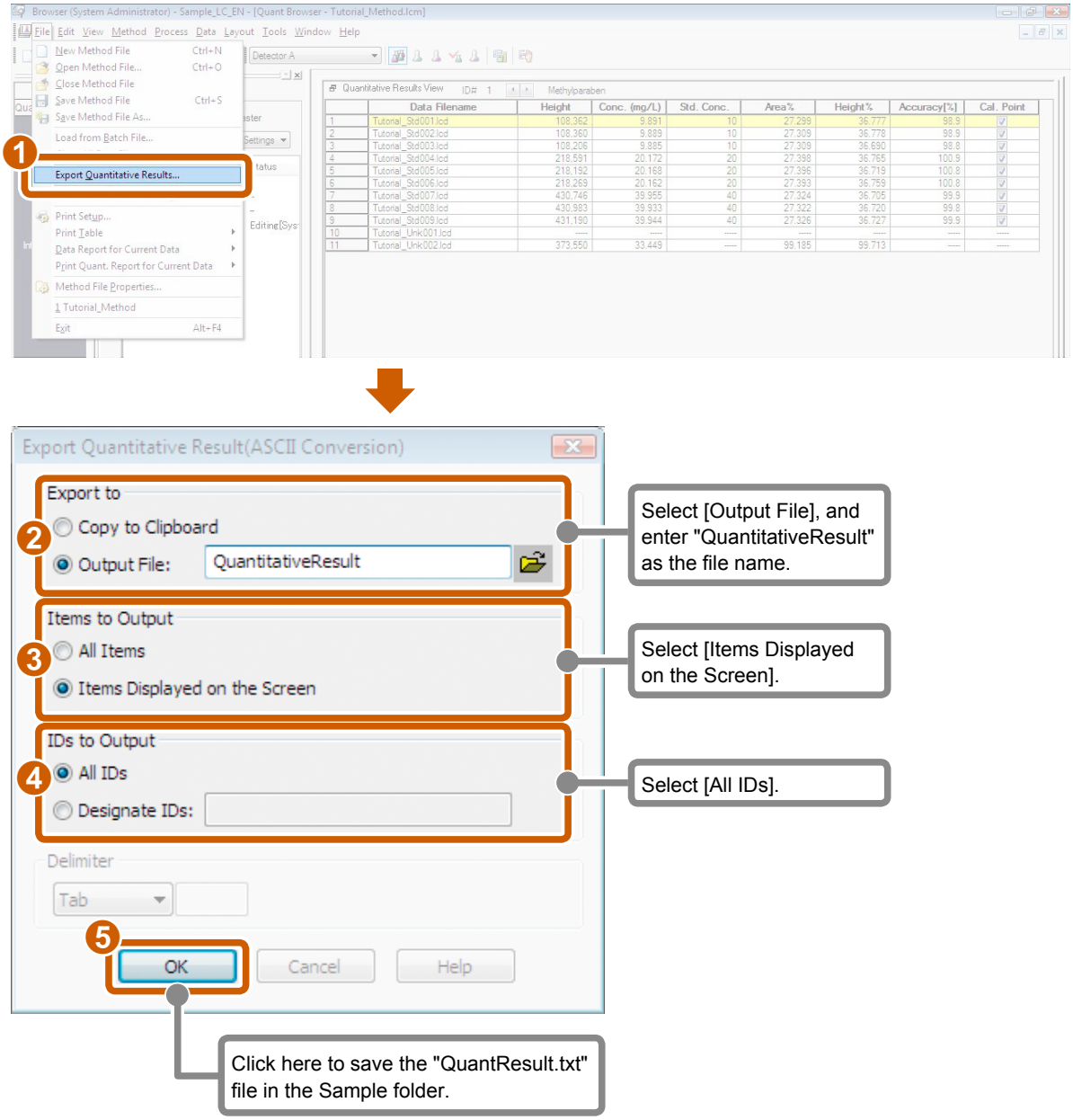


LabSolutions

SUPPLEMENT

Export Quantitative Calculation Results

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

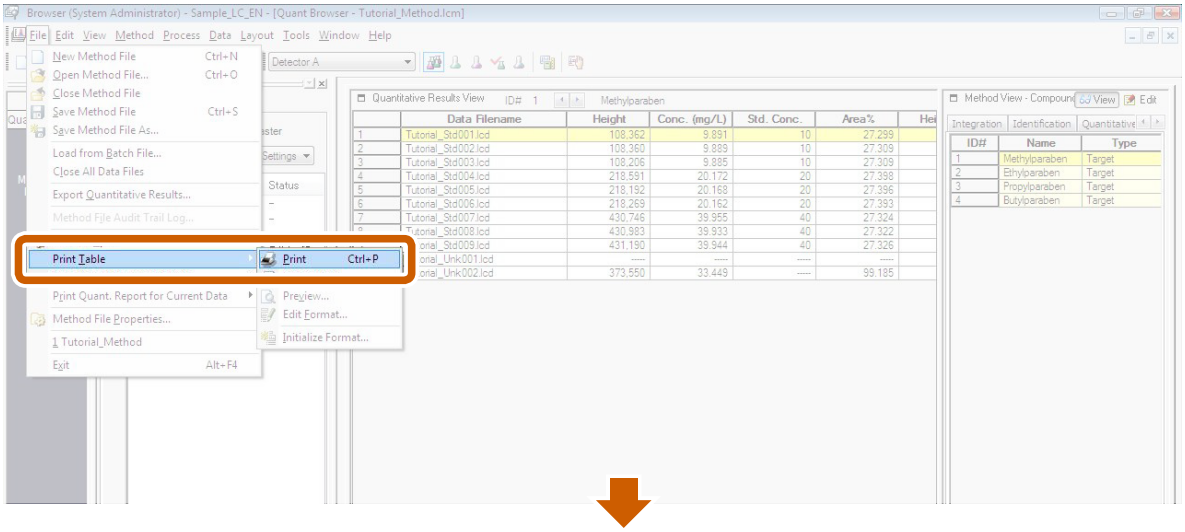


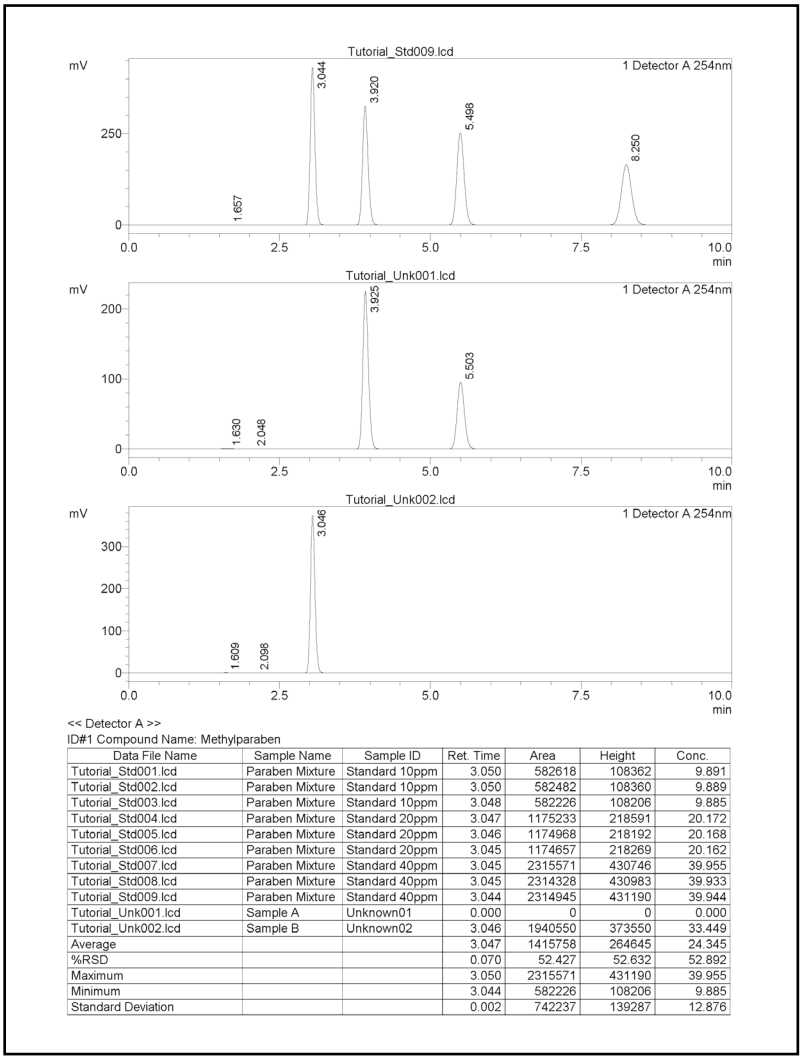
Reference Refer to "Export the Quantitative Results" of the "Quant Browser" chapter in *Operators Guide* for details on exporting quantitative results.

LabSolutions SUPPLEMENT

Print the Quantitative Results Table

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





<< Detector A >>
ID#1 Compound Name: Methylparaben

Data File Name	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Tutorial_Std001.lcd	Paraben Mixture	Standard 10ppm	3.050	582618	108362	9.891
Tutorial_Std002.lcd	Paraben Mixture	Standard 10ppm	3.050	582482	108360	9.889
Tutorial_Std003.lcd	Paraben Mixture	Standard 10ppm	3.048	582226	108206	9.885
Tutorial_Std004.lcd	Paraben Mixture	Standard 20ppm	3.047	1175233	218591	20.172
Tutorial_Std005.lcd	Paraben Mixture	Standard 20ppm	3.046	1174968	218192	20.168
Tutorial_Std006.lcd	Paraben Mixture	Standard 20ppm	3.045	1174657	218269	20.162
Tutorial_Std007.lcd	Paraben Mixture	Standard 40ppm	3.045	2315571	430746	39.955
Tutorial_Std008.lcd	Paraben Mixture	Standard 40ppm	3.045	2314328	430983	39.933
Tutorial_Std009.lcd	Paraben Mixture	Standard 40ppm	3.044	2314945	431190	39.944
Tutorial_Unk001.lcd	Sample A	Unknown01	0.000	0	0	0.000
Tutorial_Unk002.lcd	Sample B	Unknown02	3.046	1940550	373550	33.449
Average			3.047	1415758	264645	24.345
%RSD			0.070	52.427	52.632	52.892
Maximum			3.050	2315571	431190	39.955
Minimum			3.044	582226	108206	9.885
Standard Deviation			0.002	742237	139287	12.876

Hint

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

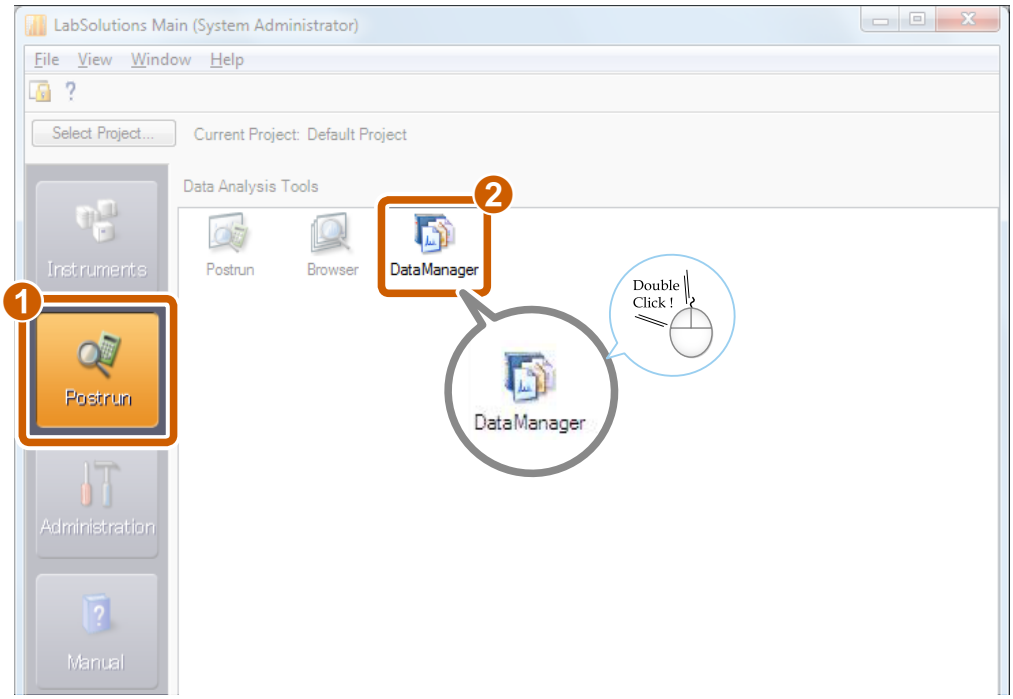
Chapter 7

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.

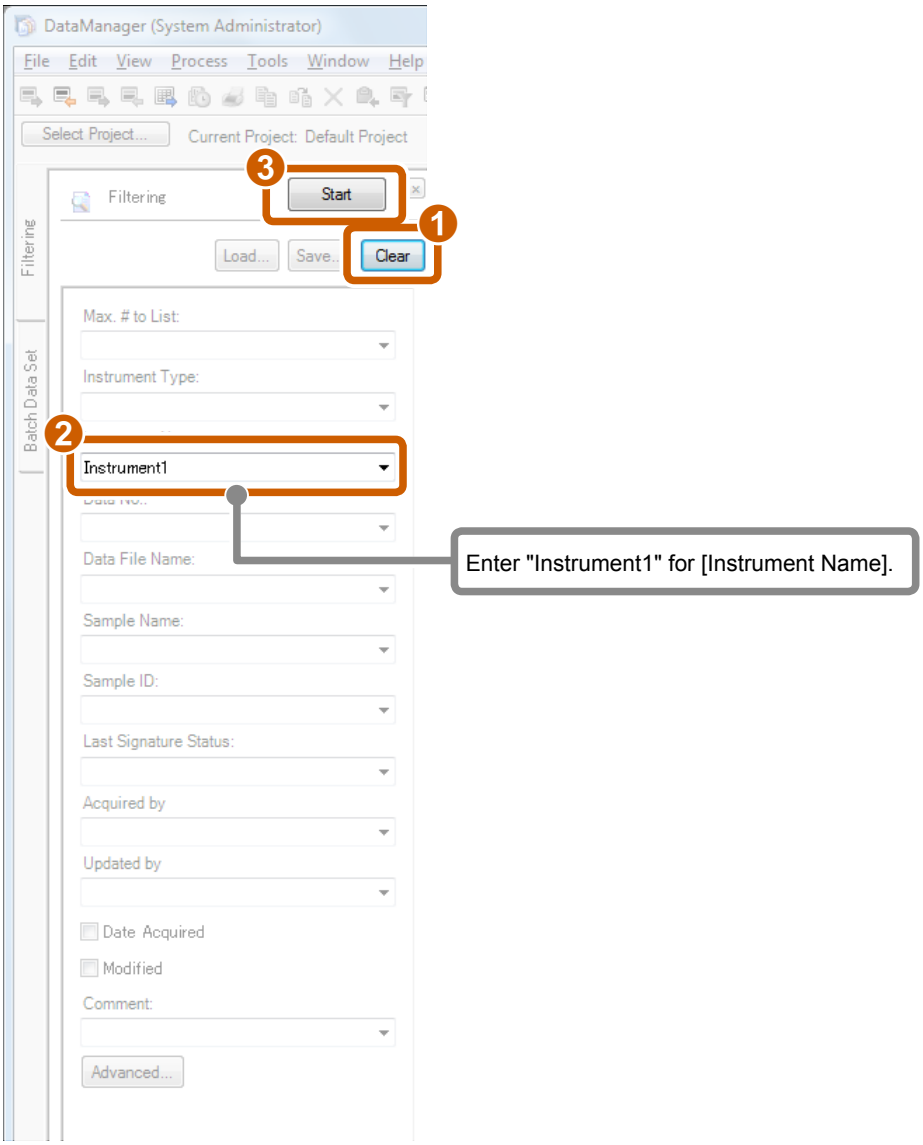
1 Open the [DataManager] program.



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

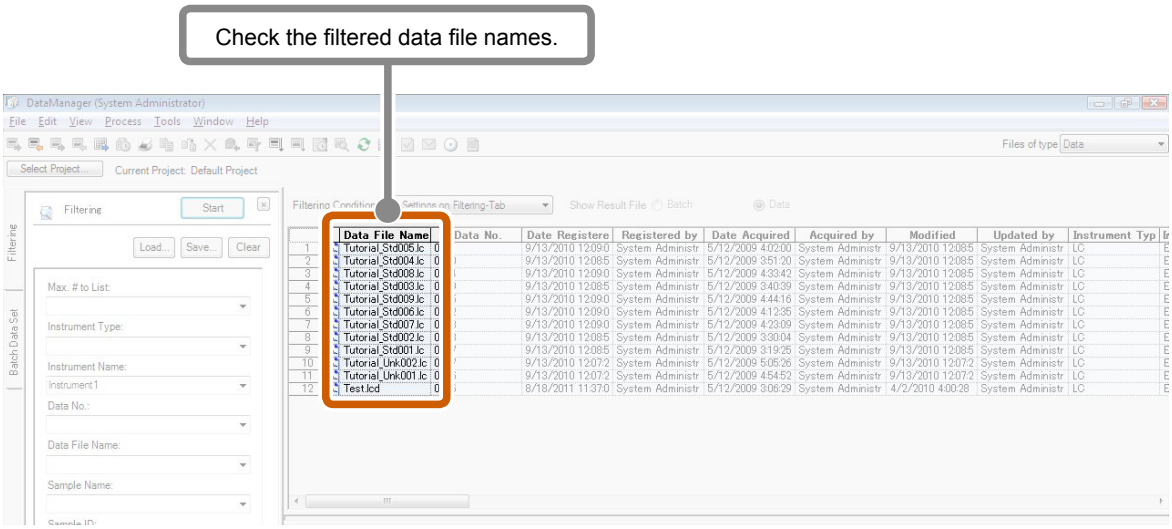
Hint The Data Manager can be used to view information on methods, batches, and report format files.
To view such information, clicking on [Show Method/Batch/Report Format in Database] in the [Tools] menu allows you to select method, batch, or report for [Files of type].

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

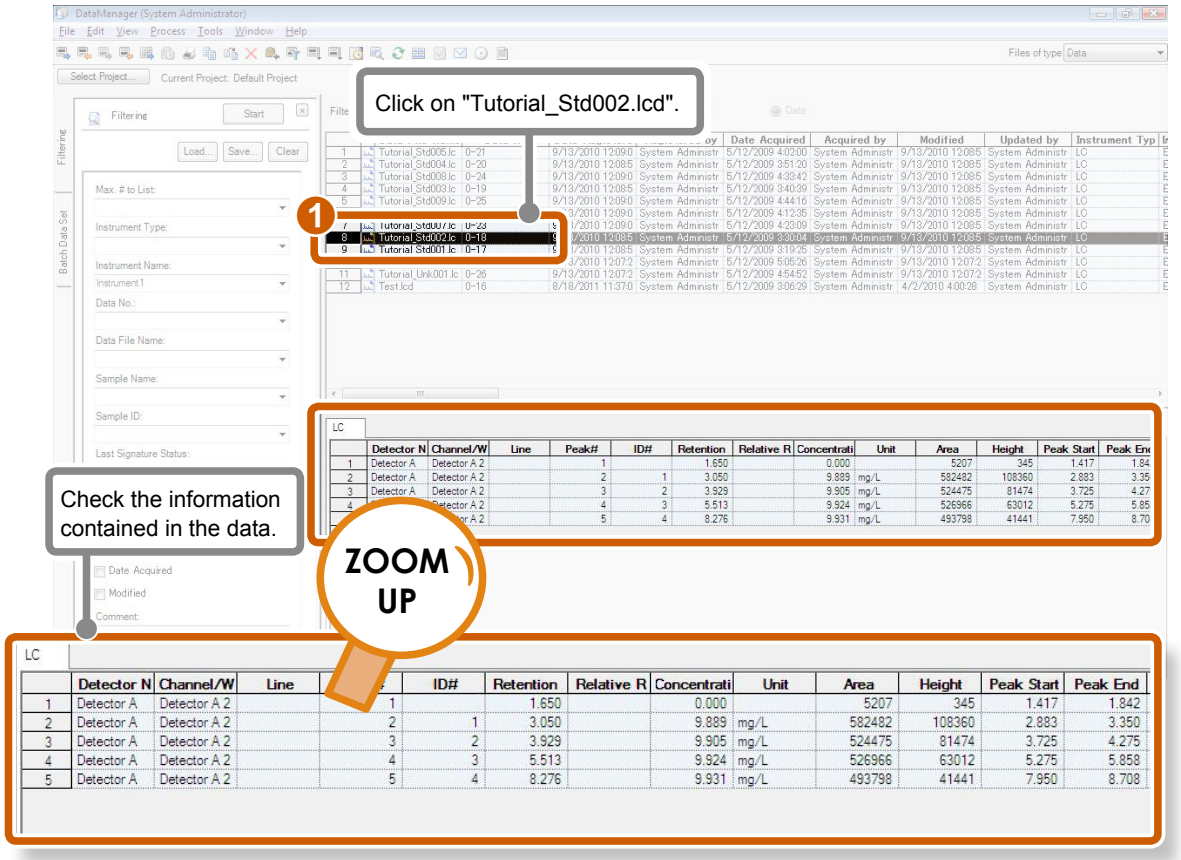


Continued on the following page

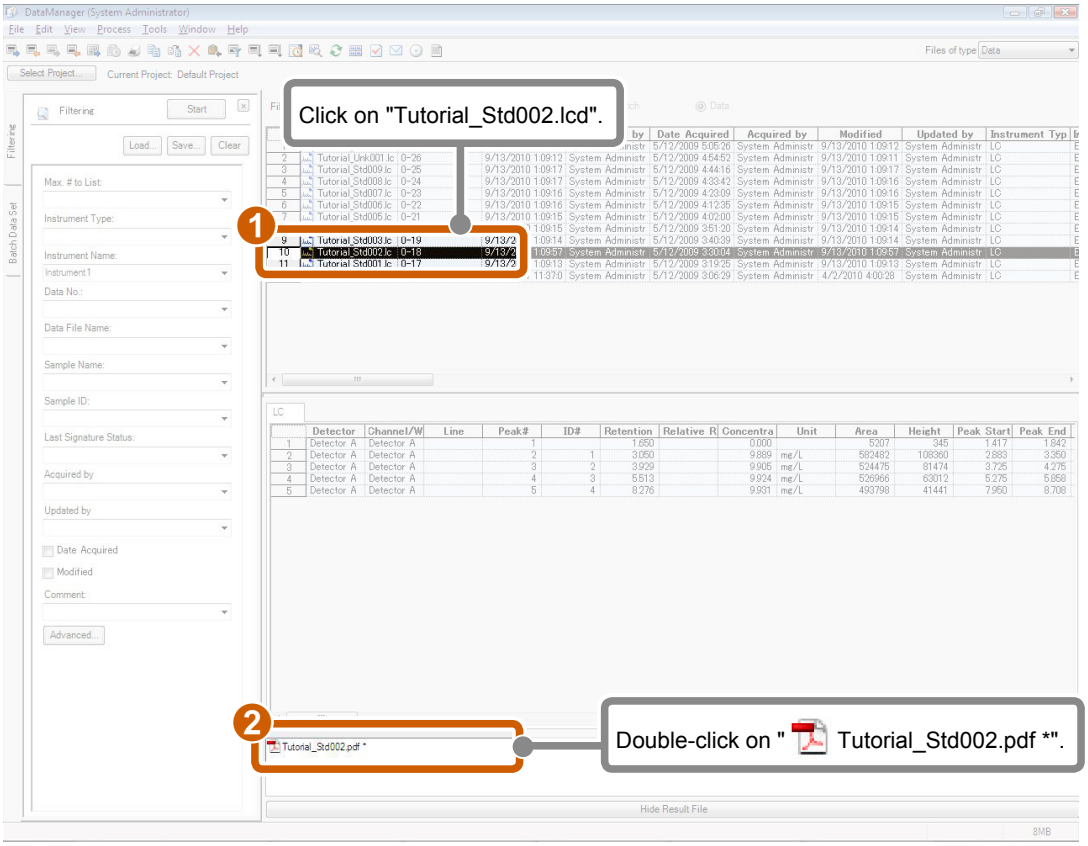
4 Check the filtered data.



5 Check the information of the selected data.



6 Display the PDF result file for the data file.



PDF Result File

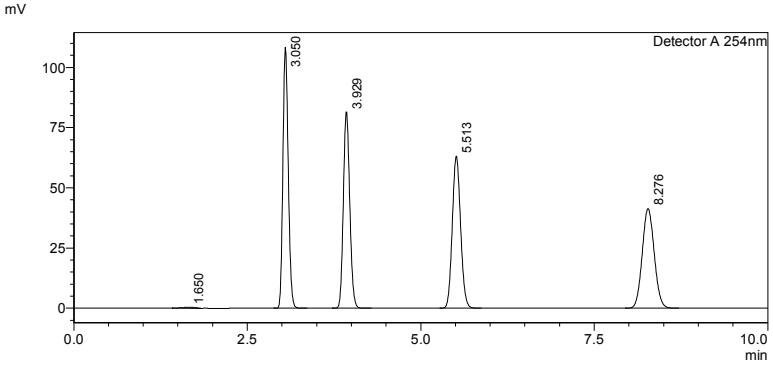
SHIMADZU LabSolutions

Analysis Report

<Sample Information>

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

<Chromatogram>



<Peak Table>

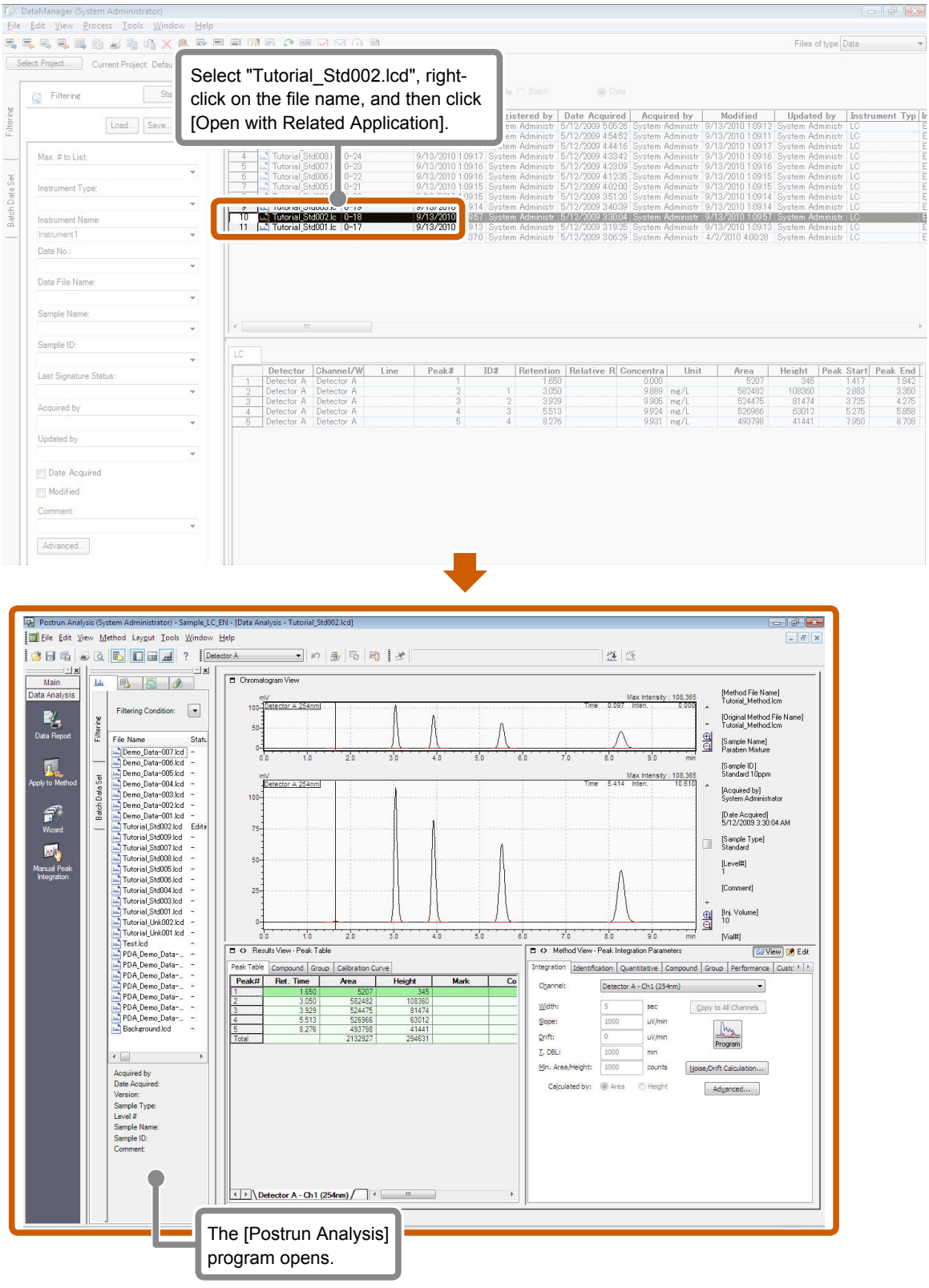
Detector A 254nm

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 SUPPLEMENT

Open the [Postrun Analysis] Program.

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



Chapter 8

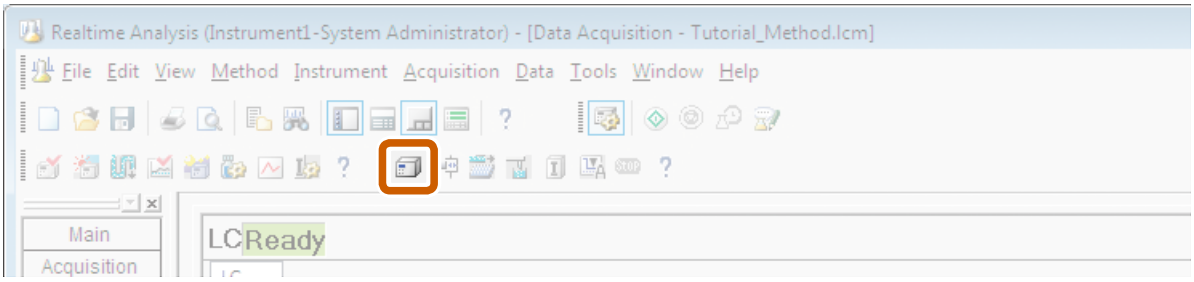
ShutDown

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

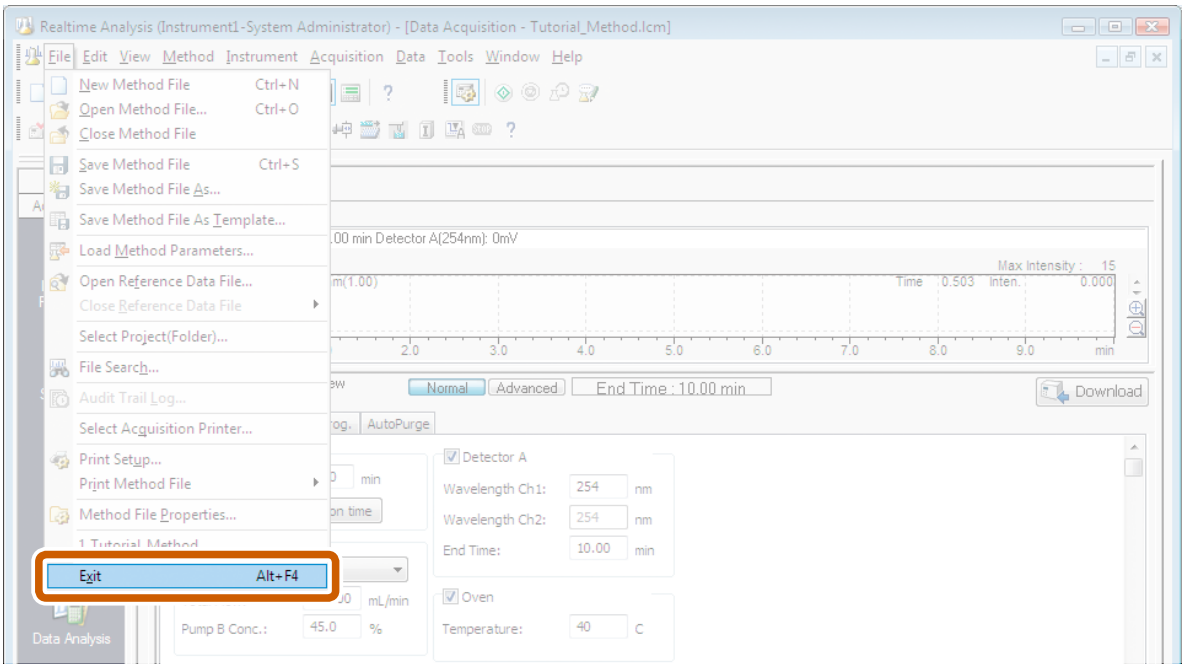
1 Stop instrument operation.

Stop pump solvent delivery and heating of the column oven.

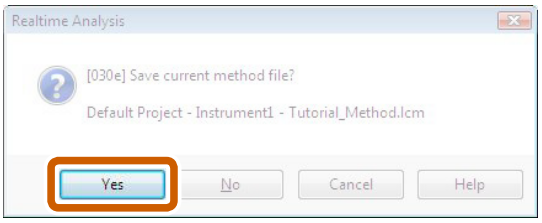
2 Set  to OFF.



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



4 Click [Yes].

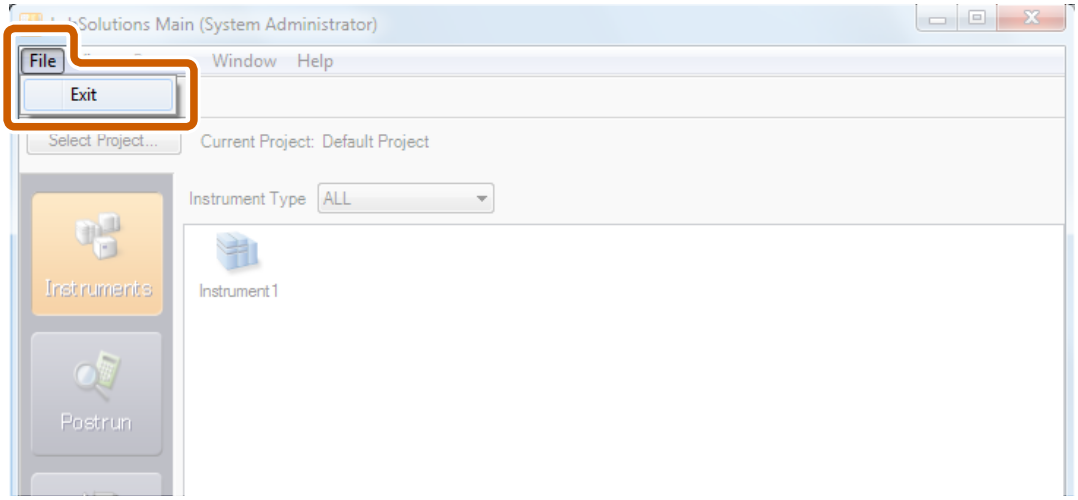


Hint

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.