

LabSolutions™ CL

Getting Started Guide

Chapters with the suffix “(LC)” is for the system without a mass spectrometer.

Chapters with the suffix “(LCMS)” is for the system with a mass spectrometer.

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Specific model names are not indicated in the descriptions common to LCMS instruments.

“LCMS/MS” is indicated in the descriptions common to LCMS-8045 CL/LCMS-8050 CL/LCMS-8060 CL/LCMS-8060NX CL.

Types of Manuals

Five Instruction Manuals are provided with LabSolutions.
You can also refer to the software [Help] menu to confirm screen settings.
The following shows how to make the best 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 describes system administration and data administration.

■ Data Acquisition & Processing Theory Guide

This manual describes the theory of peak detection and quantitation of sample components. It is written for advanced users.

■ Help

Refer to the on-screen software Help menu if you want to know more about screen settings.

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



Useful advice for convenient instrument operation



Shows where to refer to.



Additional information that may be useful for instrument operation

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 operations:

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

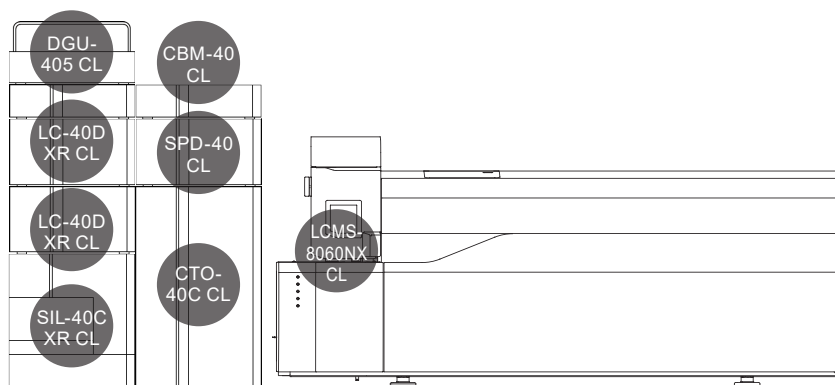
System Structure

This Getting Started Guide describes data acquisition operations with the assumption that the system includes the following instruments. Mass spectrometer is not available depending on the system configuration.

The chapters with the suffix “(LC)” is for the system without a mass spectrometer. The chapters with the suffix “(LCMS)” is for the system with a mass spectrometer.

High-pressure gradient system

- | | |
|-----------------------------------|-------------------------------------|
| • System Controller ... CBM-40 CL | • Pump LC-40D XR CL (2 units) |
| • Column Oven CTO-40C CL | • Detector SPD-40 CL |
| • Autosampler SIL-40C XR CL | • MS Detector LCMS-8060NX CL |
| • Degassing Unit DGU-405 CL | |




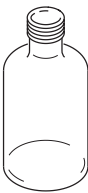

Acquisition Conditions

To acquire data as described in this Getting Started Guide, prepare a column, mobile phase, and samples as follows.

LC

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

LCMS

Column	Shim-pack XR-ODS 30 mm × 2.0 mm I.D., 2.2 µm (Shimadzu P/N 228-41605-91 or equiv.)	
Mobile Phase	Binary Gradient Mode Pump A: 0.1 % formic acid solution Pump B: 0.1 % formic acid solution / 99.9% acetonitrile	
Samples	Samples used for optimizing methods A (Procaine): 0.5 ng/µL solution B (Verapamil): 0.5 ng/µL solution C (Warfarin): 0.5 ng/µL solution Samples used for creating calibration curves A, B, C 0.01 ng/µL mixture (standard sample) A, B, C 0.05 ng/µL mixture (standard sample) A, B, C 0.1 ng/µL mixture (standard sample) A, B, C 0.5 ng/µL mixture (standard sample) Unknown (to be quantitated) sample (A, B, C 0.075 ng/µL mixture)	

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, etc.

Batch file (.lcb)

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

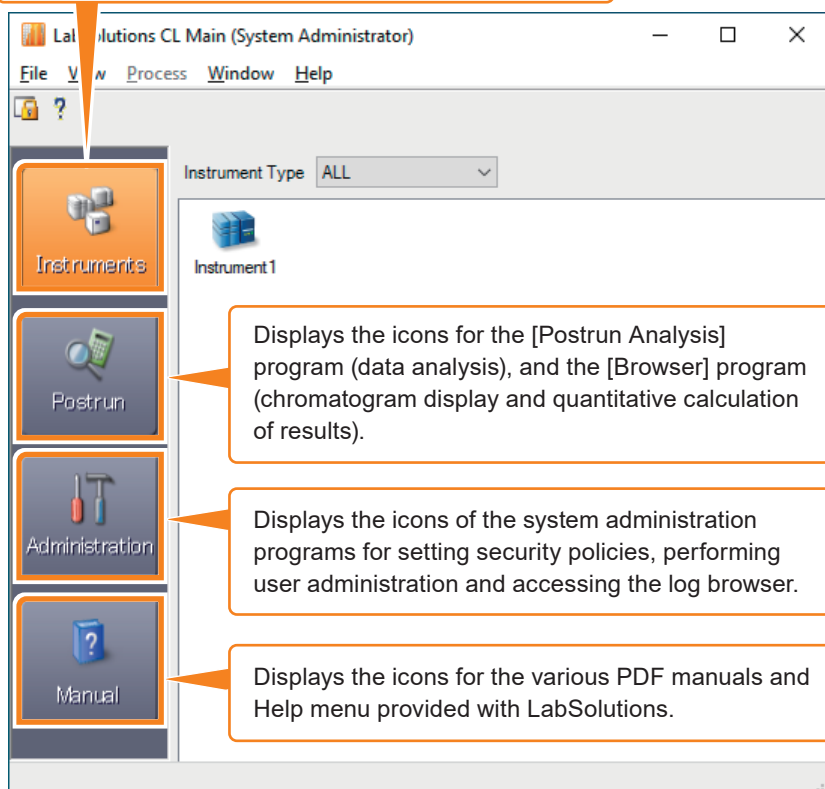
Report format file (.lsr)

This file is used to print data acquisition results.

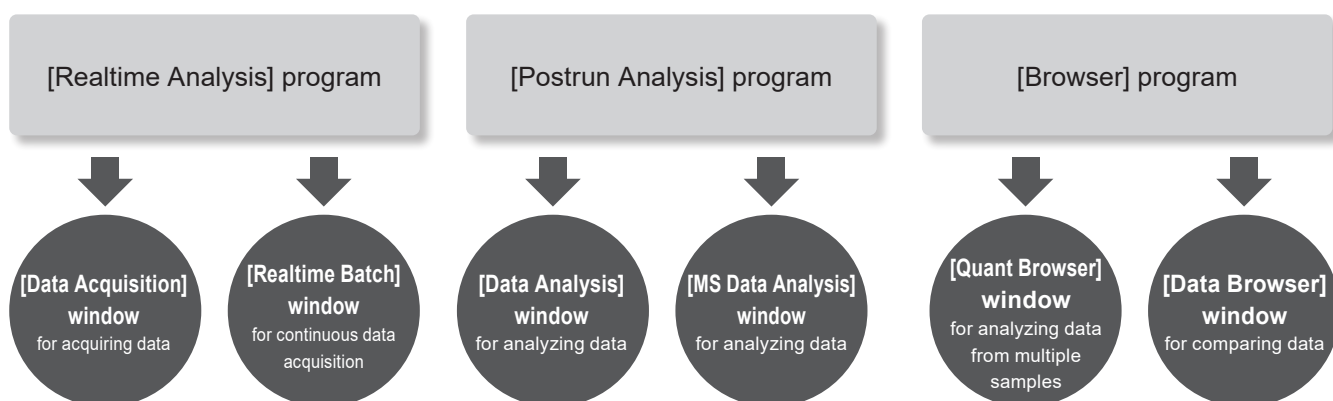
LabSolutions Main Window

The analytical instruments connected to the PC are displayed as icons.

Double-click an instrument icon to start the [Realtime Analysis] program where data acquisition settings are set and data is acquired.

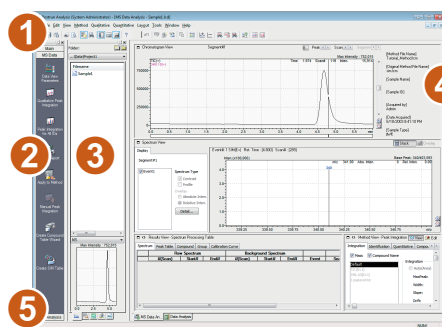


LabSolutions Main Programs and Main Windows



LabSolutions Windows

The following example describes the [Postrun 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.

3

Data Explorer

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

Click to change folders.

4

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], [Calibration Curve], [Report Format], and other windows are displayed.

Switch the windows by clicking the icons on the assistant bar.

5

Output Window

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

Message	Sub Message	Date	Time	Code
MS It is the exchange time of the oil of a rotary pump.		2/19/2008	7:57:20 AM	0x73b8 System Adm


How to Open Windows

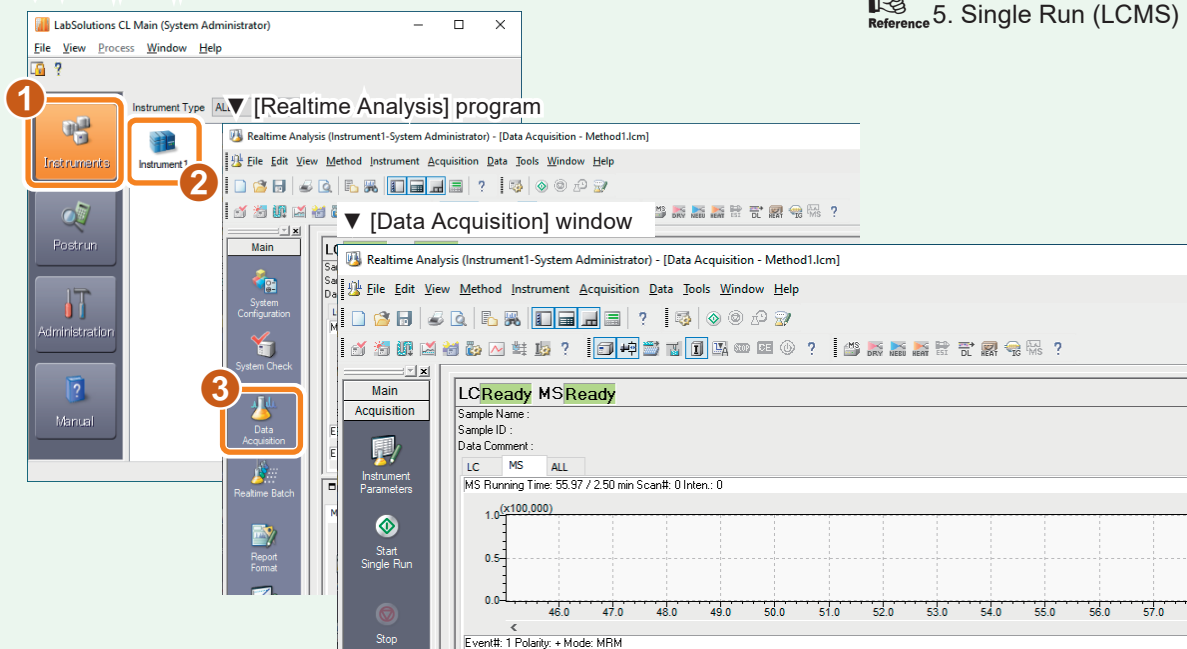
■ Set the Data Acquisition Parameters and Execute a Single Run

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

▼ Main window

 Reference 3. Single Run (LC)

 **Reference** 5. Single Run (LCMS)



■ Data Analysis and Quantitative Calculations (LC)

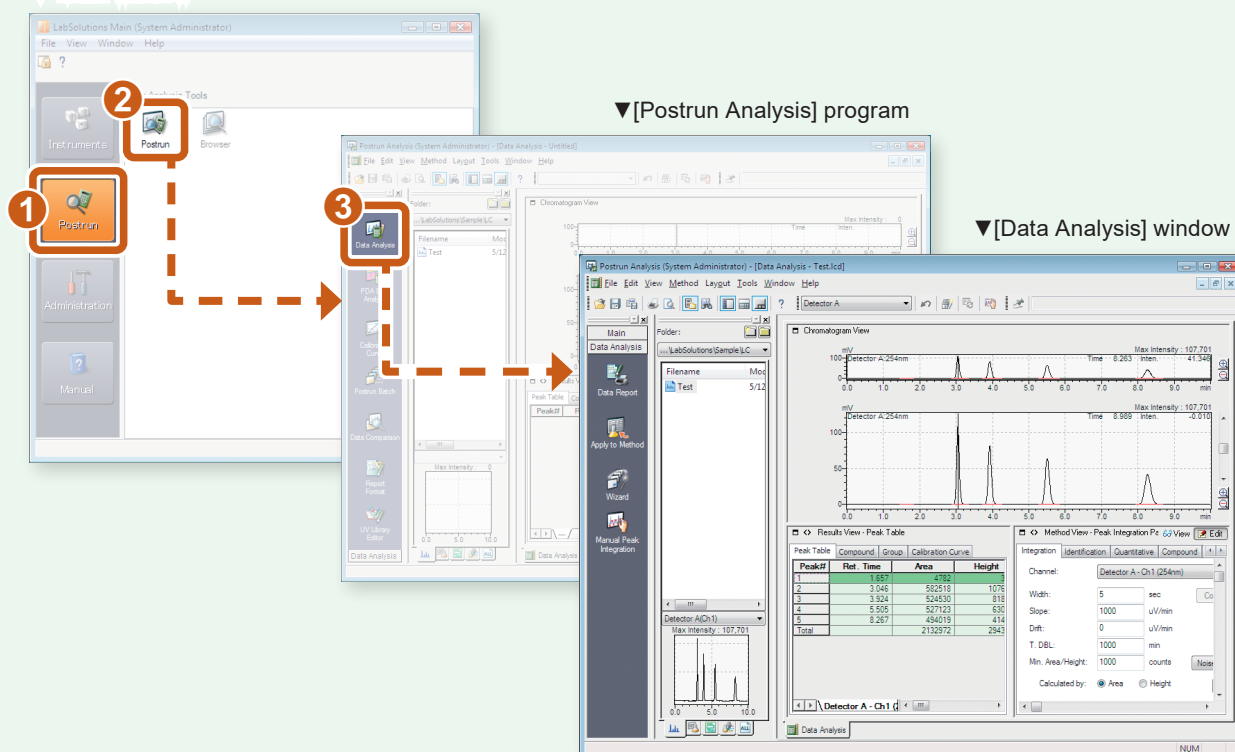
Open the [Data Analysis] window from the main window.

 Reference 4. Data Analysis (LC)

▼ Main window

▼[Postrun Analysis] program

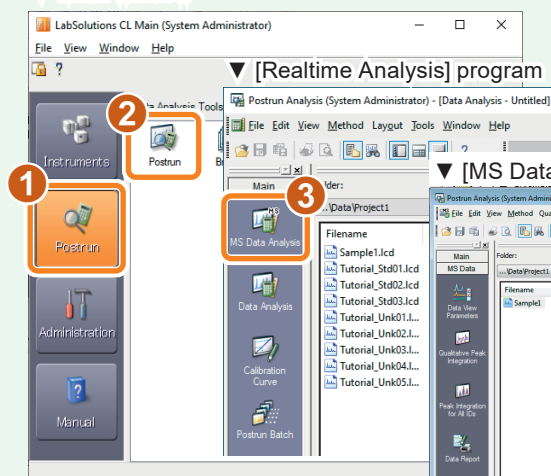
▼[Data Analysis] window



MS Data Analysis and Qualitative Calculations (LCMS)

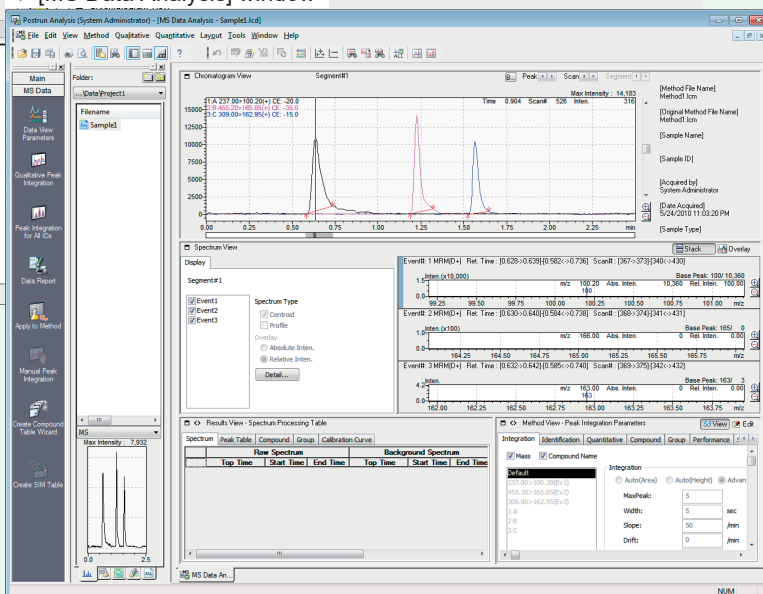
Open the [MS Data Analysis] window from the main window.

▼ Main window



6. Confirm Single Run Results (LCMS)

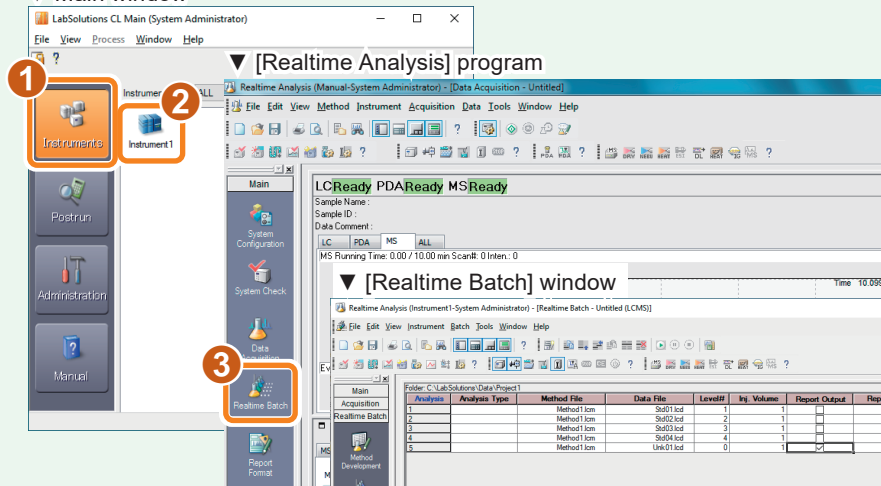
▼ [MS Data Analysis] window



Continuous Data Acquisition of Sequential Samples

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

▼ Main window




7. Realtime Batch

▼ [Realtime Batch] window

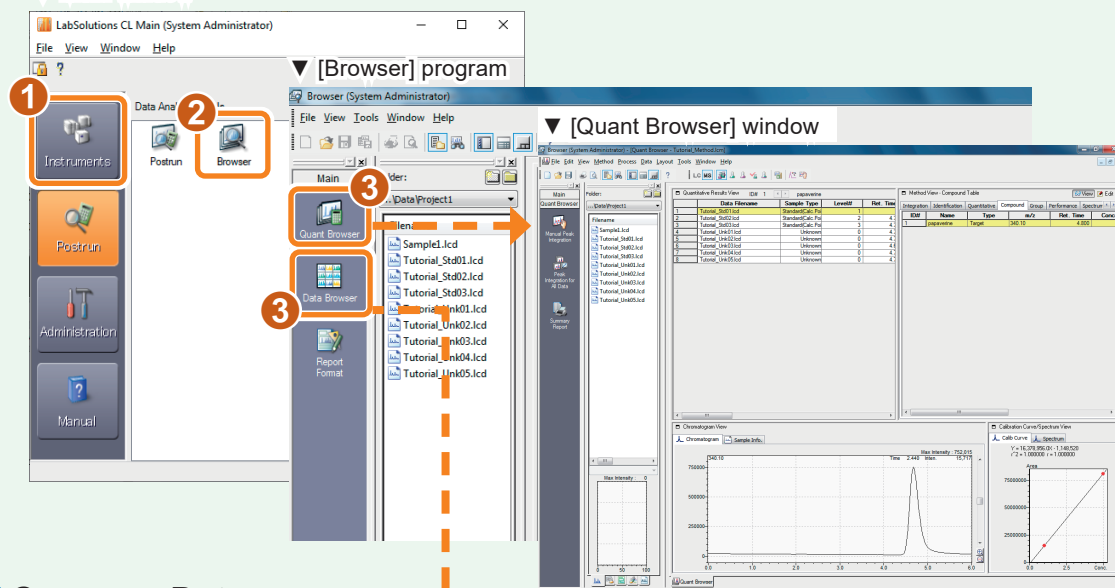
Realtime Batch - [Realtime Batch - Untitled (LCMS)]							
Analysis	Analysis Type	Method File	Data File	Level#	Inj. Volume	Report Output	Report Format File
1	Method 1	Method 1	Sample1	1	1		
2	Method 1	Method 1	Sample2	2	1		
3	Method 1	Method 1	Sample3	3	1		
4	Method 1	Method 1	Sample4	4	1		
5	Method 1	Method 1	Sample5	5	1		

Confirm Quantitative Results

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


 **Reference 8. Quantitative Data Analysis**

▼ Main window

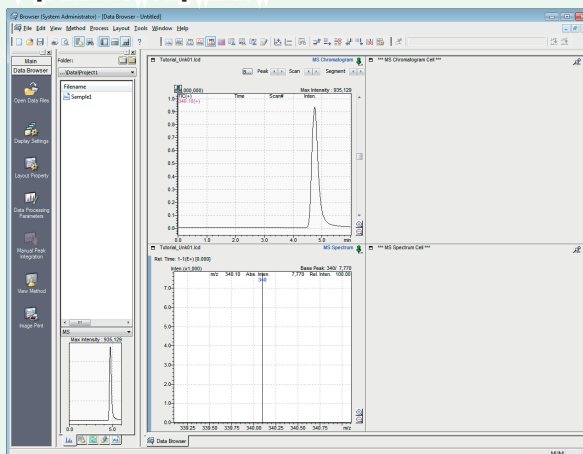


Compare Data

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

 **Reference 9. Qualitative Data Analysis**

▼ [Data Browser] window

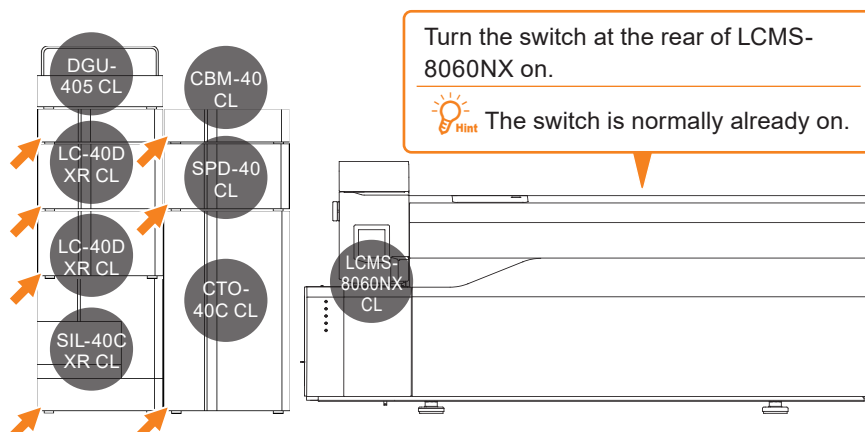


Chapter 1. Startup

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 ON all of the instruments.



3 Confirm that nitrogen gas and argon gas are being supplied to the MS instrument.

4 Start the PC.

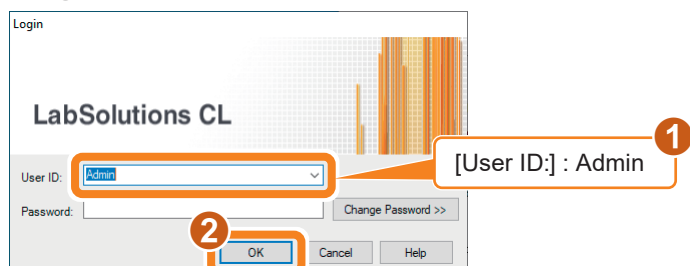
5 Verify that the [LabSolutions Service] icon in the system tray on the Taskbar is green.



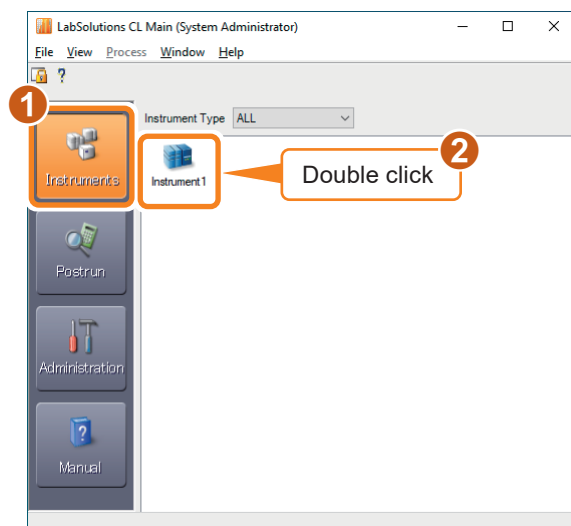
Icon Color	LabSolutions Status	Operation
Green	Normal	
Yellow	Starting up	Please wait
Red	Error	Please restart the PC.

6 Double-click  on the desktop.

7 Log in.



8 Start the [Realtime Analysis] program.




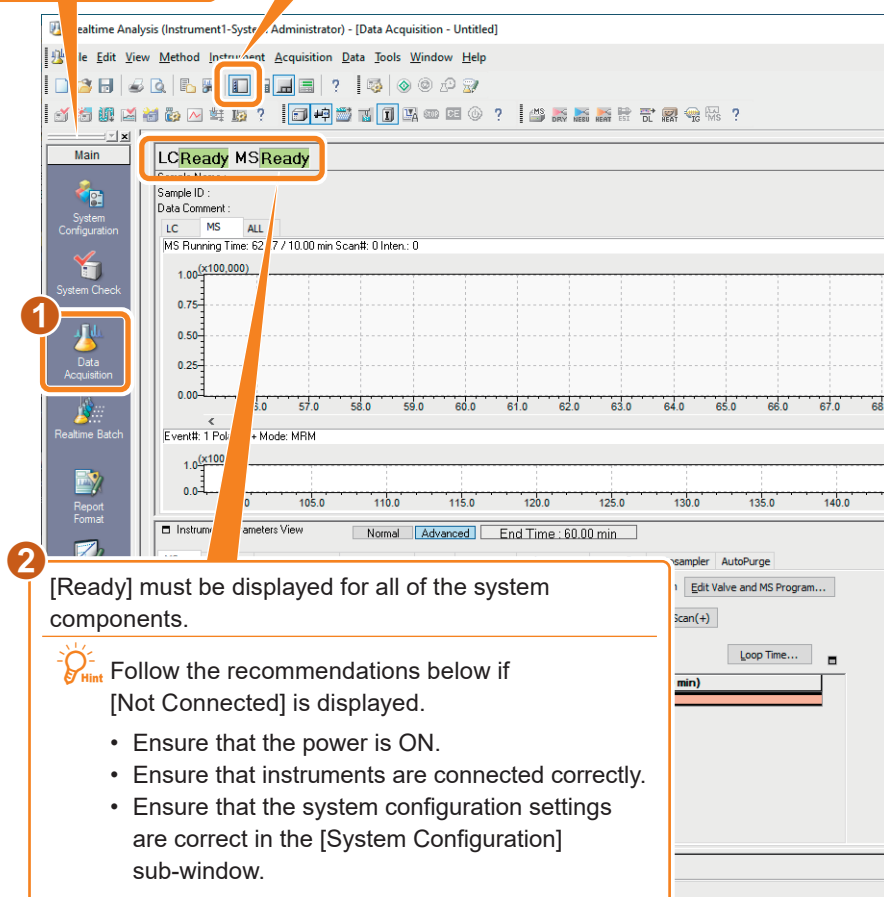
9 Open the [Data Acquisition] window.



If the [Main] assistant bar is not displayed, click the [Main] button.




Click  if the assistant bar is not displayed.



1

2

[Ready] must be displayed for all of the system components.

 Follow the recommendations below if [Not Connected] is displayed.

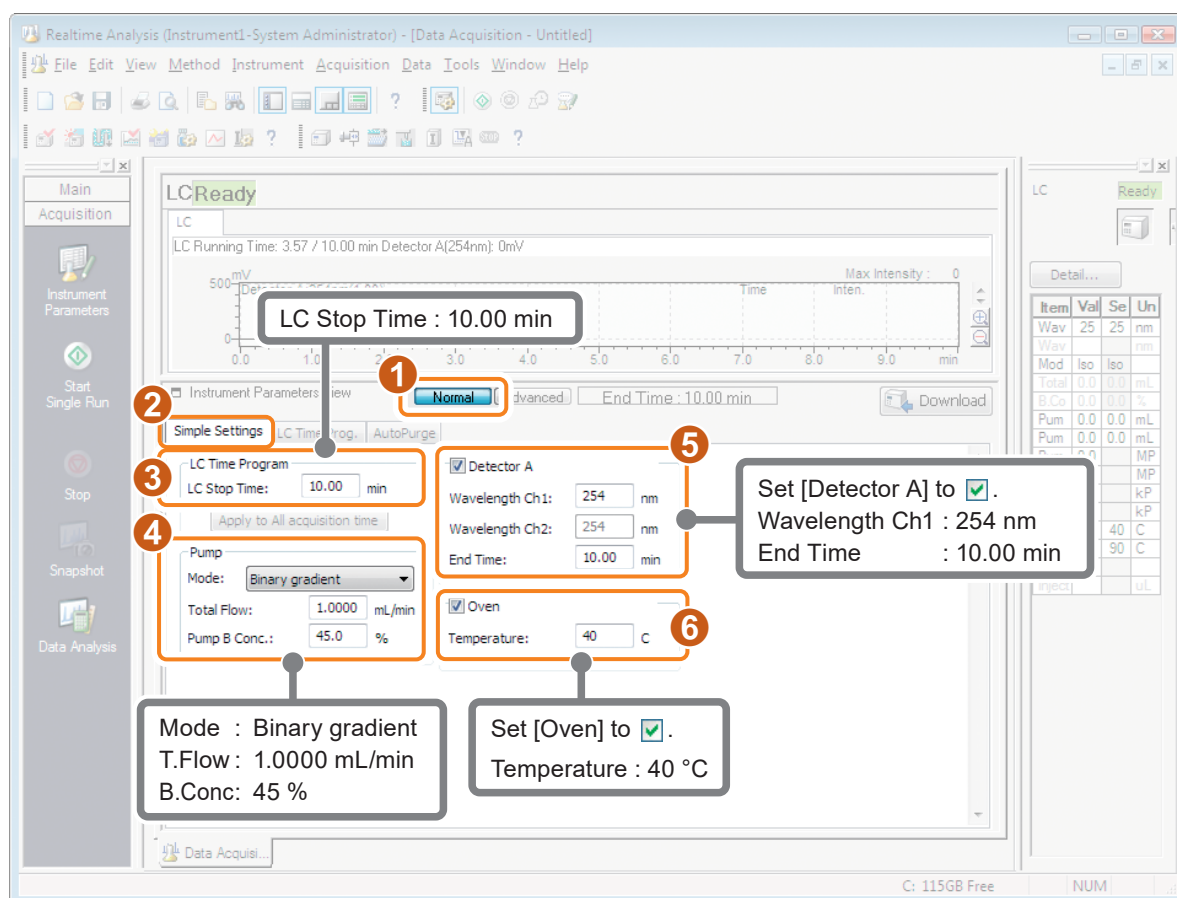
- Ensure that the power is ON.
- Ensure that instruments are connected correctly.
- Ensure that the system configuration settings are correct in the [System Configuration] sub-window.

Chapter 2. Set the Instrument Parameters (LC)

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.



Refer to P.5 for details on data acquisition conditions.



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

3 Save the data acquisition conditions.

1. Click the Save icon in the toolbar.

2. Enter "Method1".

3. Click the Save button.

4. Click the Download button to download the data acquisition conditions to the instrument.

The folder initially displayed here is the default folder.
To change the default folder, see "Default Folder and Change the Default Folder" P.16

LabSolutions



Default Folder and Change the Default Folder

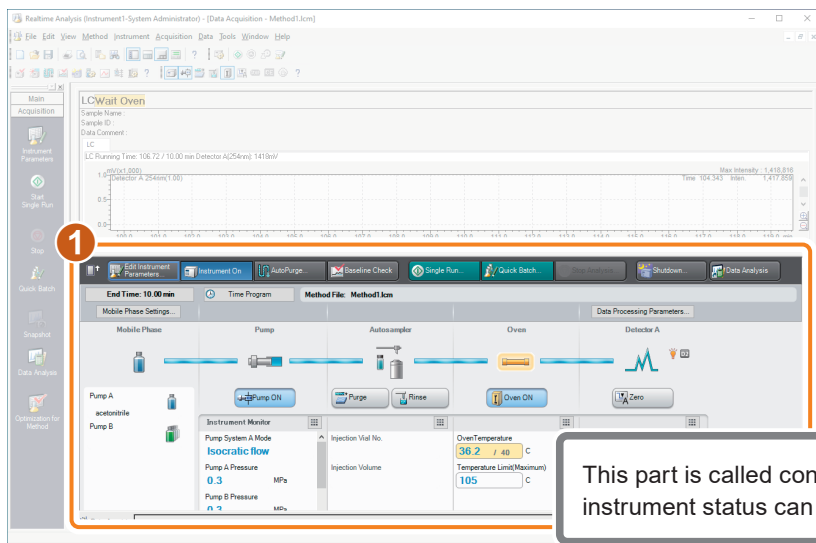
1. Click the Folder icon in the toolbar.

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

This folder is the default folder.

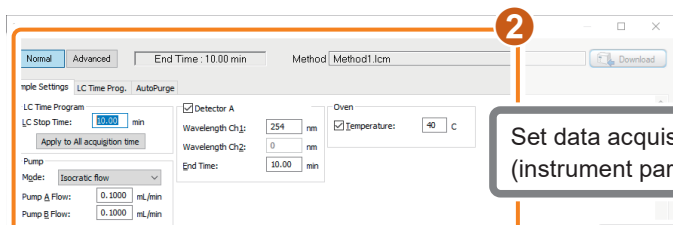
Control Panel

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




1

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



2

Set data acquisition conditions (instrument parameters).



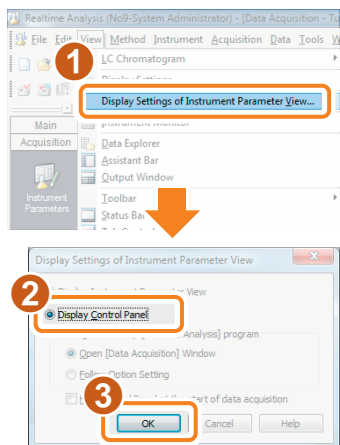
3

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



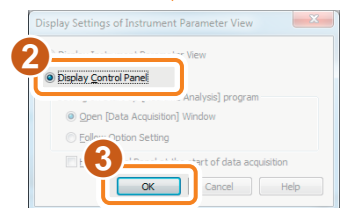
Switching Display Settings

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

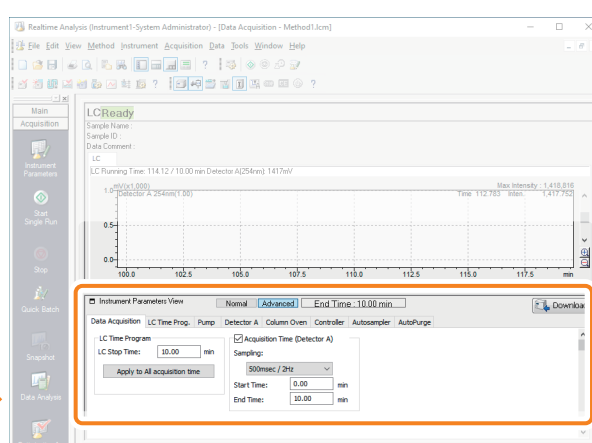


1

Display Settings of Instrument Parameter View...



2



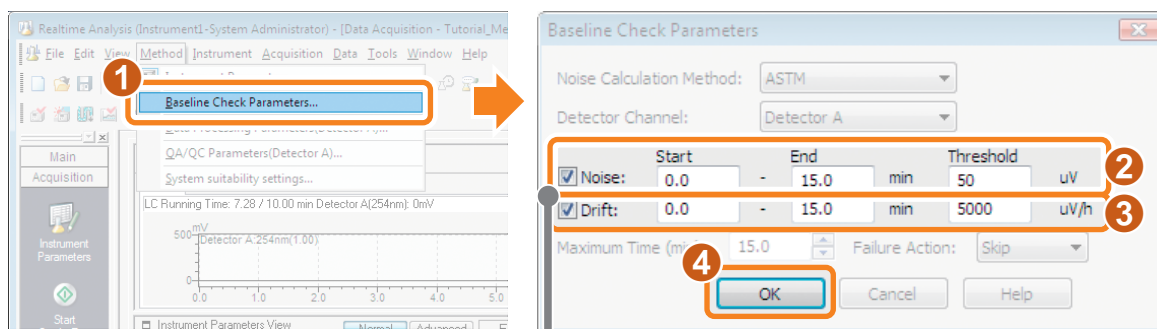
3

Baseline Check

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

Baseline check parameters are saved in the method file.

1 Set [Baseline Check Parameters].



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

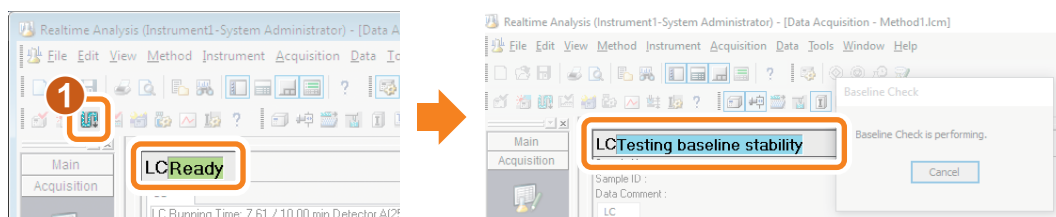


In the [Baseline Check] sub-window, the noise calculation method can be changed, and the maximum delay time when the result of the baseline check is [Fail] within the preset time.



Help for details.

2 Perform the baseline check.

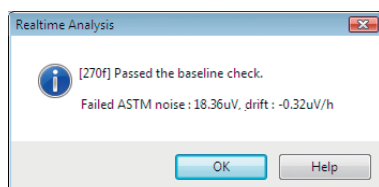


After measurement ends, the check results are displayed in [Baseline Check Results] sub-window and [Output Window].

[Output Window]

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

Baseline Check Results



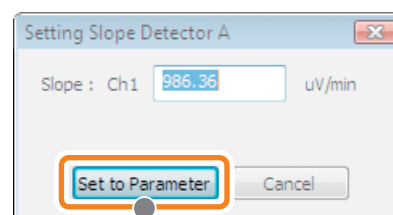
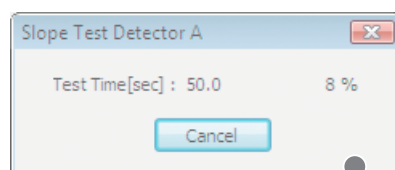
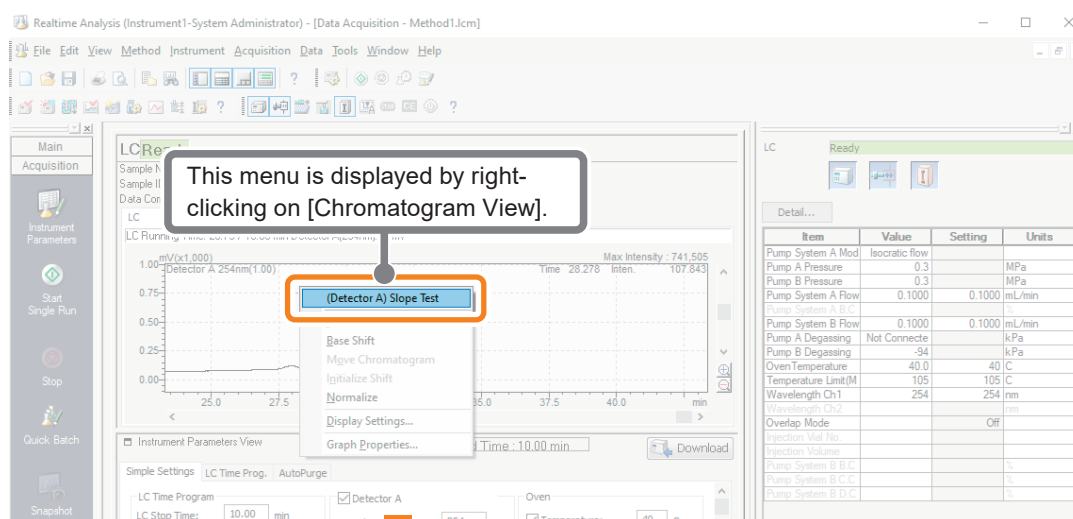
Slope Test

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

This section describes the Slope Test.



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



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".

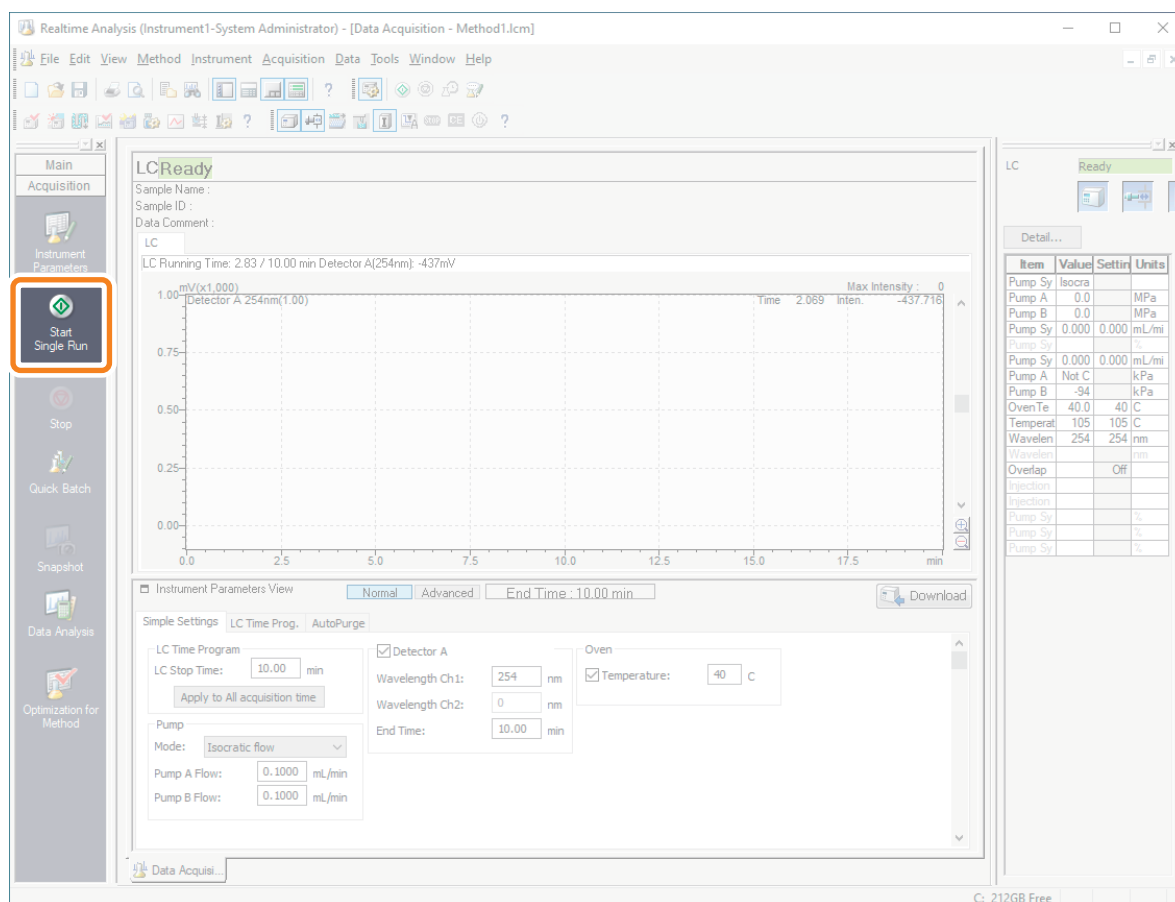
Chapter 3. Single Run (LC)

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.

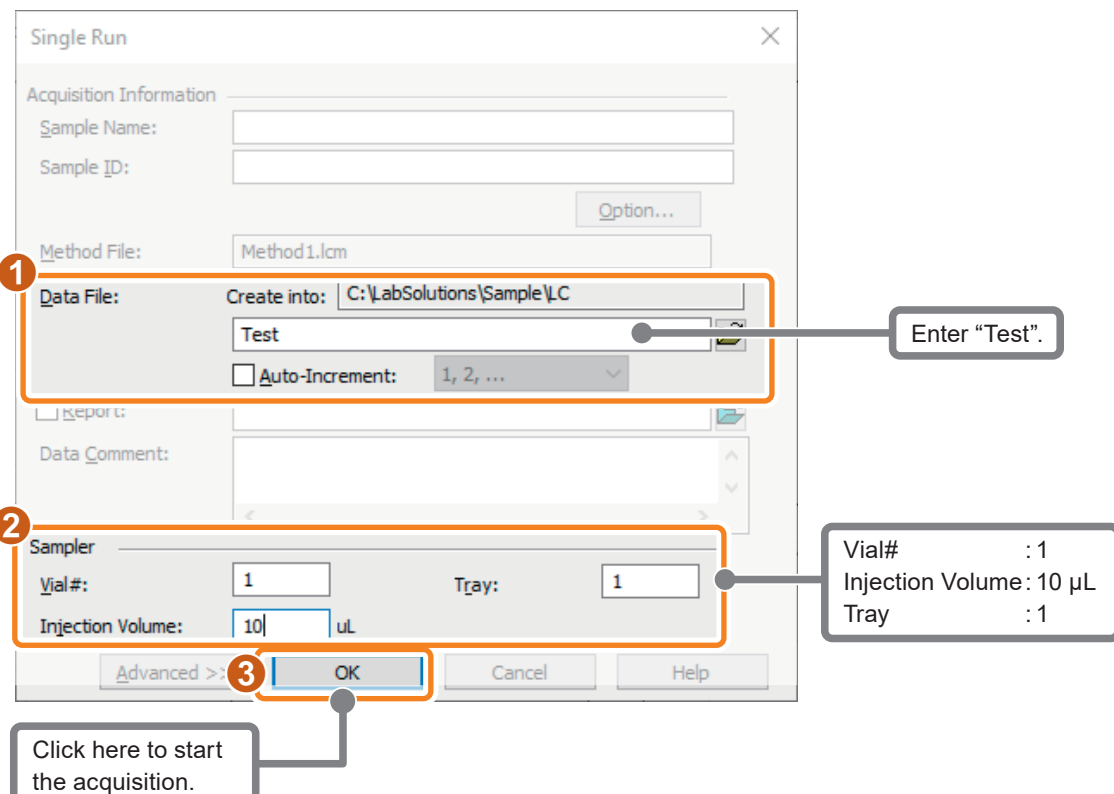
2 Open the [Single Run] sub-window.



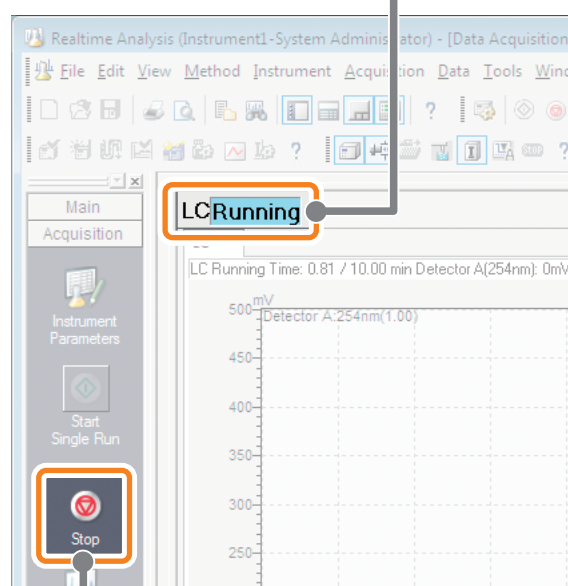
The [Single Run] sub-window opens.

3 Set the conditions for a single run.

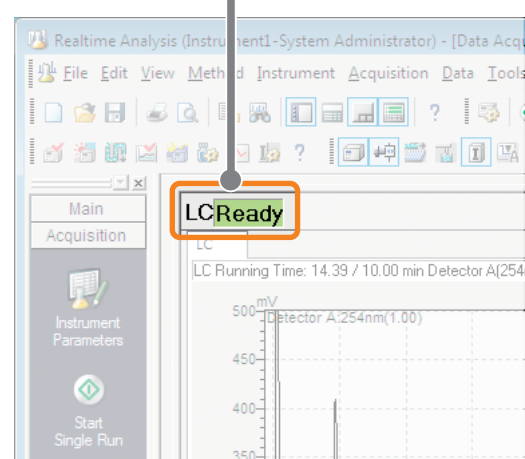
In this example, set the conditions for pouring 10 ppm of paraben mixed sample into vial No.1 on the autosampler, and injecting 10 μ L of that sample.



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.

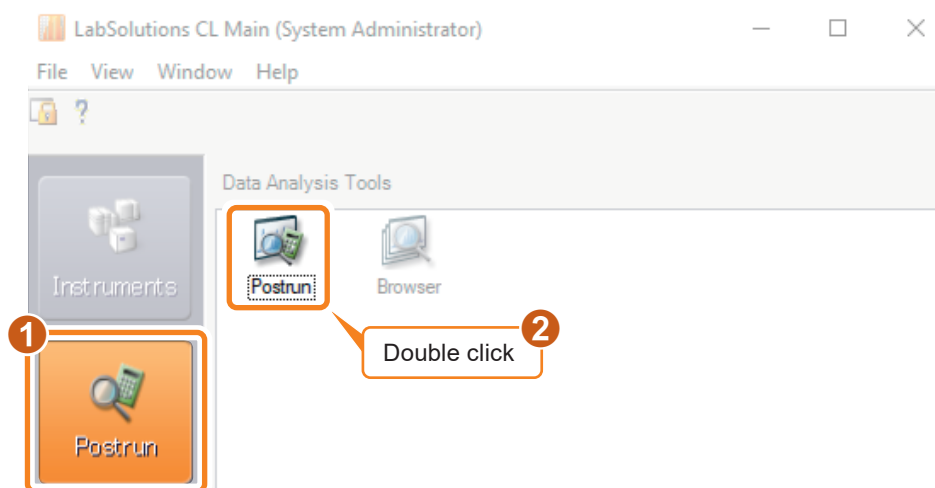


The status changes to **Ready** when data acquisition ends.

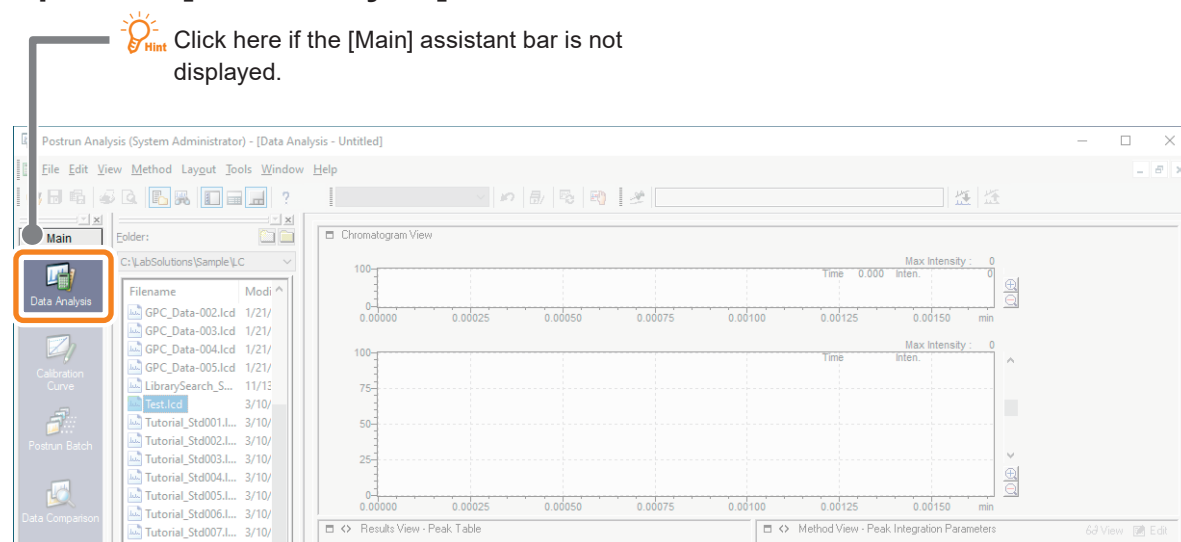
Chapter 4. Data Analysis (LC)

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.

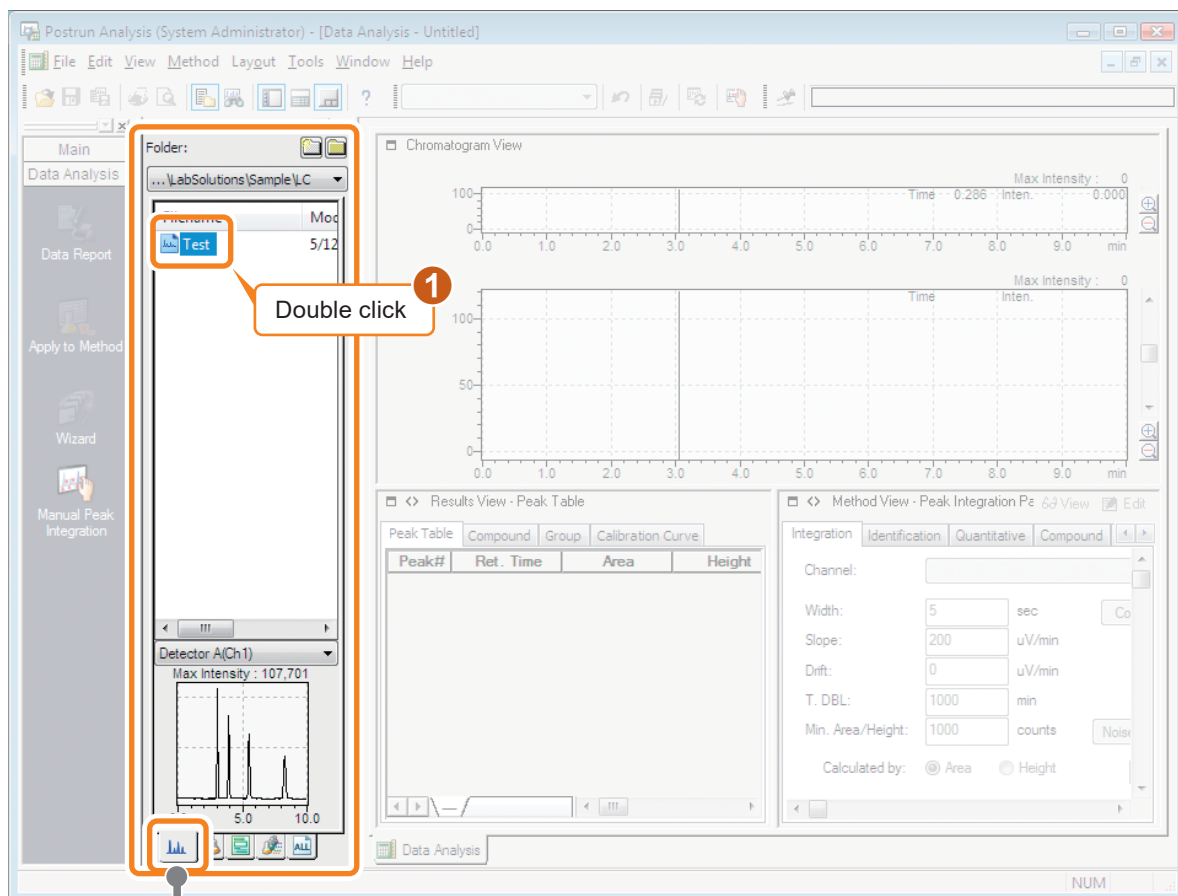


2 Open the [Data Analysis] window.



The [Data Analysis] window opens.

3 Display “Test.lcd”.



Refer to “Data Analysis” chapter in *Operators Guide for LC System* 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	8
3	3.924	524530	8
4	5.505	527123	8
5	8.267	494019	8
Total		2132972	2943

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.

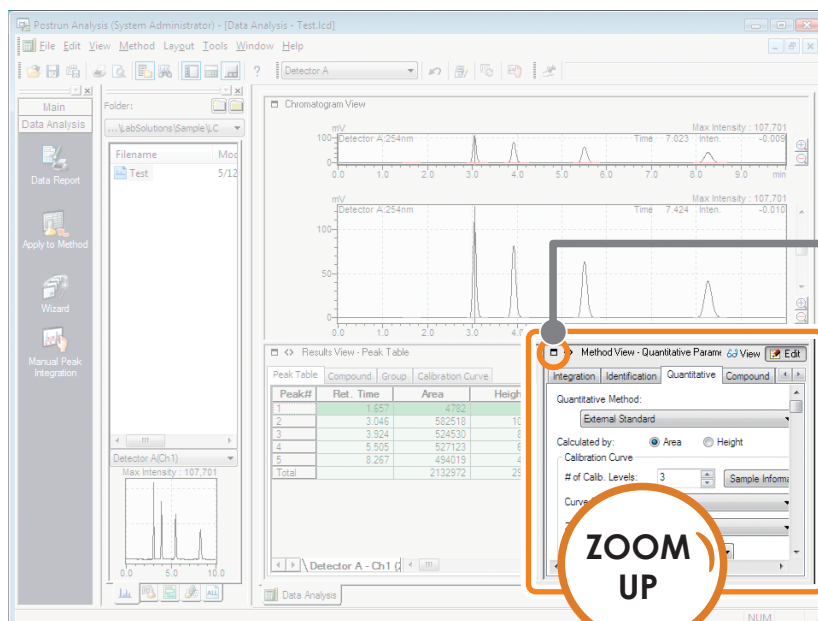
Determine the start and end points of the peak by the Slope value.

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



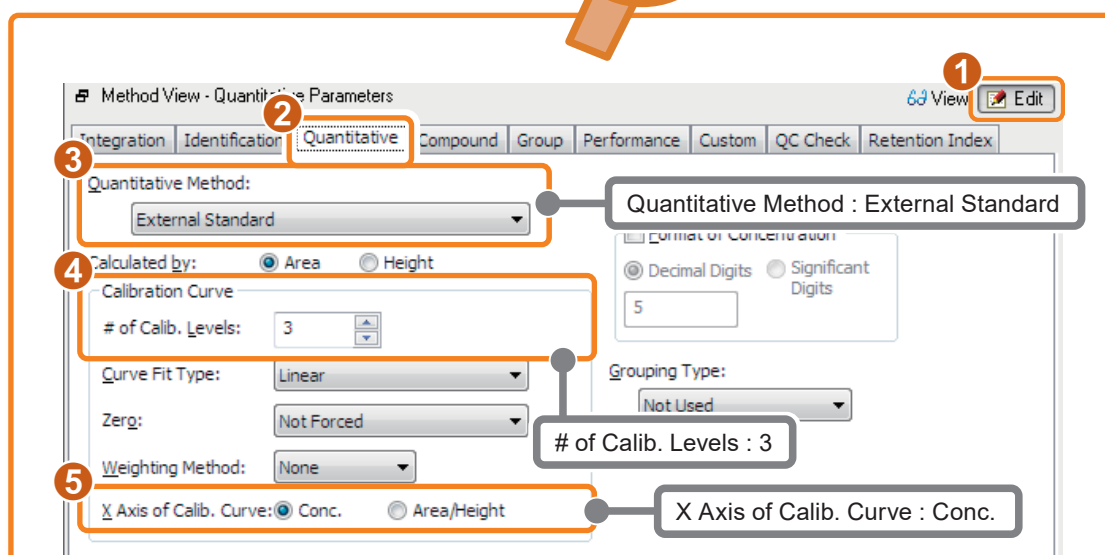
Refer to "Peak Integration Parameters" of the "Data Analysis" chapter in *LC Operators Guide* for details on the Peak Integration Parameters.

5 Enter the quantitative parameters.



 Click  to enlarge the window.

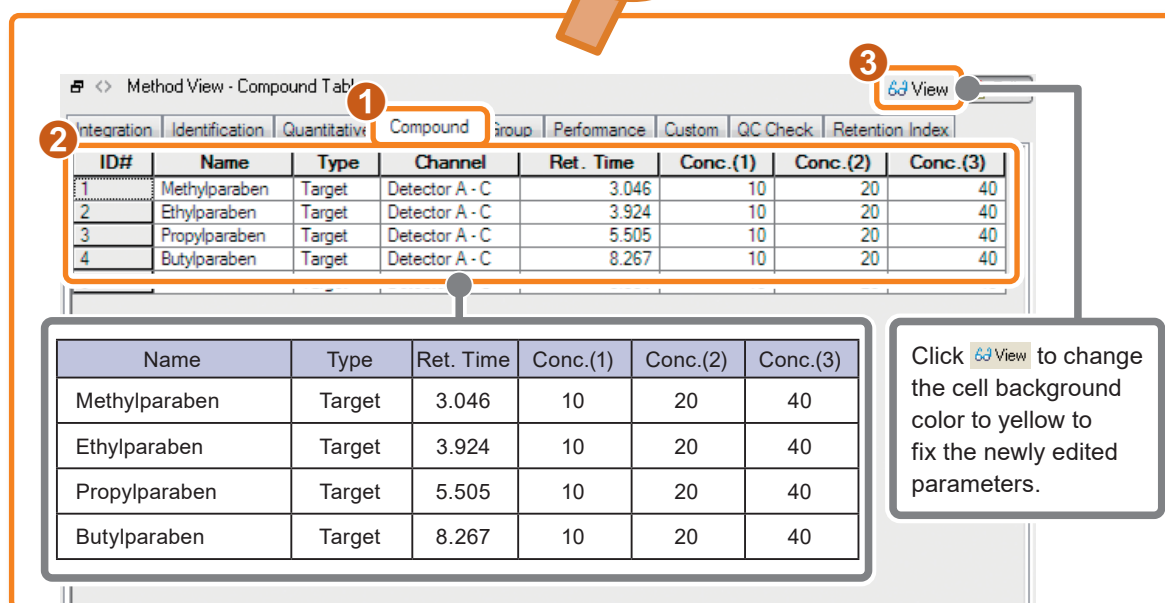
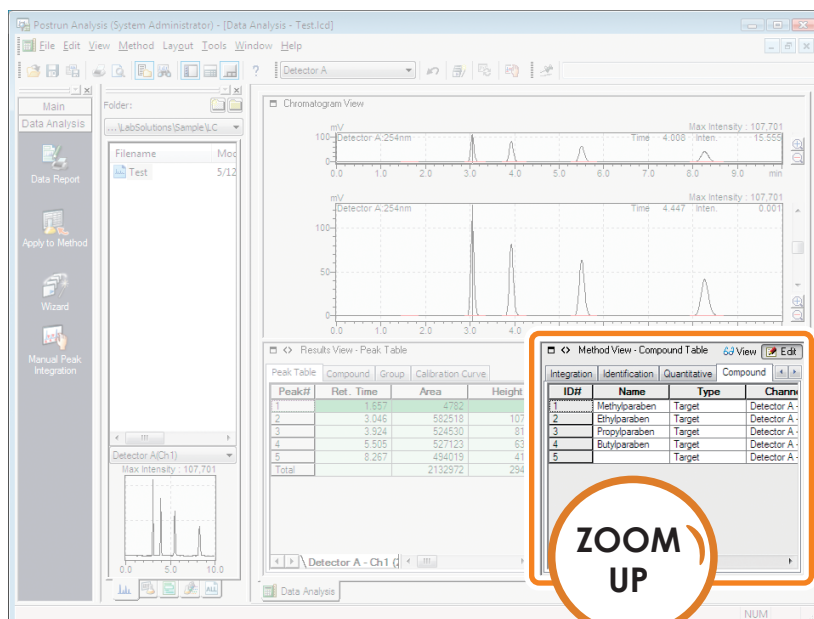
**ZOOM
UP**



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

Continued on the following page 

6 Fill in the Compound Table.



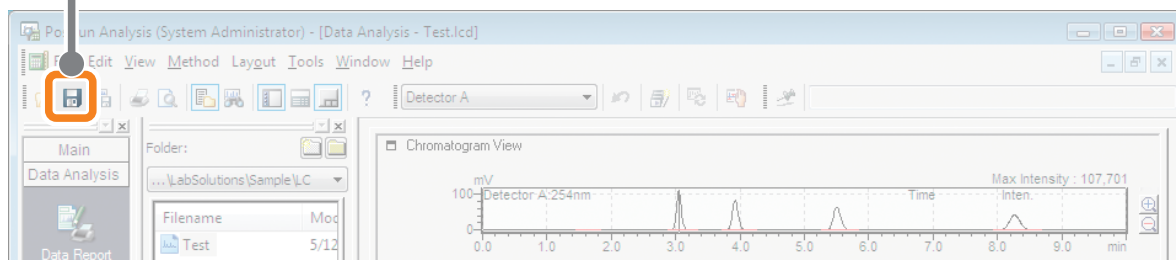
- The result obtained by performing data acquisition is used for [Ret. Time].
- Selecting the [Ret. Time] cell, and clicking the peak in [Chromatogram View] automatically enters the retention time of that peak to the currently selected [Ret. Time] cell.
The retention time can be set by simply clicking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



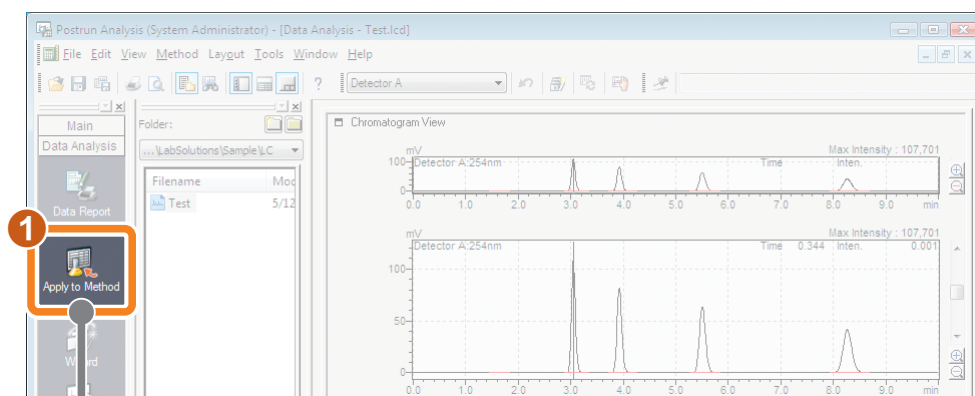
Refer to “Compound Table Retention Times Using the Mouse” of the “Data Analysis” chapter in the *Operators Guide for LC System* for details on setting retention times.

7 Save the processing results to a data file.

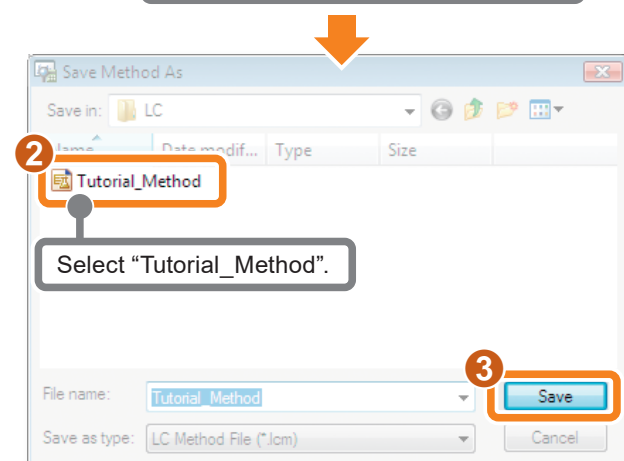
Click here to save the processing results to "test.lcd".



8 Save the method file.

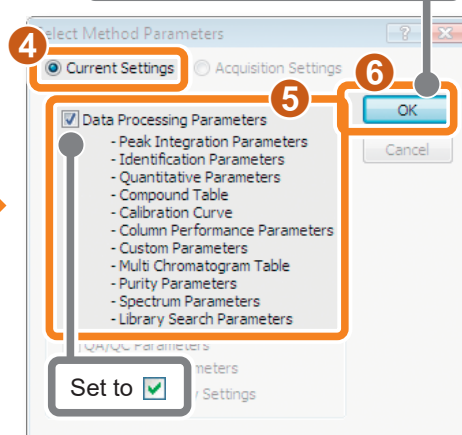


Click here to open the [Save Method As] sub-window.




Select "Tutorial_Method".

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



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. Single Run (LCMS)

Set the LC instrument parameters and MS instrument parameters (acquisition conditions) in the [Data Acquisition] window, and perform method optimization and single run.

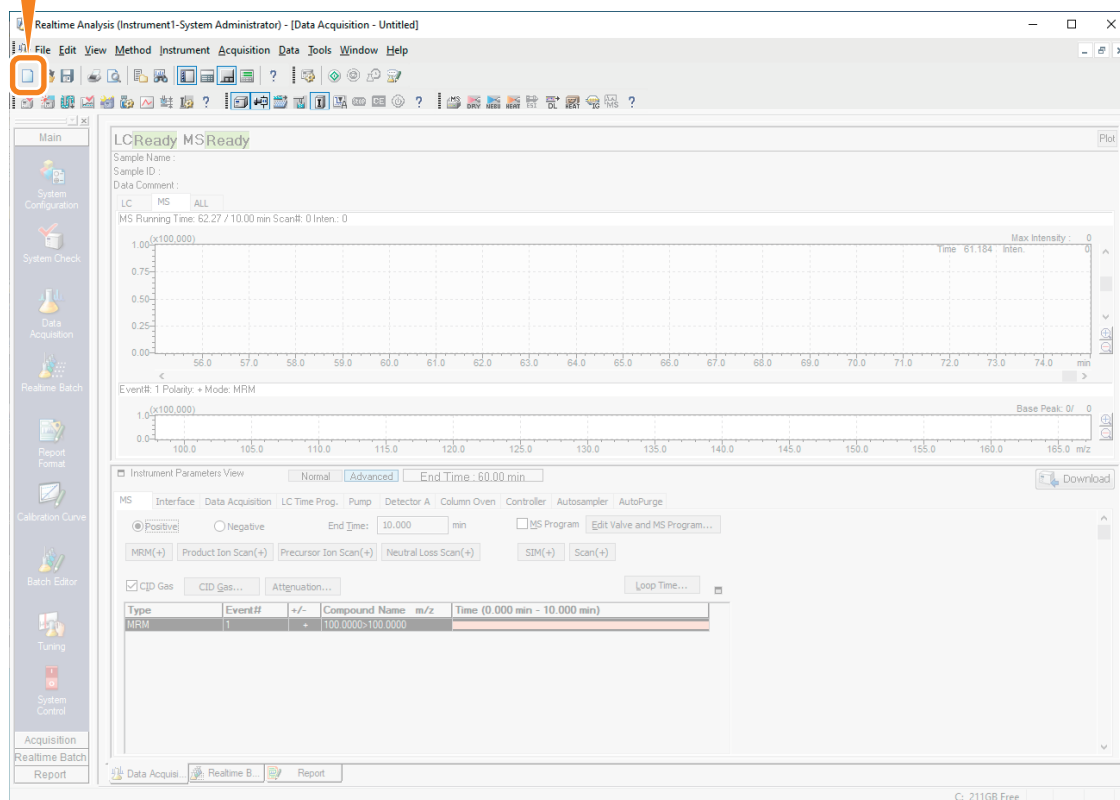
5.1 Create a Method File

1 Click [New] on the toolbar.

Click 



When the “Save current Method File?” message is displayed, select [No].



Getting Started Guide 29

3 Set the LC instrument parameters.

LC Ready MS Ready

Sample Name:
 Sample ID:
 Data Comment:

LC MS ALL

1. Normal

2. LC Stop Time: 0.50 min

3. [LC Stop Time] : 0.5

4. [Mode] : Binary gradient
[Total Flow] : 0.2
[Pump B Conc.] : 70

5. [End Time] : 0.5

6. Download

Item	Value	Setting	Units
Pump System A	Isocratic flo		
Pump A Pressure	0.1		MPa
Pump B Pressure	0.1		MPa
Pump System A	0.0500	0.0500	mL/min
Pump System B	0.0500	0.0500	mL/min
Pump A Degassi	Not Connec		kPa
Pump B Degassi	-94		kPa
Oven Temperature	40.0		°C
Temperature Lim	105		°C
Overlap Mode	Off		
Injection Val No			
Pump System B			
Pump System B			
Nebulizing Gas F		3.0	L/min
Drying Gas Flow		15.0	L/min
Heating Gas Flo		15.0	L/min
Interface	IonFocus		
Interface Voltage		0.0	kV
Interface Current		0.0	µA
Interface Temper	44		°C
Desolvation Tem	44		°C
DL Temperature	42		°C
Heat Block Tem	24		°C
Conversion Dyno		0.0	kV
Detector Voltage		0.00	kV
IG Vacuum			Pa
PG Vacuum	1.7e+02		Pa
CID Gas	17		kPa

▼ Tips

Pump Pressure Limits

The maximum column pressure (pressure resistance) value is specified in the column's instruction manual. Use the following procedure to set the pressure threshold (typically, the column's pressure resistance) at which the pump automatically stops to protect the column. This procedure changes the upper pressure value to 70 MPa, as an example.

Instrument Parameters View

Normal Advanced End Time: 3.00 min

MS Interface Data Acquisition LC Time Prc Pump for A Column Oven Controller Autosampler AutoPurge

B.GE1

Stop time: 0.50 min

Flow: 0.2000 mL/min

Time to reach the flow: 0.00 min (Off)

A.Conc: 30.0 %

B.Conc: 70.0 %

B.Curve: 0

Pressure limits

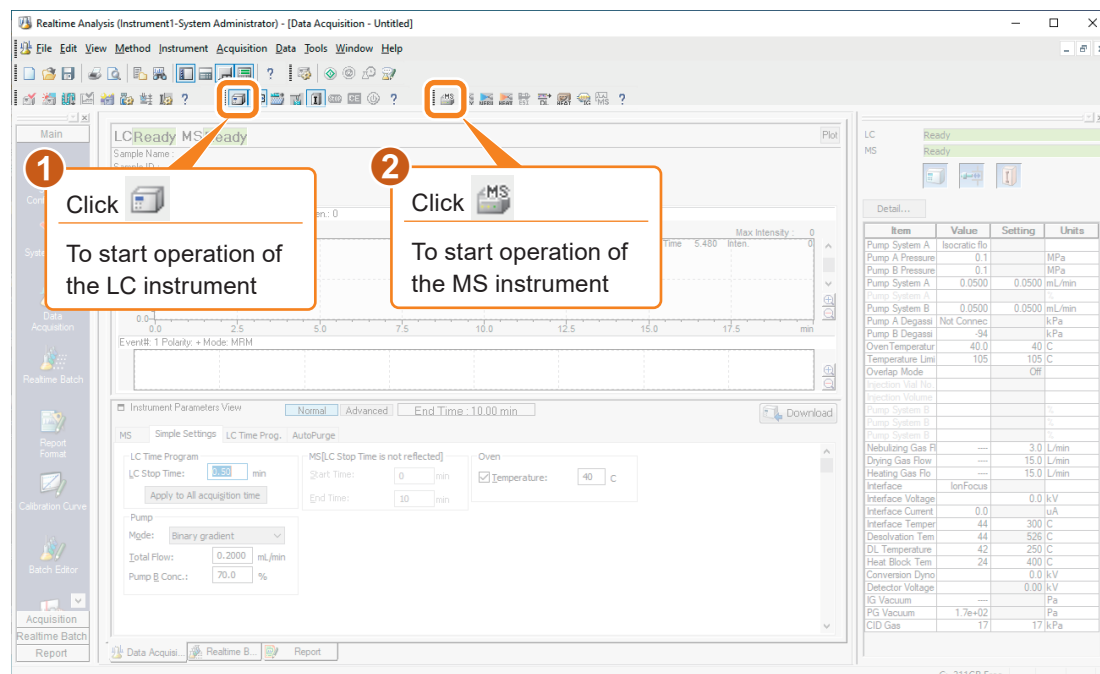
Minimum: 0.0 MPa Maximum: 70.0 MPa

3. [Maximum] : 70

5.3 Instrument Control

1 Take control of the instrument.

The DL plug must be removed before starting analysis.



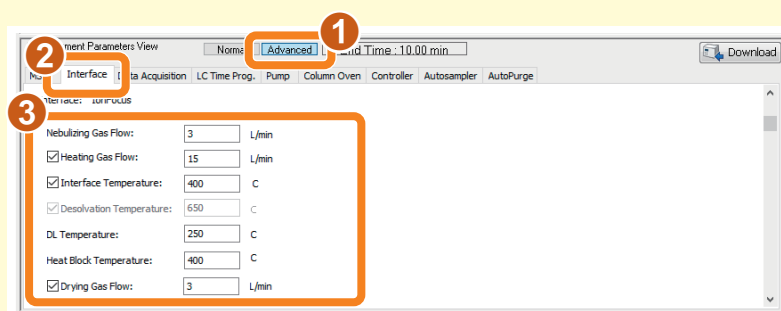
2 Purge the LC pump and the autosampler.

Always purge after changing the mobile phase.

▼ Tips

Set the interface temperature and the gas flow

The interface temperature and the gas flow are set according to the following procedure.



5.4 Execute Method Optimization

Determine the optimum parameters for MRM data acquisition of each sample by executing method optimization.



“8 Method Optimization” in *Operators Guide for LCMS/MS system*.

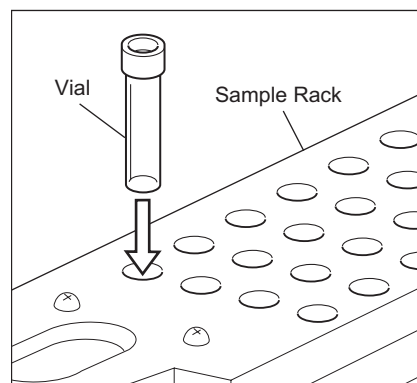
1

Place the samples in the autosampler.

Vial 1, sample A 0.5 ng/μL solution

Vial 2, sample B 0.5 ng/μL solution

Vial 3, sample C 0.5 ng/μL solution



2

Click [Optimization for Method] on the [Acquisition] assistant bar.

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

File Edit View Method Instrument Acquisition Data Tools Window Help

LCReady MSReady

Sample Name :
Sample ID :
Data Comment :

LC MS ALL

MS Running Time: 0.00 / 10.00 min Scan#: 0 Inten.: 0

Event#: 1 Polarity: + Mode: MRM

99.00 99.25 99.50 99.75 100.00 100.25 100.50 100.75 min

1.00 (x100,000)
0.75
0.50
0.25
0.00

Time 4.756 Max intensity: 0

99.00 99.25 99.50 99.75 100.00 100.25 100.50 100.75 m/z

Instrument Parameters View

Normal Advanced End Time: 10.00 min Download

MS Simple Settings LC Time Prog. AutoPurge

☒ Positive ☐ Negative End Time: 10.000 min ☐ MS Program Edit Valve and MS Program...

MRM(+) Product Ion Scan(+) Precursor Ion Scan(+) Neutral Loss Scan(+) SIM(+) Scan(+)

☒ CID Gas... CID Gas... Attenuation... Loop Time...

Type	Event#	+/-	Compound Name	m/z	Time (0.000 min - 10.000 min)
MRM	1	+	100.0000-100.0000		

MRM Acq. Time: 0 - 10 min Compound Name:

Ch	Precursor m/z	Product m/z	Dwell Time (msec)	CE
Ch1	100.0000	100.0000	100.0	35.0
Ch2				
Ch3				
Ch4				

Realtime Batch Report

Data Acqui... Realtime B... Report

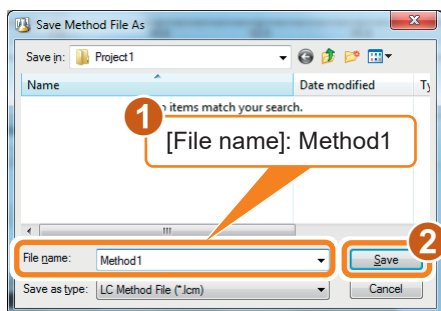
LC Ready
MS Ready

Detail...

Item	Value	Setting	Units
Pump System A Isocratic flo			
Pump A Pressure	0.0		MPa
Pump B Pressure	0.0		MPa
Pump System A	0.0500	0.0500	mL/min
Pump System A			%
Pump System B	0.0500	0.0500	mL/min
Pump A Degress	Not Connec		kPa
Pump B Degress	-94		kPa
Oven Temperature	40.0	40	C
Temperature Lim	105	105	C
Overlap Mode		Off	
Injection Val Pos			
Injection Volume			%
Pump System B			%
Pump System B			%
Nebulizing Gas Fl	---	3.0	L/min
Drying Gas Flow	---	15.0	L/min
Heating Gas Fl	---	15.0	L/min
Interface IonFocus			
Interface Voltage	0.0	0.0	kV
Interface Current	0.0		uA
Interface Temper	44	300	C
Desolvation Tem	44	250	C
DL Temperature	42	250	C
Heat Block Tem	24	400	C
Conversion Dyno		0.0	kV
Detector Voltage		0.00	kV
IG Vacuum	---		Pa
PG Vacuum	1.7e+02		Pa
CID Gas	17	17	kPa

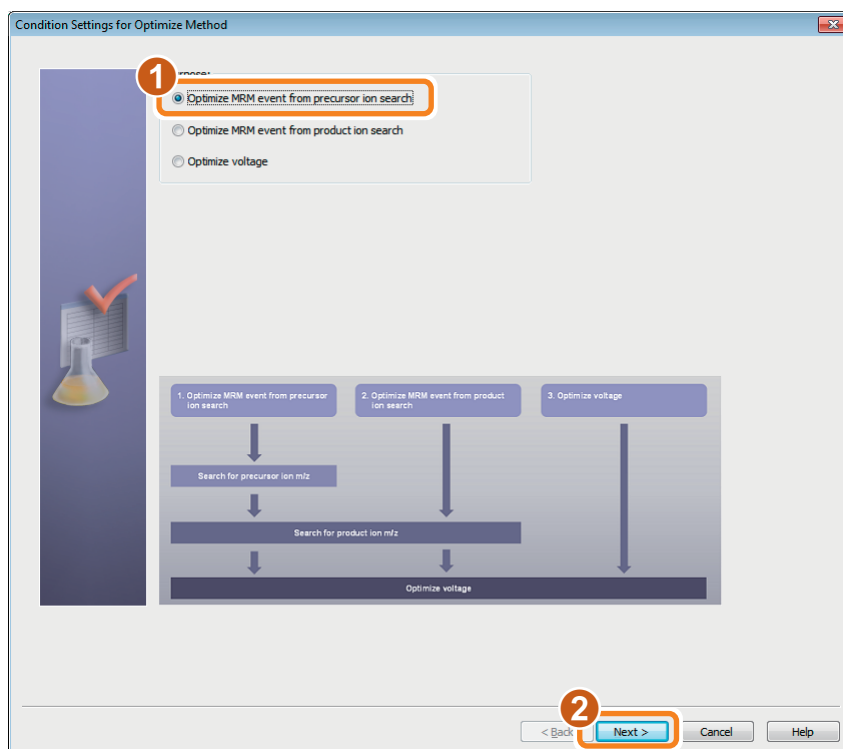
C: 211GB Free

3 Save the method file.



This sub-window is not displayed when a method file is already saved.

4 Select [Optimize MRM event from precursor ion search].



5 Set the parameters.

The screenshot shows the 'Condition Settings for Optimize Method' dialog box. Numbered callouts indicate the following steps:

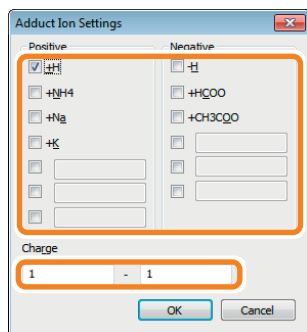
- 1** Method File: Method1.lcm
- 2** Precursor Ion Search Parameters: Min Intensity 20000, Select the Precursor m/z from All Candidate
- 3** Compound list table with columns: Compound Name, Molecular weight, +/-, Start(min), End(min), Sample ID, Vial#, Tray, Inj Vol.
- 4** Adduct Ion: Positive: +H, Charge: 1 - 1
- 5** Auto Selection Condition...
- 6** Output Folder: C:\labSolutions\Data\Project1\
- 7** Apply to method file
- 8** Next > button

	Compound Name	Molecular weight	+/-	Start(min)	End(min)	Sample ID	Vial#	Tray	Inj Vol.
1	A	236.10	+/-	0.000	0.500	1	1	1.0	
2	B	454.20	+/-	0.000	0.500	2	1	1.0	
3	C	308.10	+/-	0.000	0.500	3	1	1.0	

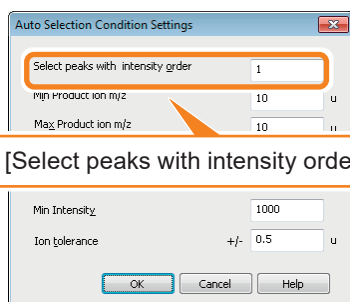
- 1 Check [Optimize Voltage].
- 2 Set the parameters for selecting precursor ions.
- 3 Set the information of compounds to be searched for.

	#1	#2	#3
[Compound Name]	A	B	C
[Molecular weight]	236.10	454.20	308.10
[+/-]	+/-	+/-	+/-
[Start (min)]	0.0	0.0	0.0
[End (min)]	0.5	0.5	0.5
[Vial#]	1	2	3
[Tray]	1	1	1
[Inj Vol.]	1.0	1.0	1.0

- 4 Set the adduct ions and the range for charge.



- 5 Set automatic selection conditions for the product m/z.



[Select peaks with intensity order] : 1

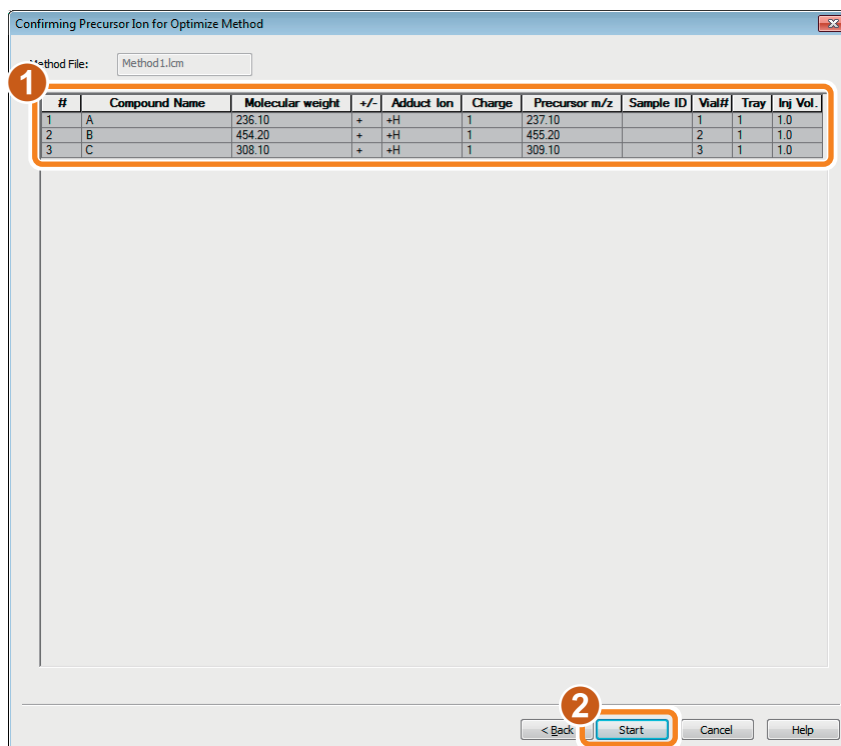
- 6 A subfolder is created under the folder specified here. The name of the subfolder is determined by the date and time. The files automatically created during the optimization are output in this folder.



Hint To check detailed results, open the target data file in the [MS Data Analysis] window.

- 7 Select [Apply to method file].
- 8 Open the [Confirming Precursor Ion for Optimize Method] sub-window.

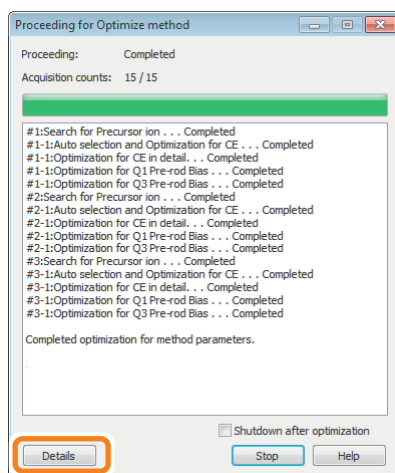
6 Confirm the calculated precursor m/z and start the method optimization.



Measurement having a data acquisition time of 0.5 minutes is repeated 15 times.

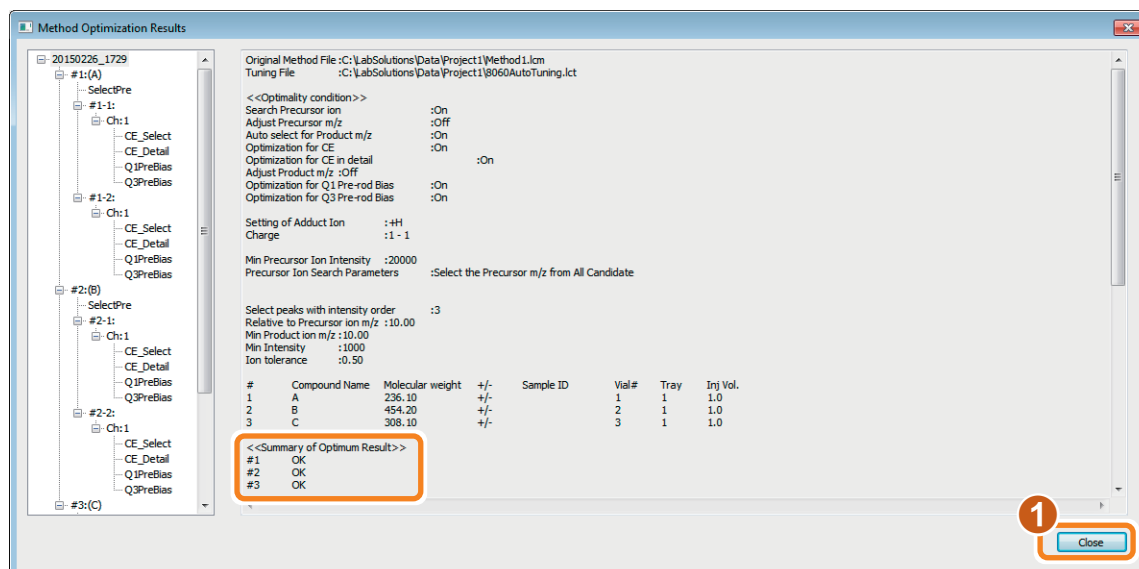


After the method optimization is completed, the word "Completed" is displayed on the window.

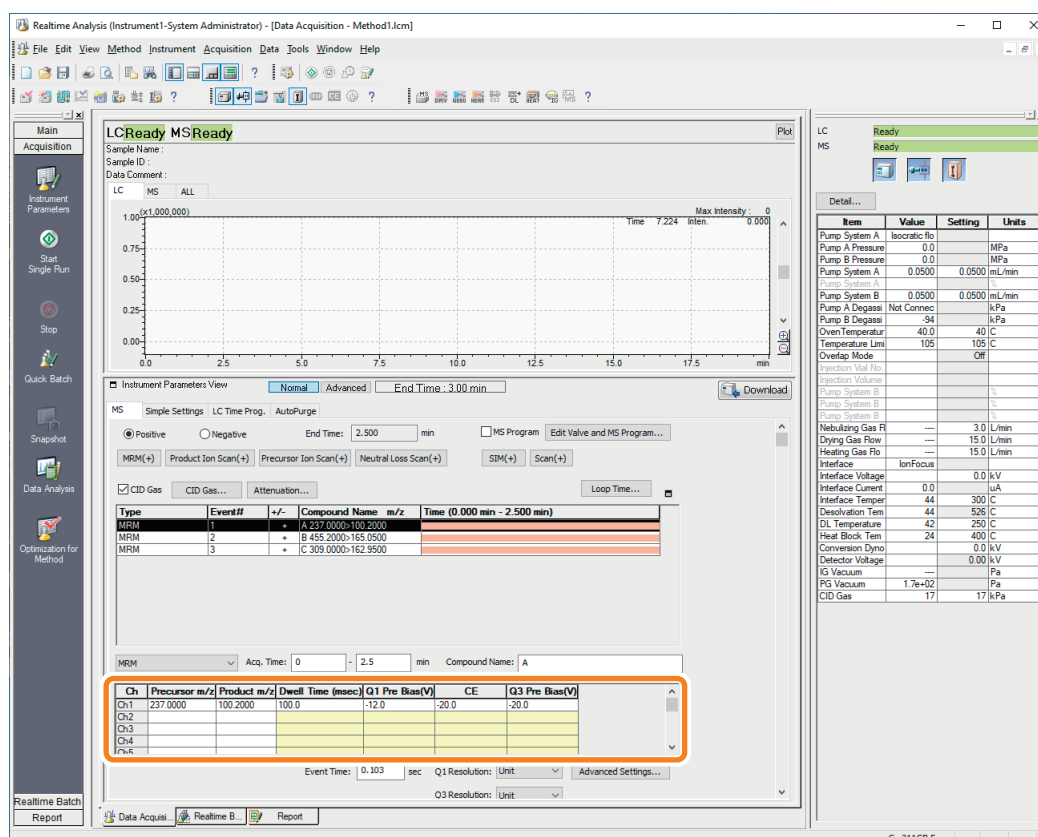


3 To check optimization results, click [Details].

7 Confirm that the summaries of the method optimization results are OK and close the [Method Optimization Results] sub-window.



The results reflected in the method parameters.



▼ Tips

Precursor ion m/z values can be easily calculated by the combination of molecular weight set in the [Condition Settings for Optimize Method] sub-window and adduct ions, polarities, and charges set in the [Adduct Ion Settings] sub-window. When the peaks of precursor ion are observed, the m/z values (molecular weight + adduct) are used. Also, the precursor ion m/z to use are not actual measured values when observing peaks but theoretical values by calculating.

Condition Settings for Optimize Method

Method File: Method1.lcm

Max Loop Time: 1.80 sec
Predicted end time: 7.50 min

☒ Search Precursor ion
☐ Adjust Precursor m/z
☒ Optimize Voltage
☒ Auto select product m/z
☐ Adjust Product m/z

Advanced Setting...
Auto Selection Condition...

Precursor Ion Search Parameters

Min Intensity: 20000

☒ Select the Precursor m/z from All Candidate
☐ Select the P...

Adduct Ign... Positive: +H
Charge: 1 - 1

#	Compound Name	Molecular weight	Start(min)	End(min)	Sample ID	Vial#	Tray	Inj Vol.
1	A	236.10	0.000	0.500		1	1	1.0
2	B	454.20	0.000	0.500		2	1	1.0
3	C	308.10	0.000	0.500		3	1	1.0



Adduct Ion Settings

DrainFlow: ☒ +H ☒ -H

☐ +H4 ☐ +HCOO
☐ +Na ☐ +CH3COO
☐ +K

Charge: 1 - 2

OK Cancel



The calculated precursor ions m/z values are displayed on a list.

Confirming Precursor Ion for Optimize Method

Method File: Method1.lcm

#	Compound Name	Molecular weight	+/-	Adduct Ion	Charge	Precursor m/z	Sample ID	Vial#	Tray	Inj Vol.
1	A	236.10	+	+H	1	237.10		1	1	1.0
2	A	236.10	+	+H	2	119.05		1	1	1.0
3	A	236.10	-	-H	1	235.10		1	1	1.0
4	A	236.10	-	-H	2	117.05		1	1	1.0
5	B	454.20	+	+H	1	455.20		2	1	1.0
6	B	454.20	+	+H	2	228.10		2	1	1.0
7	B	454.20	-	-H	1	453.20		2	1	1.0
8	B	454.20	-	-H	2	226.10		2	1	1.0
9	C	308.10	+	+H	1	309.10		3	1	1.0
10	C	308.10	+	+H	2	155.05		3	1	1.0
11	C	308.10	-	-H	1	307.10		3	1	1.0
12	C	308.10	-	-H	2	153.05		3	1	1.0

5.5 Set the Parameters for Single Run

Prepare single run for determining the retention time of the sample.

1

Install the column.

Open the CTO-40C CL door, and install the column.

2

Set the MS instrument parameters.

Realtime Analysis (Instrument1-System Administrator) - [Data Acquisition - Method1.lcm]

Sample Name:
 Sample ID:
 Data Comment:

LC MS ALL

Max Intensity: 0.0000

Time: 3.794 min

LC Ready MS Ready

Detail...

Item	Value	Setting	Units
Pump System A	Isocratic flo		
Pump A Pressure	0.0		MPa
Pump B Pressure	0.0		MPa
Pump System A	0.0500	0.0500	mL/min
Pump System B	0.0500	0.0500	mL/min
Pump A Degasser	Not Connect		kPa
Pump B Degasser	94		kPa
Oven Temperature	40.0	40	C
Oven Temperature Limit	105	105	C
Overlap Mode		Off	
Injection Valve No.			
Injection Volume			µL
Pump System B			
Pump System B			
Nebulizing Gas Flow	---	3.0	L/min
Drying Gas Flow	---	15.0	L/min
Heating Gas Flow	---	15.0	L/min
Interface	IonFocus		
Interface Voltage	0.0	0.0	kV
Interface Current			µA
Interface Temperature	44	300	C
Desolvation Temperature	44	525	C
DL Temperature	42	250	C
Heat Block Temperature	24	400	C
Conversion Dynode		0.0	kV
Detector Voltage		0.00	kV
IG Vacuum	---		Pa
PG Vacuum	1.7e-02		Pa
CID Gas	17	17	kPa

MS Simple Settings

Positive Negative

MRM(+) Product Ion Scan(+) Precursor Ion Scan(+) Neutral Loss Scan(+) SIM(+) Scan(+)

Acq. Time: 0 - 2.5 min

Ch Precursor m/z Product m/z Dwell Time (msec) Q1 Pre Bias(V)

Ch1 237.0000 100.0 100.0 12.0 20.0

Ch2 309.0000 100.0 100.0 12.0 20.0

Ch3 309.0000 100.0 100.0 12.0 20.0

Ch4 309.0000 100.0 100.0 12.0 20.0

Ch5 309.0000 100.0 100.0 12.0 20.0

Ch6 309.0000 100.0 100.0 12.0 20.0

Ch7 309.0000 100.0 100.0 12.0 20.0

Ch8 309.0000 100.0 100.0 12.0 20.0

Ch9 309.0000 100.0 100.0 12.0 20.0

Ch10 309.0000 100.0 100.0 12.0 20.0

Ch11 309.0000 100.0 100.0 12.0 20.0

Ch12 309.0000 100.0 100.0 12.0 20.0

Ch13 309.0000 100.0 100.0 12.0 20.0

Ch14 309.0000 100.0 100.0 12.0 20.0

Ch15 309.0000 100.0 100.0 12.0 20.0

Ch16 309.0000 100.0 100.0 12.0 20.0

Ch17 309.0000 100.0 100.0 12.0 20.0

Ch18 309.0000 100.0 100.0 12.0 20.0

Ch19 309.0000 100.0 100.0 12.0 20.0

Ch20 309.0000 100.0 100.0 12.0 20.0

Ch21 309.0000 100.0 100.0 12.0 20.0

Ch22 309.0000 100.0 100.0 12.0 20.0

Ch23 309.0000 100.0 100.0 12.0 20.0

Ch24 309.0000 100.0 100.0 12.0 20.0

Ch25 309.0000 100.0 100.0 12.0 20.0

Ch26 309.0000 100.0 100.0 12.0 20.0

Ch27 309.0000 100.0 100.0 12.0 20.0

Ch28 309.0000 100.0 100.0 12.0 20.0

Ch29 309.0000 100.0 100.0 12.0 20.0

Ch30 309.0000 100.0 100.0 12.0 20.0

Ch31 309.0000 100.0 100.0 12.0 20.0

Ch32 309.0000 100.0 100.0 12.0 20.0

Ch33 309.0000 100.0 100.0 12.0 20.0

Ch34 309.0000 100.0 100.0 12.0 20.0

Ch35 309.0000 100.0 100.0 12.0 20.0

Ch36 309.0000 100.0 100.0 12.0 20.0

Ch37 309.0000 100.0 100.0 12.0 20.0

Ch38 309.0000 100.0 100.0 12.0 20.0

Ch39 309.0000 100.0 100.0 12.0 20.0

Ch40 309.0000 100.0 100.0 12.0 20.0

Ch41 309.0000 100.0 100.0 12.0 20.0

Ch42 309.0000 100.0 100.0 12.0 20.0

Ch43 309.0000 100.0 100.0 12.0 20.0

Ch44 309.0000 100.0 100.0 12.0 20.0

Ch45 309.0000 100.0 100.0 12.0 20.0

Ch46 309.0000 100.0 100.0 12.0 20.0

Ch47 309.0000 100.0 100.0 12.0 20.0

Ch48 309.0000 100.0 100.0 12.0 20.0

Ch49 309.0000 100.0 100.0 12.0 20.0

Ch50 309.0000 100.0 100.0 12.0 20.0

Ch51 309.0000 100.0 100.0 12.0 20.0

Ch52 309.0000 100.0 100.0 12.0 20.0

Ch53 309.0000 100.0 100.0 12.0 20.0

Ch54 309.0000 100.0 100.0 12.0 20.0

Ch55 309.0000 100.0 100.0 12.0 20.0

Ch56 309.0000 100.0 100.0 12.0 20.0

Ch57 309.0000 100.0 100.0 12.0 20.0

Ch58 309.0000 100.0 100.0 12.0 20.0

Ch59 309.0000 100.0 100.0 12.0 20.0

Ch60 309.0000 100.0 100.0 12.0 20.0

Ch61 309.0000 100.0 100.0 12.0 20.0

Ch62 309.0000 100.0 100.0 12.0 20.0

Ch63 309.0000 100.0 100.0 12.0 20.0

Ch64 309.0000 100.0 100.0 12.0 20.0

Ch65 309.0000 100.0 100.0 12.0 20.0

Ch66 309.0000 100.0 100.0 12.0 20.0

Ch67 309.0000 100.0 100.0 12.0 20.0

Ch68 309.0000 100.0 100.0 12.0 20.0

Ch69 309.0000 100.0 100.0 12.0 20.0

Ch70 309.0000 100.0 100.0 12.0 20.0

Ch71 309.0000 100.0 100.0 12.0 20.0

Ch72 309.0000 100.0 100.0 12.0 20.0

Ch73 309.0000 100.0 100.0 12.0 20.0

Ch74 309.0000 100.0 100.0 12.0 20.0

Ch75 309.0000 100.0 100.0 12.0 20.0

Ch76 309.0000 100.0 100.0 12.0 20.0

Ch77 309.0000 100.0 100.0 12.0 20.0

Ch78 309.0000 100.0 100.0 12.0 20.0

Ch79 309.0000 100.0 100.0 12.0 20.0

Ch80 309.0000 100.0 100.0 12.0 20.0

Ch81 309.0000 100.0 100.0 12.0 20.0

Ch82 309.0000 100.0 100.0 12.0 20.0

Ch83 309.0000 100.0 100.0 12.0 20.0

Ch84 309.0000 100.0 100.0 12.0 20.0

Ch85 309.0000 100.0 100.0 12.0 20.0

Ch86 309.0000 100.0 100.0 12.0 20.0

Ch87 309.0000 100.0 100.0 12.0 20.0

Ch88 309.0000 100.0 100.0 12.0 20.0

Ch89 309.0000 100.0 100.0 12.0 20.0

Ch90 309.0000 100.0 100.0 12.0 20.0

Ch91 309.0000 100.0 100.0 12.0 20.0

Ch92 309.0000 100.0 100.0 12.0 20.0

Ch93 309.0000 100.0 100.0 12.0 20.0

Ch94 309.0000 100.0 100.0 12.0 20.0

Ch95 309.0000 100.0 100.0 12.0 20.0

Ch96 309.0000 100.0 100.0 12.0 20.0

Ch97 309.0000 100.0 100.0 12.0 20.0

Ch98 309.0000 100.0 100.0 12.0 20.0

Ch99 309.0000 100.0 100.0 12.0 20.0

Ch100 309.0000 100.0 100.0 12.0 20.0

Ch101 309.0000 100.0 100.0 12.0 20.0

Ch102 309.0000 100.0 100.0 12.0 20.0

Ch103 309.0000 100.0 100.0 12.0 20.0

Ch104 309.0000 100.0 100.0 12.0 20.0

Ch105 309.0000 100.0 100.0 12.0 20.0

Ch106 309.0000 100.0 100.0 12.0 20.0

Ch107 309.0000 100.0 100.0 12.0 20.0

Ch108 309.0000 100.0 100.0 12.0 20.0

Ch109 309.0000 100.0 100.0 12.0 20.0

Ch110 309.0000 100.0 100.0 12.0 20.0

Ch111 309.0000 100.0 100.0 12.0 20.0

Ch112 309.0000 100.0 100.0 12.0 20.0

Ch113 309.0000 100.0 100.0 12.0 20.0

Ch114 309.0000 100.0 100.0 12.0 20.0

Ch115 309.0000 100.0 100.0 12.0 20.0

Ch116 309.0000 100.0 100.0 12.0 20.0

Ch117 309.0000 100.0 100.0 12.0 20.0

Ch118 309.0000 100.0 100.0 12.0 20.0

Ch119 309.0000 100.0 100.0 12.0 20.0

Ch120 309.0000 100.0 100.0 12.0 20.0

Ch121 309.0000 100.0 100.0 12.0 20.0

Ch122 309.0000 100.0 100.0 12.0 20.0

Ch123 309.0000 100.0 100.0 12.0 20.0

Ch124 309.0000 100.0 100.0 12.0 20.0

Ch125 309.0000 100.0 100.0 12.0 20.0

Ch126 309.0000 100.0 100.0 12.0 20.0

Ch127 309.0000 100.0 100.0 12.0 20.0

Ch128 309.0000 100.0 100.0 12.0 20.0

Ch129 309.0000 100.0 100.0 12.0 20.0

Ch130 309.0000 100.0 100.0 12.0 20.0

Ch131 309.0000 100.0 100.0 12.0 20.0

Ch132 309.0000 100.0 100.0 12.0 20.0

Ch133 309.0000 100.0 100.0 12.0 20.0

Ch134 309.0000 100.0 100.0 12.0 20.0

Ch135 309.0000 100.0 100.0 12.0 20.0

Ch136 309.0000 100.0 100.0 12.0 20.0

Ch137 309.0000 100.0 100.0 12.0 20.0

Ch138 309.0000 100.0 100.0 12.0 20.0

Ch139 309.0000 100.0 100.0 12.0 20.0

Ch140 309.0000 100.0 100.0 12.0 20.0

Ch141 309.0000 100.0 100.0 12.0 20.0

Ch142 309.0000 100.0 100.0 12.0 20.0

Ch143 309.0000 100.0 100.0 12.0 20.0

Ch144 309.0000 100.0 100.0 12.0 20.0

Ch145 309.0000 100.0 100.0 12.0 20.0

Ch146 309.0000 100.0 100.0 12.0 20.0

Ch147 309.0000 100.0 100.0 12.0 20.0

Ch148 309.0000 100.0 100.0 12.0 20.0

Ch149 309.0000 100.0 100.0 12.0 20.0

Ch150 309.0000 100.0 100.0 12.0 20.0

Ch151 309.0000 100.0 100.0 12.0 20.0

Ch152 309.0000 100.0 100.0 12.0 20.0

Ch153 309.0000 100.0 100.0 12.0 20.0

Ch154 309.0000 100.0 100.0 12.0 20.0

Ch155 309.0000 100.0 100.0 12.0 20.0

Ch156 309.0000 100.0 100.0 12.0 20.0

Ch157 309.0000 100.0 100.0 12.0 20.0

Ch158 309.0000 100.0 100.0 12.0 20.0

Ch159 309.0000 100.0 100.0 12.0 20.0

Ch160 309.0000 100.0 100.0 12.0 20.0

Ch161 309.0000 100.0 100.0 12.0 20.0

Ch162 309.0000 100.0 100.0 12.0 20.0

Ch163 309.0000 100.0 100.0 12.0 20.0

Ch164 309.0000 100.0 100.0 12.0 20.0

Ch165 309.0000 100.0 100.0 12.0 20.0

Ch166 309.0000 100.0 100.0 12.0 20.0

Ch167 309.0000 100.0 100.0 12.0 20.0

Ch168 309.0000 100.0 100.0 12.0 20.0

Ch169 309.0000 100.0 100.0 12.0 20.0

Ch170 309.0000 100.0 100.0 12.0 20.0

Ch171 309.0000 100.0 100.0 12.0 20.0

Ch172 309.0000 100.0 100.0 12.0 20.0

Ch173 309.0000 100.0 100.0 12.0 20.0

Ch174 309.0000 100.0 100.0 12.0 20.0

Ch175 309.0000 100.0 100.0 12.0 20.0

Ch176 309.0000 100.0 100.0 12.0 20.0

Ch177 309.0000 100.0 100.0 12.0 20.0

Ch178 309.0000 100.0 100.0 12.0 20.0

Ch179 309.0000 100.0 100.0 12.0 20.0

Ch180 309.0000 100.0 100.0 12.0 20.0

Ch181 309.0000 100.0 100.0 12.0 20.0

Ch182 309.0000 100.0 100.0 12.0 20.0

Ch183 309.0000 100.0 100.0 12.0 20.0

Ch184 309.0000 100.0 100.0 12.0 20.0

Ch185 309.0000 100.0 100.0 12.0 20.0

Ch186 309.0000 100.0 100.0 12.0 20.0

Ch187 309.0000 100.0 100.0 12.0 20.0

Ch188 309.0000 100.0 100.0 12.0 20.0

Ch189 309.0000 100.0 100.0 12.0 20.0

Ch190 309.0000 100.0 100.0 12.0 20.0

Ch191 309.0000 100.0 100.0 12.0 20.0

Ch192 309.0000 100.0 100.0 12.0 20.0

Ch193 309.0000 100.0 100.0 12.0 20.0

Ch194 309.0000 100.0 100.0 12.0 20.0

Ch195 309.0000 100.0 100.0 12.0 20.0

Ch196 309.0000 100.0 100.0 12.0 20.0

Ch197 309.0000 100.0 100.0 12.0 20.0

Ch198 309.0000 100.0 100.0 12.0 20.0

Ch199 309.0000 100.0 100.0 12.0 20.0

Ch200 309.0000 100.0 100.0 12.0 20.0

Ch201 309.0000 100.0 100.0 12.0 20.0

Ch202 309.0000 100.0 100.0 12.0 20.0

Ch203 309.0000 100.0 100.0 12.0 20.0

Ch204 309.0000 100.0 100.0 12.0 20.0

Ch205 309.0000 100.0 100.0 12.0 20.0

Ch206 309.0000 100.0 100.0 12.0 20.0

Ch207 309.0000 100.0 100.0 12.0 20.0

Ch208 309.0000 100.0 100.0 12.0 20.0

Ch209 309.0000 100.0 100.0 12.0 20.0

Ch210 309.0000 100.0 100.0 12.0 20.0

Ch211 309.0000 100.0 100.0 12.0 20.0

Ch212 309.0000 100.0 100.0 12.0 20.0

Ch213 309.0000 100.0 100.0 12.0 20.0

Ch214 309.0000 100.0 100.0 12.0 20.0

Ch215 309.0000 100.0 100.0 12.0 20.0

Ch216 309.0000 100.0 100.0 12.0 20.0

Ch217 309.0000 100.0 100.0 12.0 20.0

Ch218 309.0000 100.0 100.0 12.0 20.0

Ch219 309.0000 100.0 100.0 12.0 20.0

Ch220 309.0000 100.0 100.0 12.0 20.0

Ch221 309.0000 100.0 100.0 12.0 20.0

Ch222 309.0000 100.0 100.0 12.0 20.0

Ch223 309.0000 100.0 100.0 12.0 20.0

Ch224 309.0000 100.0 100.0 12.0 20.0

Ch225 309.0000 100.0 100.0 12.0 20.0

Ch226 309.0000 100.0 100.0 12.0 20.0

Ch227 309.0000 100.0 100.0 12.0 20.0

Ch228 309.0000 100.0 100.0 12.0 20.0

Ch229 309.0000 100.0 100.0 12.0 20.0

Ch230 309.0000 100.0 100.0 12.0 20.0

Ch231 309.0000 100.0 100.0 12.0 20.0

Ch232 309.0000 100.0 100.0 12.0 20.0

Ch233 309.0000 100.0 100.0 12.0 20.0

Ch234 309.0000 100.0 100.0 12.0 20.0

Ch235 309.0000 100.0 100.0 12.0 20.0

Ch236 309.0000 100.0 100.0 12.0 20.0

Ch237 309.0000 100.0 100.0 12.0 20.0

Ch238 309.0000 100.0 100.0 12.0 20.0

Ch239 309.0000 100.0 100.0 12.0 20.0

Ch240 309.0000 100.0 100.0 12.0 20.0

Ch241 309.0000 100.0 100.0 12.0 20.0

Ch242 309.0000 100.0 100.0 12.0 20.0

Ch243 309.0000 100.0 100.0 12.0 20.0

Ch244 309.0000 100.0 100.0 12.0 20.0

Ch245 309.0000 100.0 100.0 12.0 20.0

Ch246 309.0000 100.0 100.0 12.0 20.0

Ch247 309.0000 100.0 100.0 12.0 20.0

Ch248 309.0000 100.0 100.0 12.0 20.0

Ch249 309.0000 100.0 100.0 12.0 20.0

Ch250 309.0000 100.0 100.0 12.0 20.0

Ch251 309.0000 100.0 100.0 12.0 20.0

Ch252 309.0000 100.0 100.0 12.0 20.0

Ch253 309.0000 100.0 100.0 12.0 20.0

Ch254 309.0000 100.0 100.0 12.0 20.0

Ch255 309.0000 100.0 100.0 12.0 20.0

Ch256 309.0000 100.0 100.0 12.0 20.0

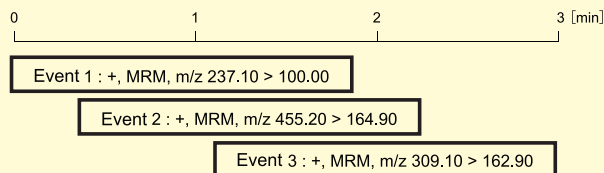
Ch257 309.0000 100.0 100.0 12.0 20.0

Ch258 309.0000 100.0 100.0 12.0 2

Tips

Switch the Polarity for Each Event

On the LCMS/MS, MS conditions are switched successively in a single data acquisition. Each individual MS condition is called an “event,” and polarity can be set to each event. When “MRM” is selected as the acquisition type for an event, set a combination of [Precursor m/z] and [Product m/z] for each channel (Ch) in the MRM Table. When optimizing methods, create one event for each single component. In this guide, three “MRM” events are prepared for quantitative acquisition of three components, and method optimization is executed for determining the optimum [Product m/z]. If multiple events are registered, when the “event time” set for the currently executed event elapses, the next scheduled event is executed. When the last event registered to a specific time ends the first event starts over. (In the case of 1 [min] in the example in the figure below, Event 1 → Event 2 → Event 1, and in the case of 2 [min], Event 2 → Event 3 → Event 2, and so forth) The time taken to complete a single cycle is called the “loop time.”



Select the event polarity.

Click the acquisition type of the event.

The Event Table is displayed.

Enter a combination of [Precursor m/z] and [Product m/z] for each channel (Ch) in the MRM Table.

Type	Event#	Compound Name	m/z	Time (0.000 min - 2.500 min)
MRM	1	A 237.0000-100.0000		
MRM	2	B 455.2000-164.9000		
MRM	3	C 309.1000-162.9000		

Ch	Precursor m/z	Product m/z	Dwell Time (msec)	Q1 Pre Bias(V)	CE	Q3 Pre Bias(V)
Ch1	237.0000	100.0000	100.0	-12.0	-20.0	-20.0
Ch2						
Ch3						
Ch4						



“237.10 > 100.00” indicates migration of MRM. The left side separated by the “>” is expressed as [Precursor m/z] and the right side is expressed as [Product m/z].



When compounds are different, please change and set the event number.



Ch1 is used for the quantitative calculation.



“2 Data Acquisition” in *Operators Guide for LCMS/MS system*.

Tips

Check the loop time

Click on **Loop Time...** to show the loop time.

Maximum Loop Time

Target Value: 0.309 sec

Calculate Dwell Time

Start - End Time(min)	Event	Loop Time(sec)	Dwell Time(msec)
0.000 - 10.000	3	0.309	100.0

Maximum Event: 3

Minimum Dwell Time(msec): 100.0

Maximum Dwell Time(msec): 100.0

Maximum Loop Time(sec): 0.309

Apply to Method Close

The maximum loop time is set to approximately 1/20 of the peak width by adjusting the Dwell Time.

3 Set the LC instrument parameters.

Realtime Analysis (Instrument1-System Administrator) - [Data Acquisition - Method1.lcm]

LC Ready MS Ready

Sample Name :
Sample ID :
Data Comment :

LC MS ALL

Time 13.342 Max Intensity: 0

Intensity 0.000

LC Stop Time : 3.00 min

MS/LC Stop Time is not reflected

Start Time: 0 min
End Time: 2.5 min

Oven Temperature: 40.0 C

Mode: Binary gradient

LC Time Program: 3.00 min
Apply to All acquisition time

Total Flow: 0.4000 mL/min
Pump B Conc.: 8.0 %

[Download]

Item	Value	Setting	Units
Pump System A	Isocratic flow		
Pump A Pressure	0.0		MPa
Pump B Pressure	0.0		MPa
Pump System A	0.0500	0.0500	mL/min
Pump System B	0.0500	0.0500	mL/min
Pump A Degass	-34		kPa
Pump B Degass	40.0	40	C
Oven Temperature	105	105	C
Overlap Mode		Off	
Direction Valve No.			
Injection Volume			
Pump System B			
Pump System B			
Nebulizing Gas B		3.0	L/min
Drying Gas Flow		15.0	L/min
Heating Gas Flow		15.0	L/min
Interface	IonFocus		
Interface Voltage		0.0	kV
Interface Current	0.0		uA
Interface Temperature	43	300	C
Desolvation Temp	43	526	C
DL Temperature	42	250	C
Heat Block Temp	24	400	C
Conversion Dyno		0.0	kV
Detector Voltage		0.00	kV
IG Vacuum			Pa
PG Vacuum	1.7e+02		Pa
CID Gas	17	17	kPa

4 Set the Gradient conditions.

Change the mobile phase mixture ratio.

Instrument Parameters View

MS Interface Data Acquisition LC Time Program Pump Detector A Column Oven Controller Autosampler AutoPurge

Advanced End Time: 3.00 min

Stop time: 3.00 min

Flow: 0.4000 mL/min

Time to reach the flow: 0.00 min (Off)

A.Conc: 92.0 %

B.Conc: 8.0 %

B.Curve: 0

Pressure limits
Minimum: 0.0 MPa Maximum: 10.0 MPa

Gradient

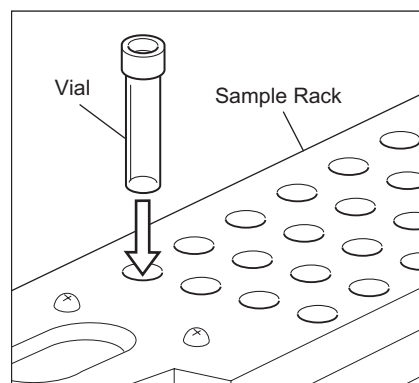
Time	Flow	A.Conc	B.Conc	B.Curve
1.50	0.4000	92.0	8.0	0
2.50	0.4000	10.0	90.0	0
2.60	0.4000	92.0	8.0	0

Set the [Time], [Flow], [A.Conc], [B.Conc] and [B.Curve] as shown.

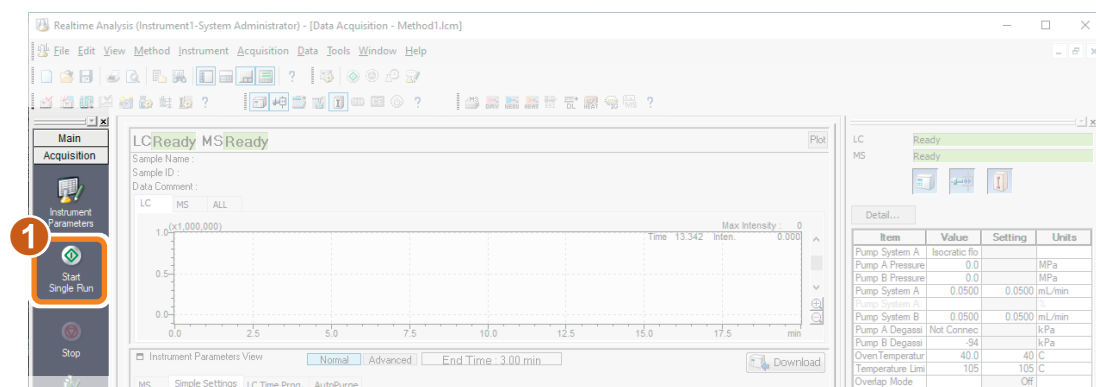
5.6 Execute Single Run to Determine Retention Time

1 Place the samples in the autosampler.

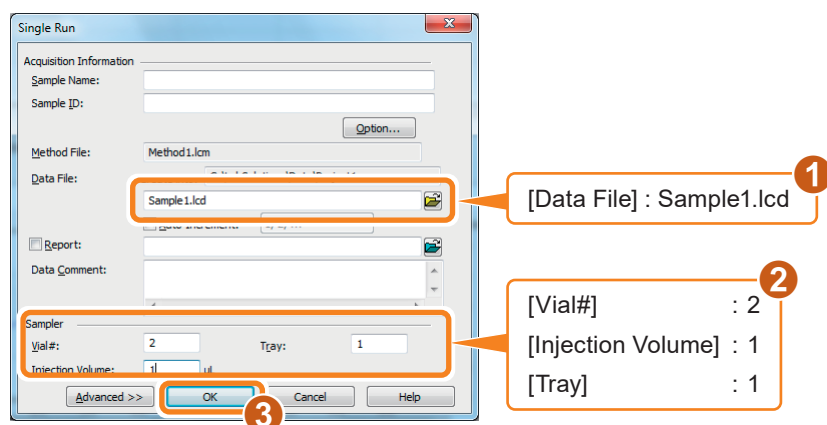
Vial 2, analytes A, B, C 0.05 ng/ μ L mixture



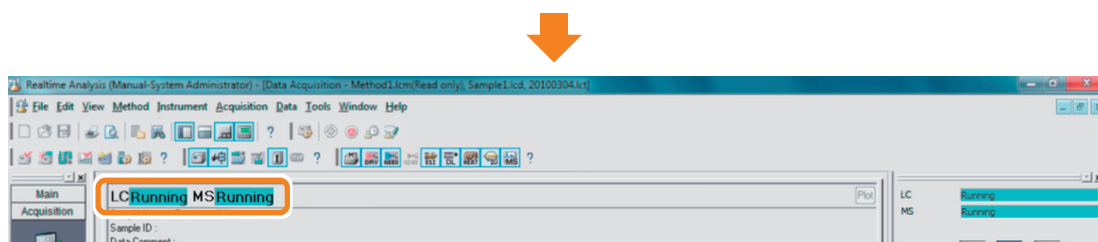
2 Open the [Single Run] sub-window.



3 Set the conditions for a single run.



3 Click [OK] to start the acquisition.

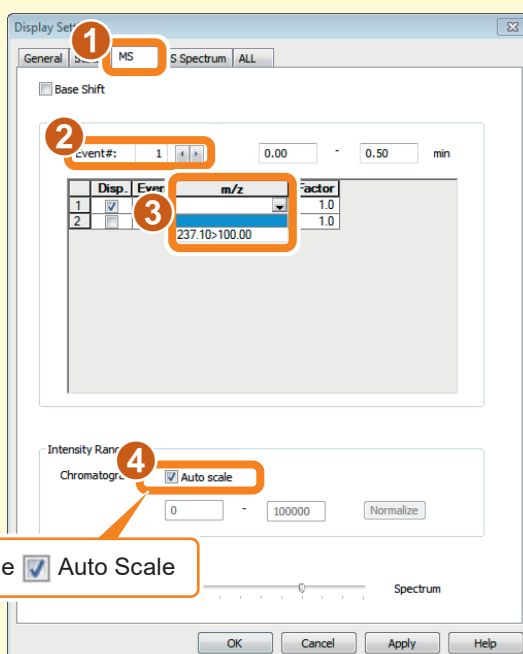


Data acquisition ends automatically when the [Acquisition Time] set in the method file has elapsed.

▼ Tips

Change the Displayed Chromatograph

To change the chromatogram to display in the [Data Acquisition] window, right-click on the chromatogram and select [Display Settings].

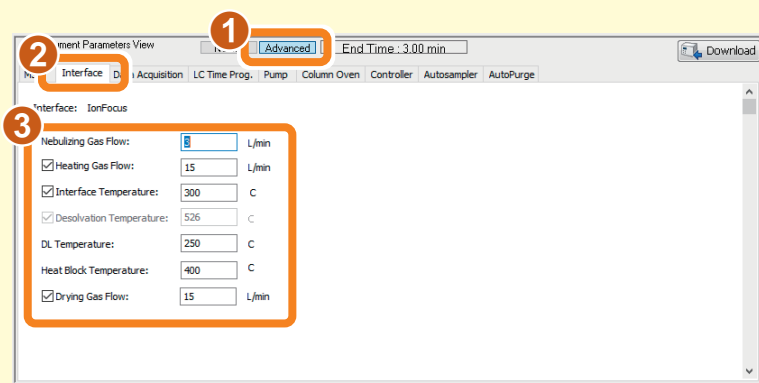


Select in the ☒ Auto Scale

▼ Tips

Set the interface temperature and the gas flow

The interface temperature and the gas flow are set according to the following procedure.

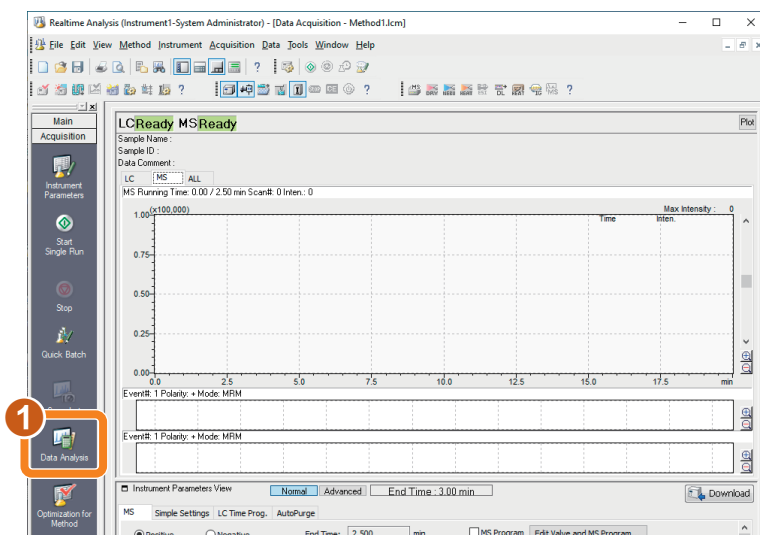


Chapter 6. Confirm Single Run Results (LCMS)

6.1 Open the Results of Single Run in the [MS Data Analysis] Window

Display the results of single run in the [MS Data Analysis] window, and set the parameters for quantitative data acquisition.

1 Click [Data Analysis] in the [Acquisition] assistant bar.

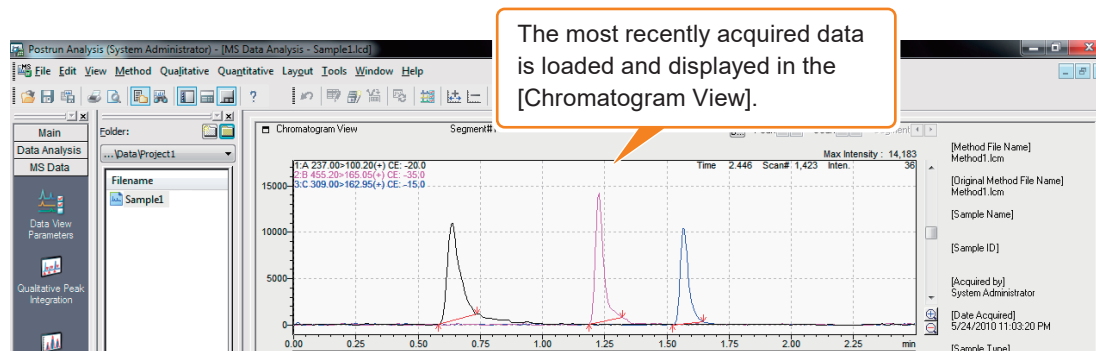


The [Postrun Analysis] program starts.

2 Click [MS Data Analysis] in the [Main] assistant bar.



The [MS Data Analysis] window opens.

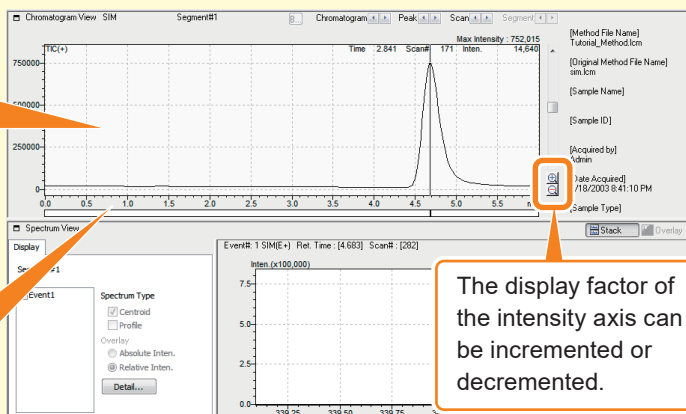


▼ Tips

About viewing operations

An area on a graph can be zoomed and displayed by dragging over it with the mouse. The [Initialize Zoom], [Redo Zoom] and [Undo Zoom] menus can be selected by right-clicking on the graph.

Drag the frame border to change the relative size of each view.



The display factor of the intensity axis can be incremented or decremented.

6.2 Compound Table Setup

For quantitative processing, use a “standard sample” with a known concentration to create a “calibration curve”.

Use this calibration curve to calculate the concentration of the components in the unknown data source.

In this example, we create a calibration curve by injecting 1 μL of 0.01, 0.05, 0.1 and 0.5 $\text{ng}/\mu\text{L}$ standard sample containing analytes A, B and C.

1 Set the peak integration parameters from [MS Data Analysis].

1. Edit

2. Integration

3. Advanced

4. [Slope] : 100

Hint Enter one thousandth of the anticipated peak amplitude. If no peak is detected, halve the Slope setting and try again.

Hint The [Edit] and [View] switch between the [Edit Mode] and the [View Mode]. Parameters cannot be altered in the [View Mode]. Switching from [Edit Mode] to [View Mode] applies the changes and executes the related operations.

2 Enter the quantitative parameters.

[Quantitative Method] : External Standard

[# of Calib. Levels] : 4

Quantitative Parameters

Quantitative Method: External Standard

of Calib. Levels: 4

Curve Fit Type: Linear

Zero: Not Forced

Weighting Method: $1/C^2$

Unit: ppm

Format of Concentration: Decimal Digits (5)

Grouping Type: Not Used

3 Enter the retention time of the sample in the Compound Table.

Click the peak in [Chromatogram View].

Click

Compound

The time is automatically entered.

ID#	Name	Type	Retention Time	Conc. (1)	Conc. (2)
1	A	Target	237.00-100.20	0.633	0.01
2	B	Target	455.20-165.05	0.01	0.0
3	C	Target	309.00-162.95	0.630	0.01
4	TIC	Target		0.001	0.0

4 Enter the concentration of the standard sample in the Compound Table.

[Type]: Target
[Conc. (1)]: 0.01
[Conc. (2)]: 0.05
[Conc. (3)]: 0.1
[Conc. (4)]: 0.5

ID#	m/z	Ret. Time	Conc. (1)	Conc. (2)	Conc. (3)	Conc. (4)
1	237.00-100.20	0.633	0.01	0.05	0.1	0.5
2	455.20-165.05	1.229	0.01	0.05	0.1	0.5
3	309.00-162.95	0.630	0.01	0.05	0.1	0.5
4	TIC	0.001	0.01	0.05	0.1	0.5

5 Click the View to exit [Edit Mode] and execute quantitative peak integration.

Peak integration for all IDs will be performed. Continue?

Yes No

View

Integration	Identification	Quantitative	Compound	Group	Performance	Spectrum	Library	Check
ID#	m/z	Ret. Time	Conc. (1)	Conc. (2)	Conc. (3)	Conc. (4)		
1	237.00-100.20	0.633	0.01	0.05	0.1	0.5		
2	455.20-165.05	1.229	0.01	0.05	0.1	0.5		
3	309.00-162.95	0.630	0.01	0.05	0.1	0.5		

6 Confirm the results of quantitative peak integration, and save the method file.

Look at the identified peak mark (▼) on the chromatogram peak to confirm that the standard sample is identified correctly.

The ↑ and ↓ marks indicate the peak detection start and end points. If integration fails, adjust the Slope peak integration parameter.

Click to save. This will overwrite the quantitation parameters in the current method.

Sound Table

ID#	Name	Ret. Time	Conc.
1	A	0.637	0.010
2	B	1.226	0.009
3	C	1.566	0.010

ID#	m/z	Ret. Time	Conc. (1)
1	237.00-100.20	0.633	0.01
2	455.20-165.05	1.229	0.01
3	309.00-162.95	0.630	0.01

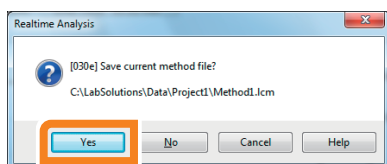
Confirm that "Method1" is selected.

If a peak is detected but not identified, check the retention time in the compound table and window width in the identification parameters.

The method file is overwritten and saved.



The following message is displayed when [Method1] in the [Data Acquisition] window is being edited.



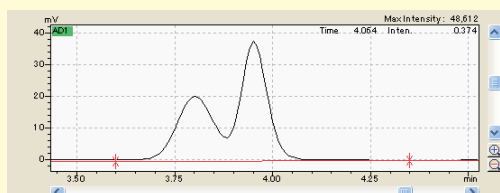
Click [Yes] to continue processing.

▼ Tips

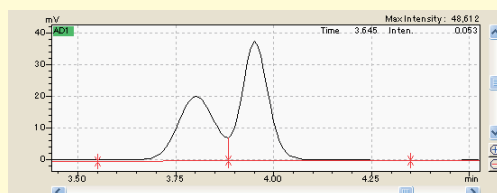
Simple Peak Integration Parameters

First set smaller values for the width and slope. Then double the values to confirm the peak detection status. Setting a large width value prevents detection of peaks in background noise. Also, setting a large slope value prevents detection of peaks in slow baseline undulations. Repeat the above setting adjustments until no unwanted peaks are detected, then use those settings as the peak integration parameters.

Width Setting Example

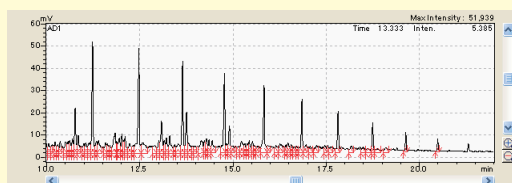


With the [Width] set to 30, the data is processed as one peak.

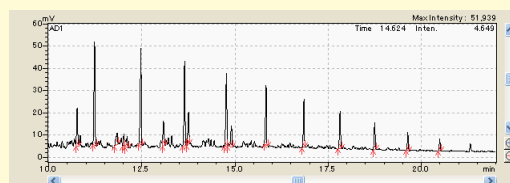


With the [Width] set to 10, the data is processed as two peaks.

Slope Setting Example



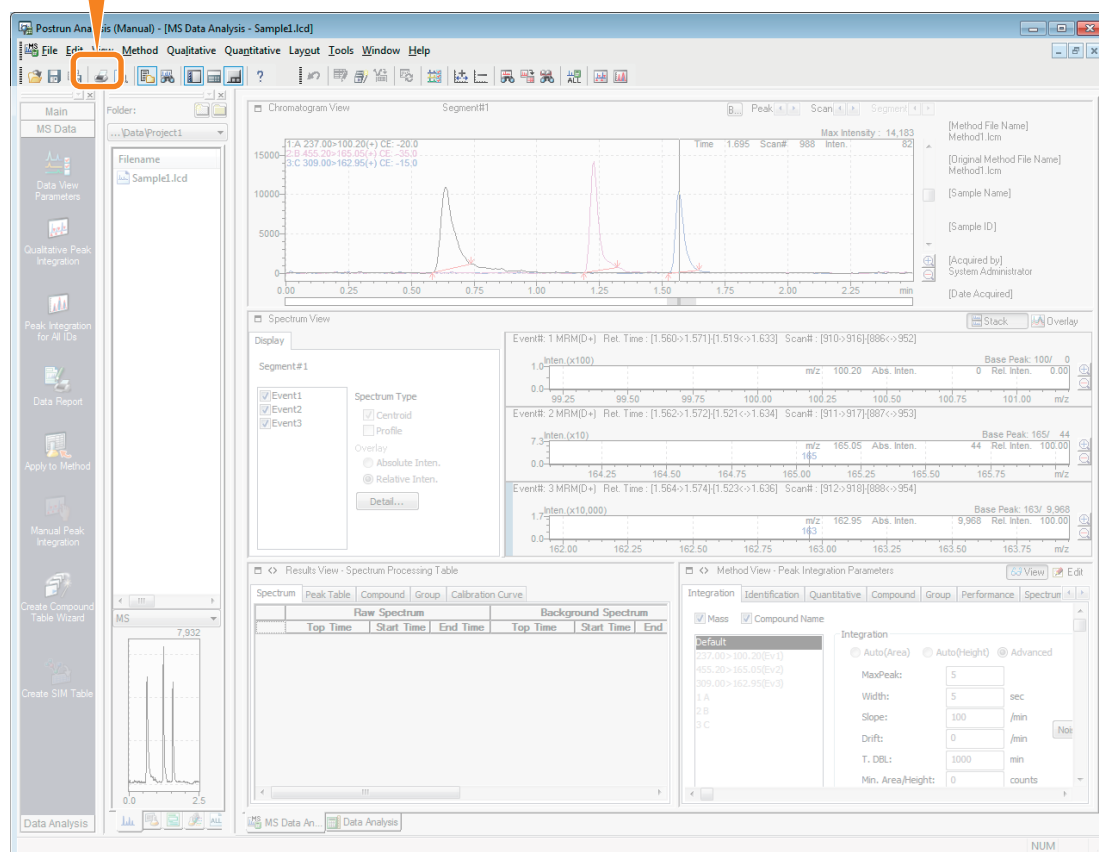
When the [Slope] is set to 1000, even small noise peaks are detected.



When the [Slope] is set to 100000, only those peaks larger than the slope setting are detected.

6.3 Print Results

■ Print the Information Displayed in the Window

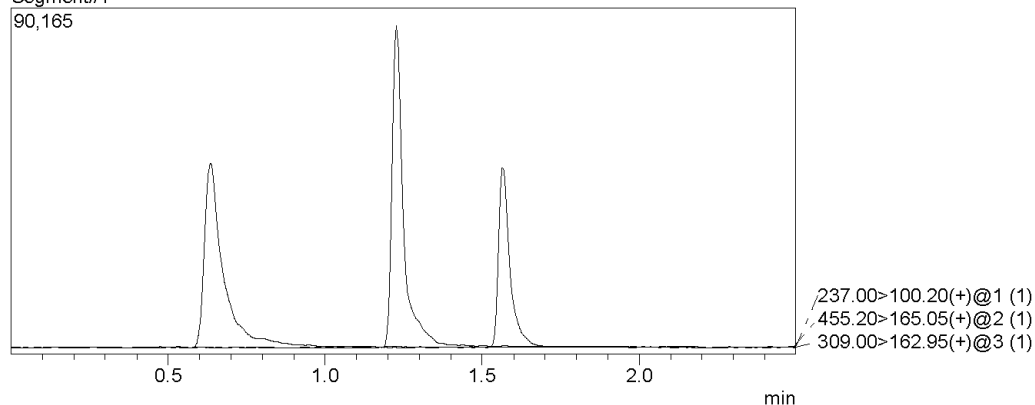


==== Shimadzu Labolutions Data Report ====

Sample ID :
Data Filename : Sample1.lcd
Date Acquired : 5/25/2010 2:38:05 PM

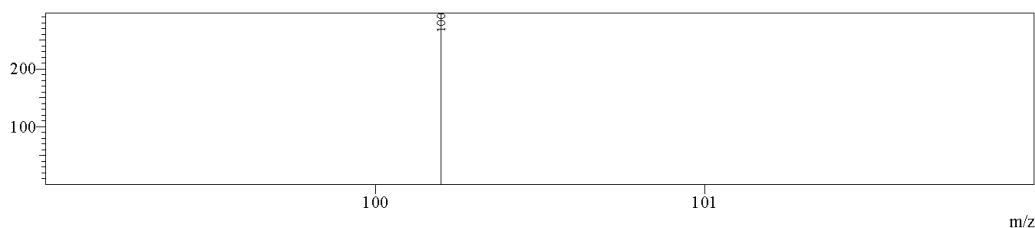
<Chromatogram>

Segment#1

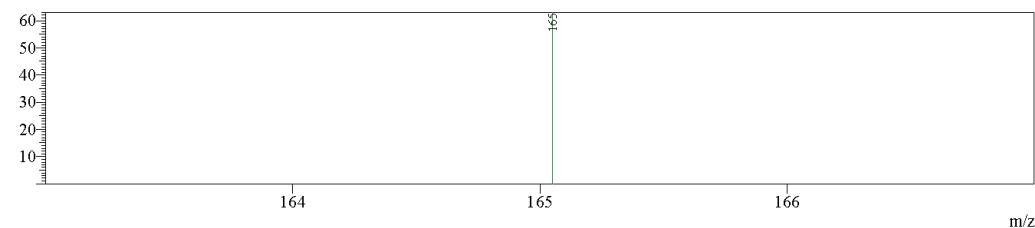


<Spectrum>

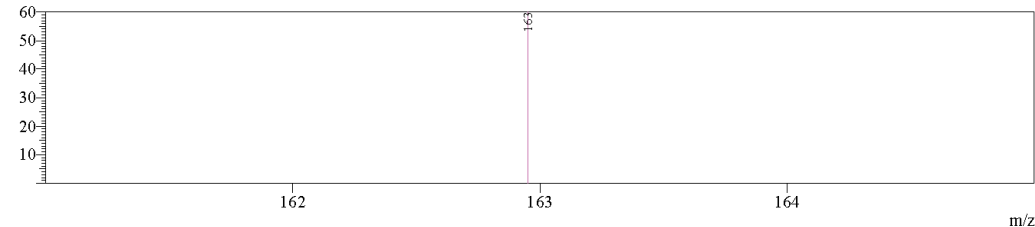
R.Time:0.999(Scan#:583)
MassPeaks:1 BasePeak:100(297)
Polarity:Positive Segment 1 - Event 1



R.Time:1.001(Scan#:584)
MassPeaks:1 BasePeak:165(63)
Polarity:Positive Segment 1 - Event 2



R.Time:1.003(Scan#:585)
MassPeaks:1 BasePeak:163(60)
Polarity:Positive Segment 1 - Event 3

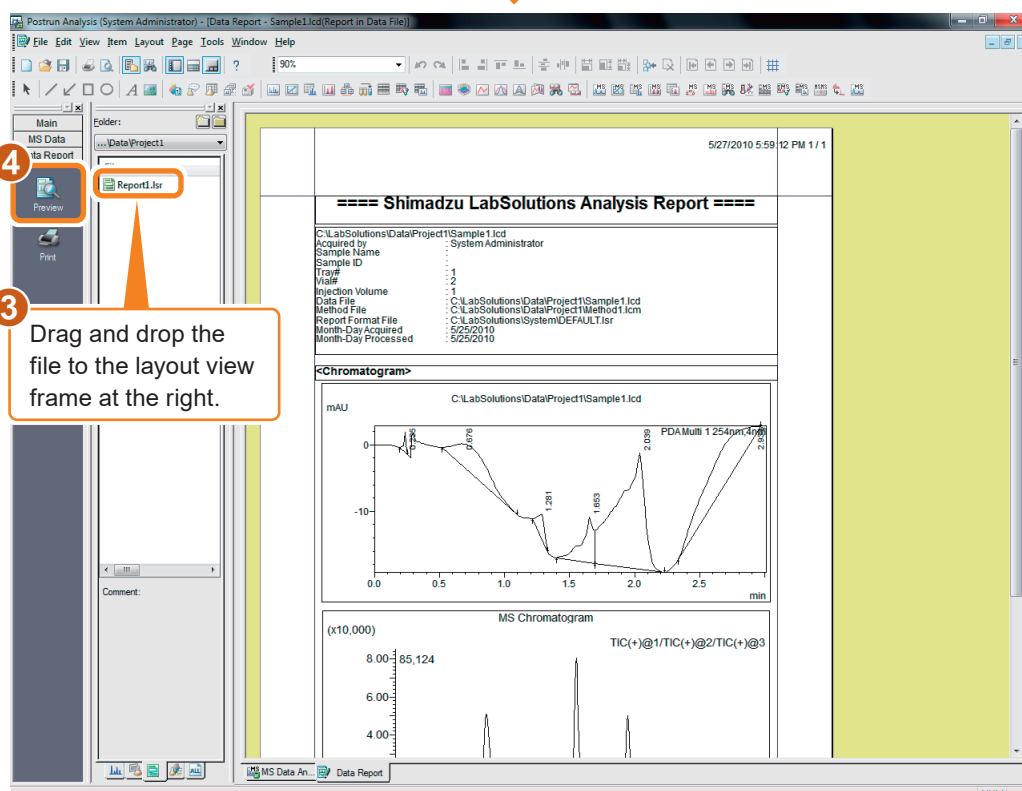
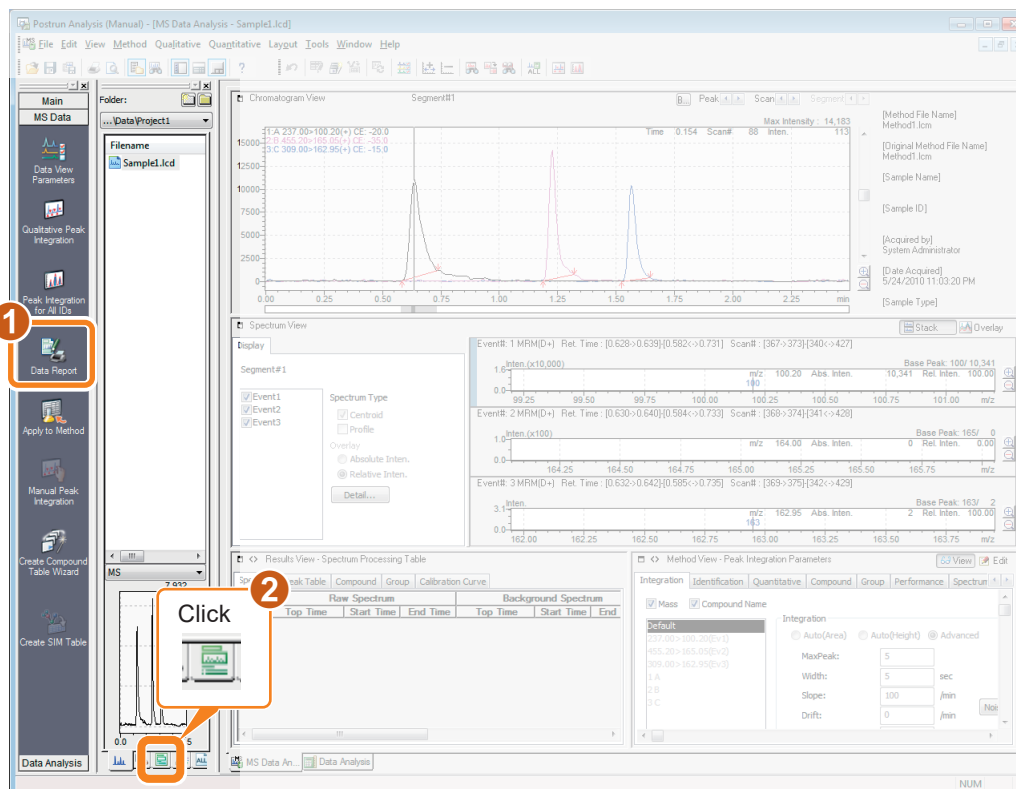


Layout the report format

The print layout of data reports can be edited.

This procedure loads and prints the report of the Report.lsr file.

1 Select [Data Report] to open the [Report] window.

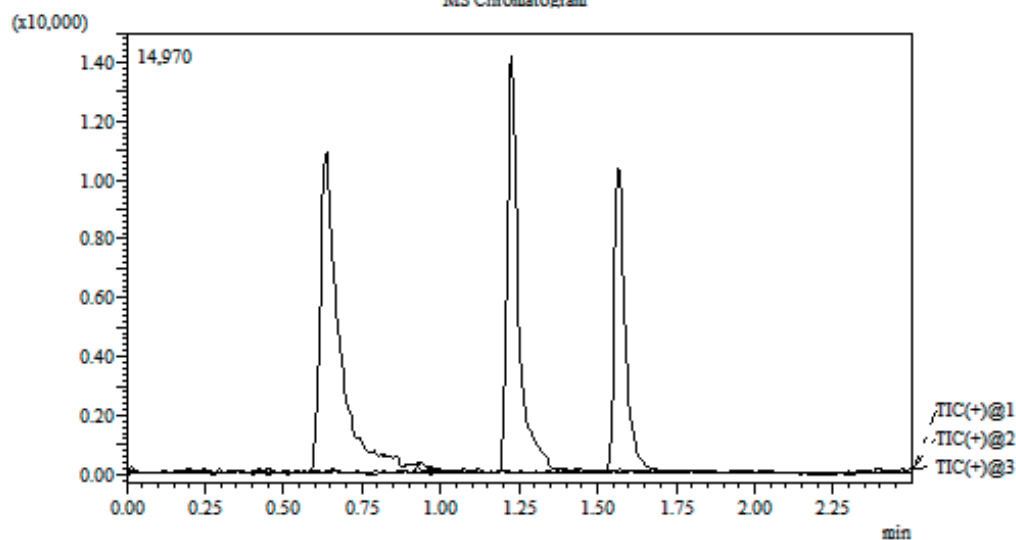


Report Format Printout Example

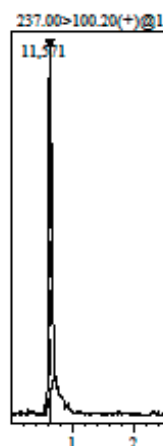
Acquired by : System Administrator
 Date Acquired : 5/24/2010 11:03:20 PM
 Sample Type : Standard
 Level# : 1
 Sample Name :
 Sample ID :
 ISTD Amount : (Level1 Conc.)
 Sample Amount : 1
 Dilution Factor : 1
 Tray# : 1
 Vial# : 1
 Injection Volume : 1
 Data File : Sample1.tcd
 Method File : Method1.lcm
 Original Method File : Method1.lcm
 Report Format File : DEFAULT.rpt
 Tuning File : Tuning.lct
 Processed by : Manual
 Date Processed : 6/14/2013 3:09:25 PM

Sample Information

MS Chromatogram

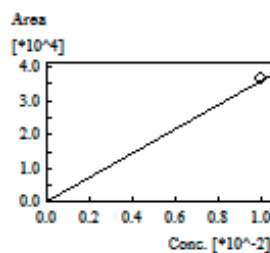


Mass Quant Graph



ID# 1
 Type: Name:
 RetTime: 0.637
 Area: 35904
 Conc.: 0.010ppm
 Event: 1

m/z: 237. ID# : 1 m/z : 237.00>
 Name : A
 Target Function : $f(x) = 3.61950e+006 \cdot x + 0$
 R₁=1.000000 R₂=1.000000
 MeanRF: 3.619502e+006 RF SD: 0.000000e+000 RF %RSD: 0.000000
 FitType : Linear
 ZeroThrough : Not Through
 Weighted Regression : 1/C²
 Quantitation Method : External Standard



#	Conc./Ratio
1	0.01

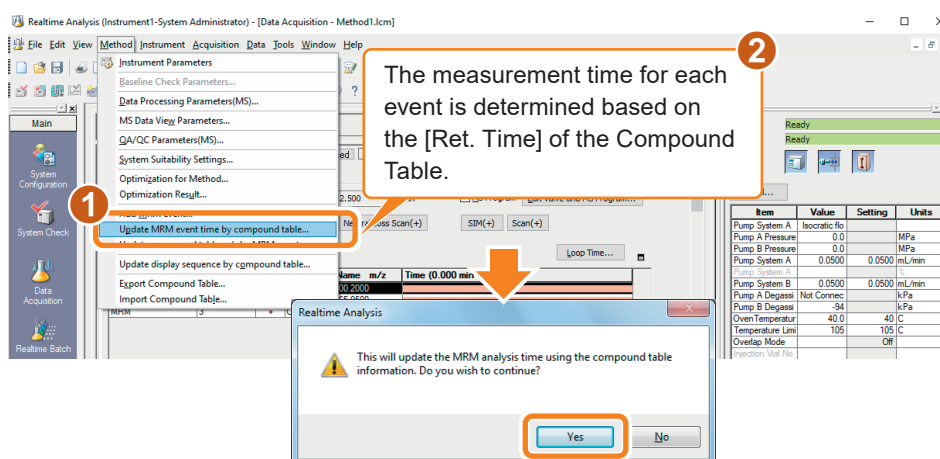
MeanArea	Area
36195	36195

Chapter 7. Realtime Batch

7.1 Create a Batch Table

Select a batch table using the method file created for realtime sequential batch analysis.
Here we perform quantitative calculation for a sample containing A, B and C at 0.075 ng/ μ L each.

1 Change the measurement time for each event on the [Data Acquisition] window.



The measurement time for each event is determined based on the [Ret. Time] of the Compound Table.

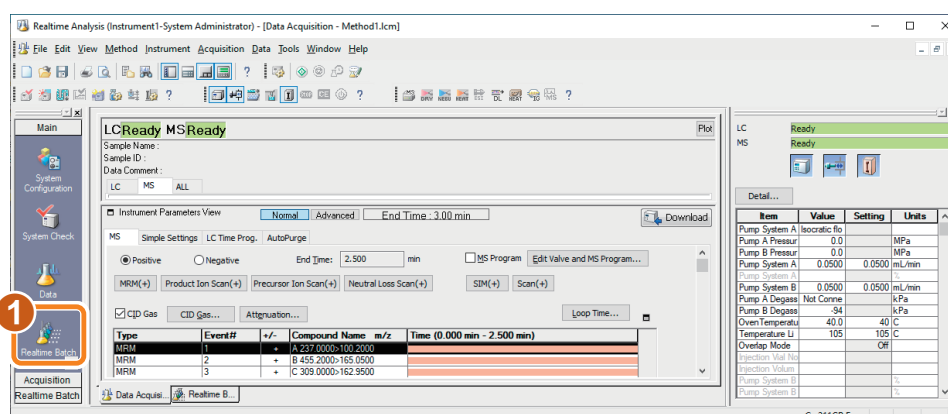
The start time of measurement = [Ret. Time]

- [process time in the identification parameters]

The end time of measurement = [Ret. Time]

+ [process time in the identification parameters]

2 Click [Realtime Batch] in the [Main] assistant bar.

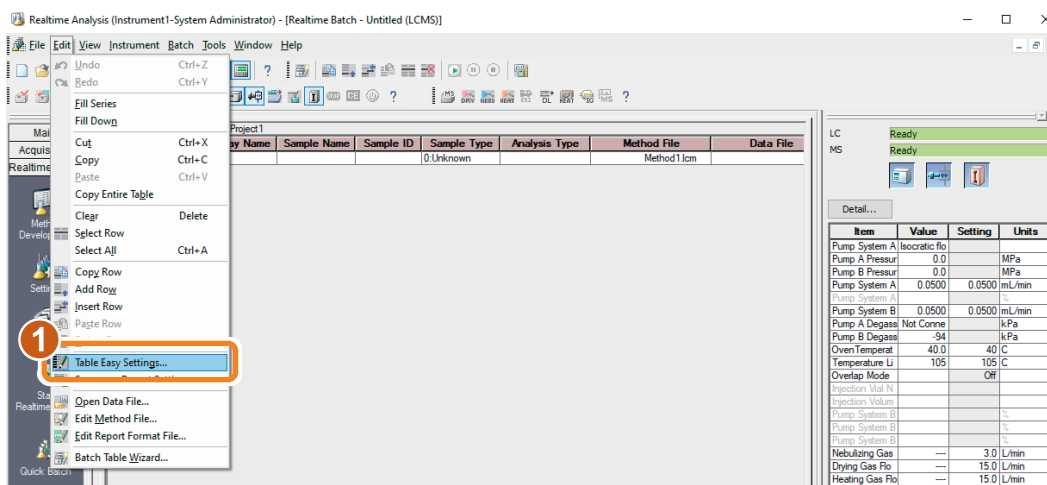


The [Batch Table] window is displayed.

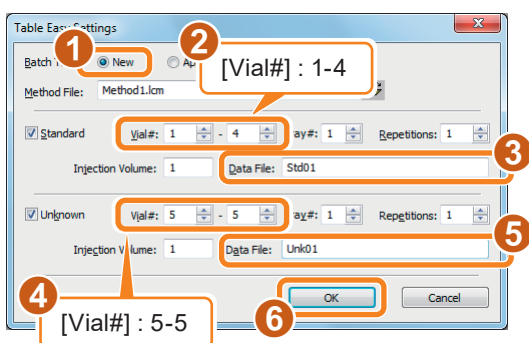
Create the Batch Table using the following procedure.

Use the first four rows for the standard sample and the fifth row for the unknown sample.

3 Select [Table Easy Settings] in the [Edit] menu.

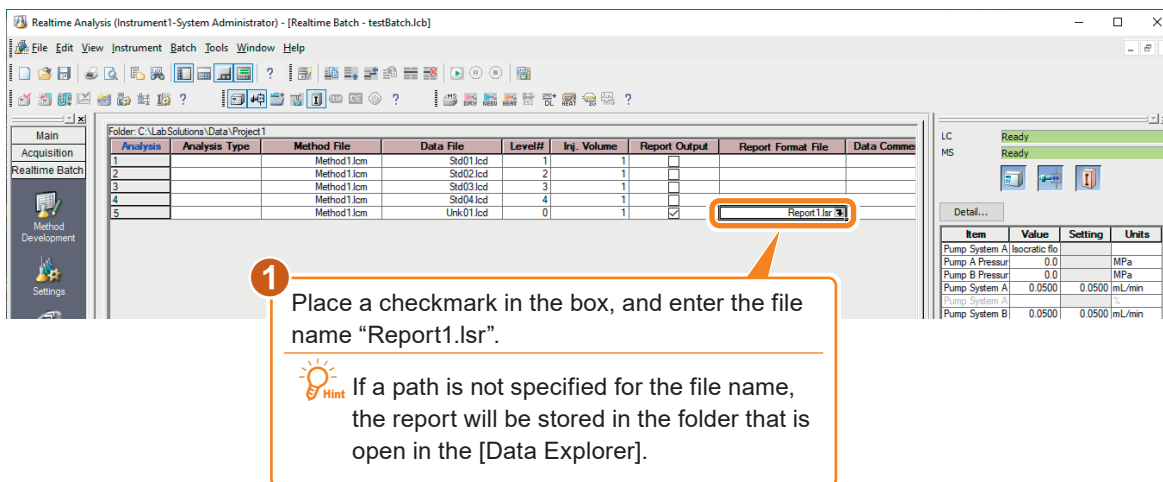


4 Make the following settings on the [Table Easy Settings] sub-window.

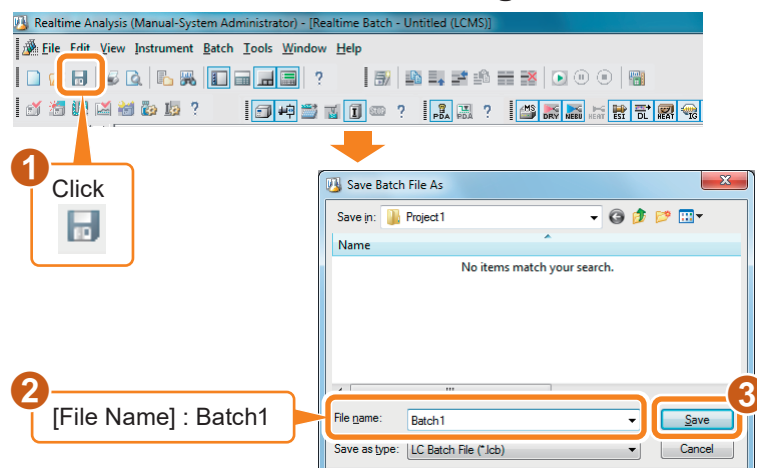


A five-row Batch Table is created.

5 Specify the fifth row (unknown sample) for report output.




6 Save the Batch Table settings.

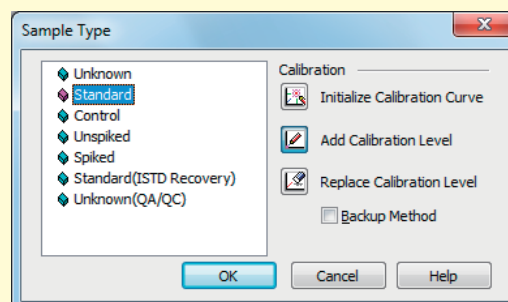


▼ Tips


Batch Table Settings

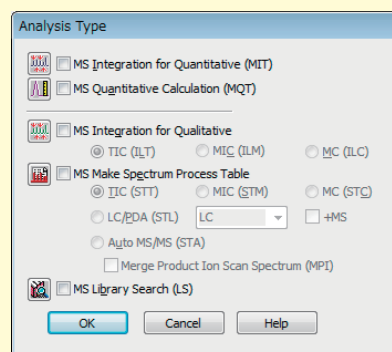
Sample Type

Click  in a cell to open the [Sample Type] sub-window. Select the type of sample in this sub-window. Select [Standard] for grouping types of samples, or [Unknown] to use a sample for quantitation. Enable [Initialize Calibration Curve] for the first standard sample in a grouping type.



Analysis Type

Select the type of analysis for MS data. Set whether or not to perform analysis processing on MS data. Click  in a cell to open the [Analysis Type] sub-window. In this sub-window, click the items to be executed. Peak integration and quantitative calculation are automatically performed on the LC data.




Level Number

Enter a level number for all of the standard samples.

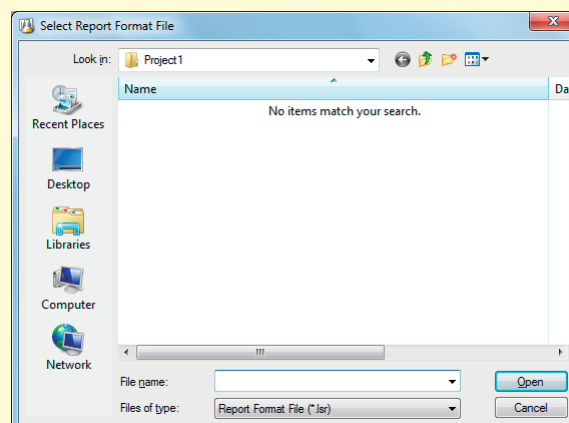
Report Output

Check this box to automatically print an analysis report.

Report Format Files

Click  in a cell to open the [Select Report Format File] sub-window.

Analysis reports are printed in the specified format.



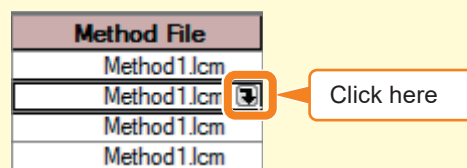
Help for details

▼ Tips

Table Entries

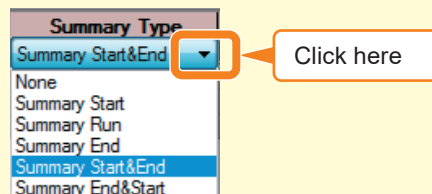
Popup Windows (for complex settings)

After selecting a cell, click the button at the right end of the cell to open the popup window to make settings for that cell.



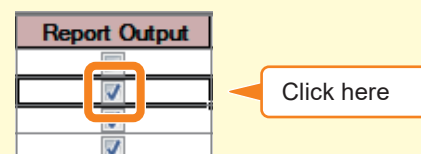
Drop-Down List (to select from a list of choices)

After selecting a cell, click the down arrow at the right end of the cell to display a list of choices. Select a choice from the list.



Check Box (to select on/off)

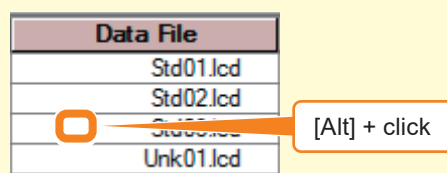
Click the displayed check box to select or clear a checkmark.



[Alt] + click (to open a file)

In file-related windows, this function opens the specified file.

The data or method file for the selected row in a Batch Table can also be opened from the [Edit] menu.

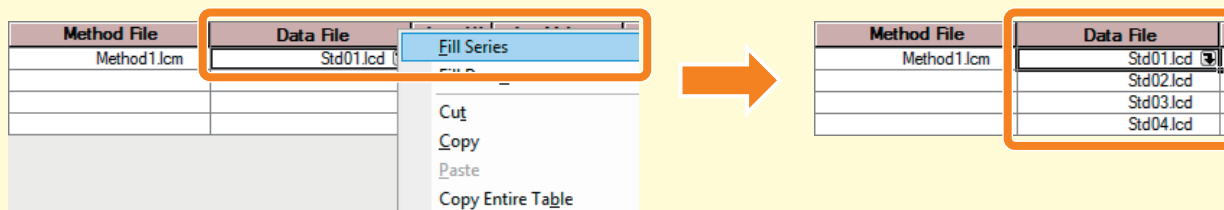


▼ Tips

Fill Series and Fill Down

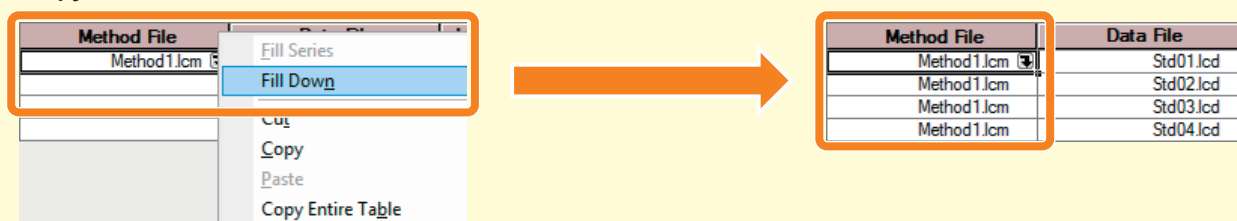
Use the right-click menu on the Batch Table to select [Fill Series] to enter a numbered series or [Fill Down] to copy a particular cell entry to the rest of the cells in the column.

To enter a numbered series



Enter "Std01.lcd" in the top row of the [Data File] column, then right click and select [Fill Series] to fill each cell in the column with "Std01.lcd" to "Std04.lcd".

To copy a cell



Enter "Method1.lcm" in the top row of the [Method File] column, then right click and select [Fill Down] to copy "Method1.lcm" into all cells in the [Method File] column.



To add rows, select [Add Row] from the right-click menu of the batch table.

LabSolutions



Create a Batch Table Using Quick Batch

You can also create a Batch Table using quick batch.

1 Click **Quick Batch...** (F6) in the **Tools** menu.

2 Enter the sample information.

3 Select a sample type and vials.

4 Click **Add Batch Table** to add the settings to the Batch Table.

5 Click **Start** to start the realtime batch.

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

Batch Table

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

Batch Setting

Folder: C:\LabSolutions\Sample\LC

Batch Table

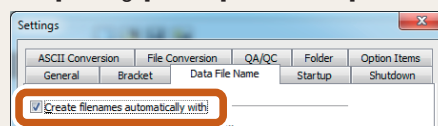
Start realtime batch.



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



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.



7.2 Realtime Batch Processing

Execute batch processing.

1 Place the samples in the autosampler.

Vial 1, sample solution containing A, B, C at 0.01 ng/μL each (standard sample)

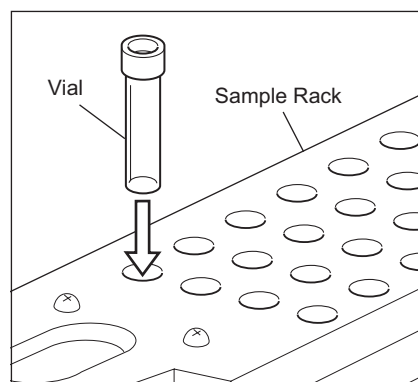
Vial 2, sample solution containing A, B, C at 0.05 ng/μL each (standard sample)

Vial 3, sample solution containing A, B, C at 0.1 ng/μL each (standard sample)

Vial 4, sample solution containing A, B, C at 0.5 ng/μL each (standard sample)

Vial 5, unknown (to be quantitated) sample

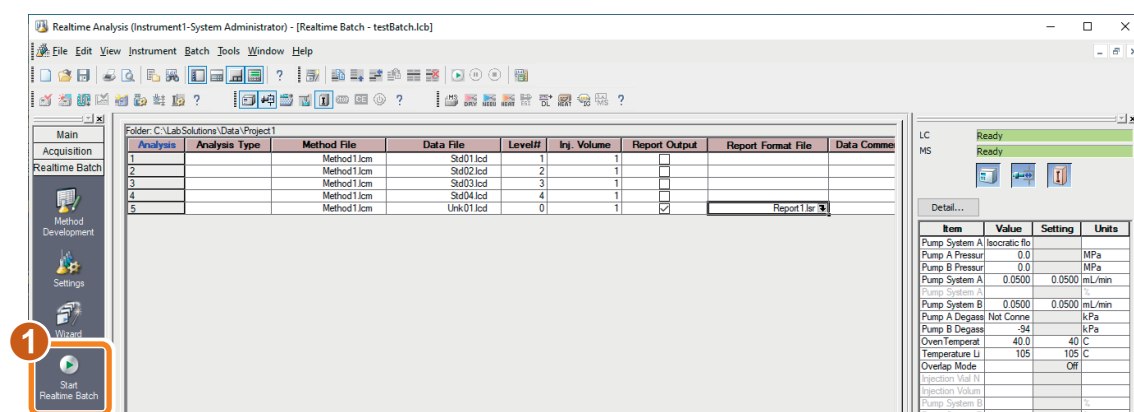
In this example, a sample solution containing A, B, C at 0.075 ng/μL each is taken as the unknown sample.



2 Start realtime batch processing.

During realtime batch processing, the [Realtime Batch] and [Data Acquisition] windows are displayed side by side.

A report is output after analysis of the unknown sample is complete.




Click  to stop batch processing.



By pausing the Batch Table, modifications can be made while measurements for the current analysis continue.



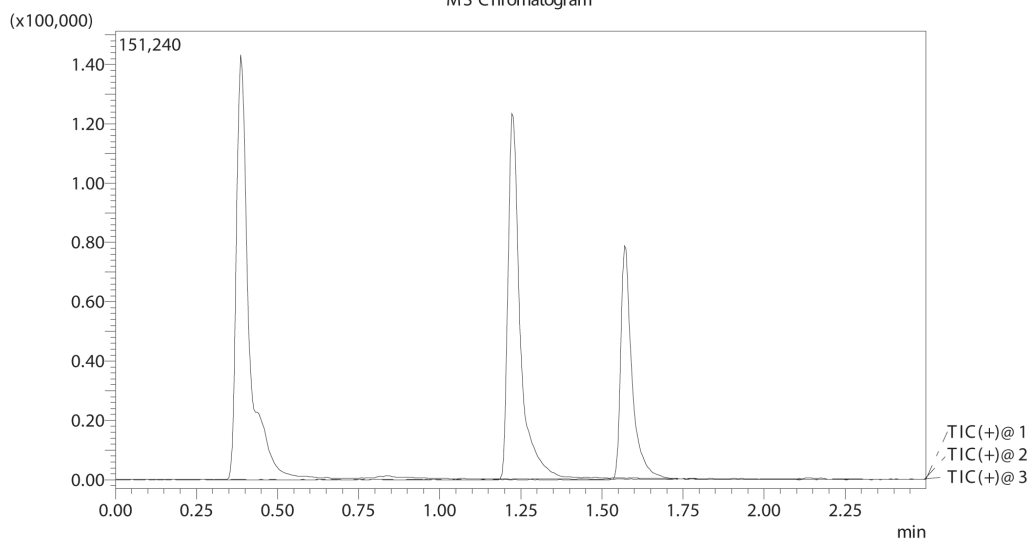
You can take a snapshot to view the data during acquisition. To take a snapshot, click  in the [Data Acquisition] assistant bar during acquisition.

Realtime Batch Report Printout Example

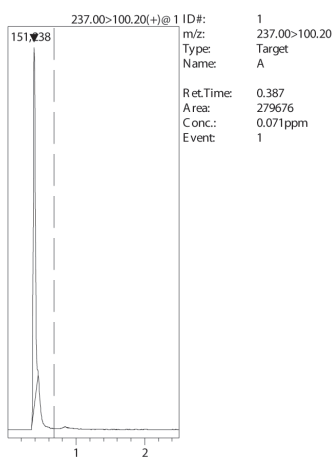
Acquired by : System Administrator
 Date Acquired : 5/25/2010 7:45:59 PM
 Sample Type : Unknown
 Level# : 0
 Sample Name :
 Sample ID :
 Sample Amount : 1
 Dilution Factor : 1
 Tray# : 1
 Vial# : 5
 Injection Volume : 1
 Data File : Unk01.lcd
 Method File : Method1.lcm
 Original Method File : Method1.lcm
 Report Format File : Report1.lsr
 Tuning File : Tuning.lct
 Processed by : System Administrator
 Date Processed : 7/5/2010 5:01:46 PM

Sample Information

MS Chromatogram

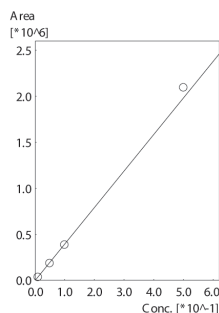


Mass Quant Graph

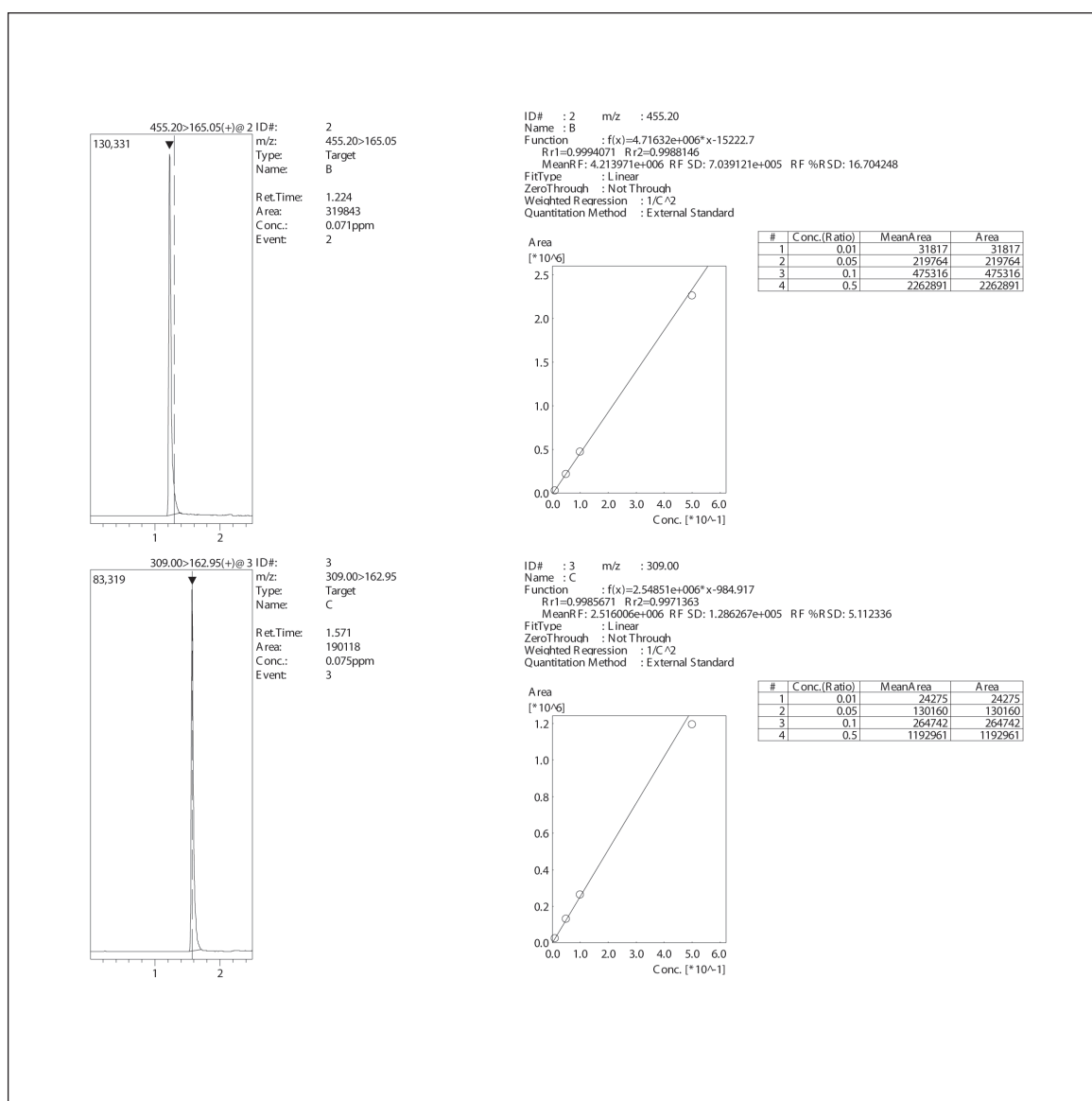


Calibration Curve

ID# : 1 m/z : 237.00
 Name : A
 Function : $f(x) = 3.98377e+006 \cdot x - 4014.10$
 $R^2 = 0.9988958$ $R^2 = 0.9977929$
 MeanRF: 3.851308e+006 RF SD: 2.457992e+005 RF %RSD: 6.382226
 FitType : Linear
 ZeroThrough : Not Through
 Weighted Regression : 1/C^2
 Quantitation Method : External Standard



#	Conc.(Ratio)	MeanArea	Area
1	0.01	36195	36195
2	0.05	187076	187076
3	0.1	385310	385310
4	0.5	2095553	2095553



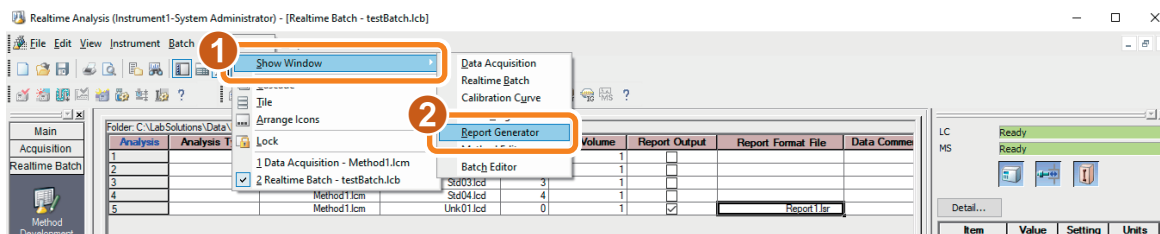
This example report for unknown sample (vial 5) shows the quantitated values for A, B and C. Also shown are the method calibration curves for A, B and C.

The method calibration information resulted from method integration of peaks A, B and C in standard vials 1-4.

7.3 Print Batch Processing Reports

Prints a batch processing summary report (a simple combined report of two or more sets of analysis results).

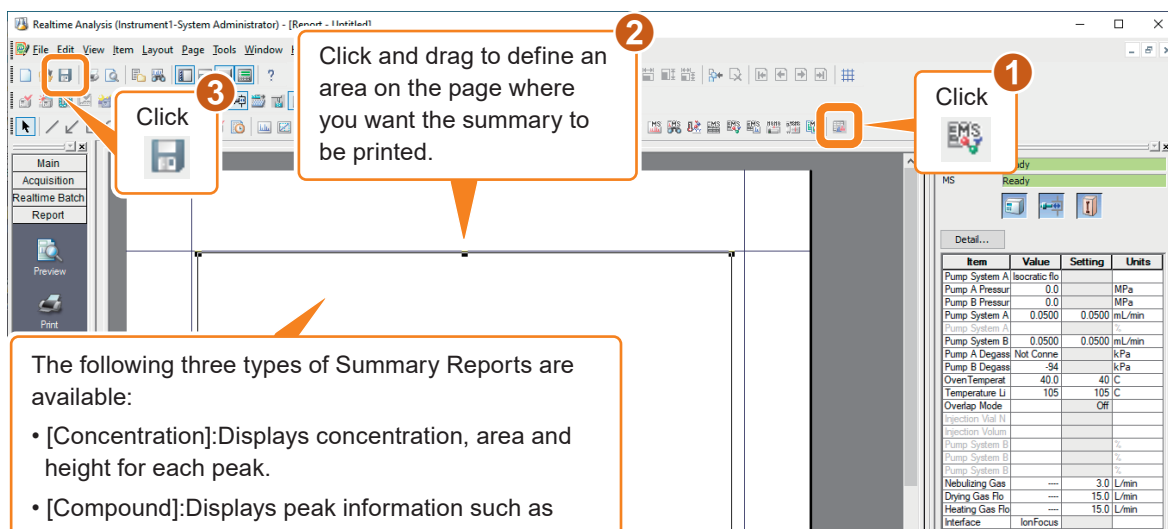
1 Open the [Report] window.



2 Create a summary report format with the [MS Summary (Compound)] report item.

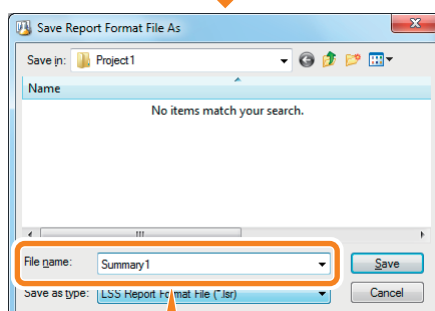


“6.4 Create a Report Format File” in *Operators Guide for LCMS/MS system*.



The following three types of Summary Reports are available:

- [Concentration]: Displays concentration, area and height for each peak.
- [Compound]: Displays peak information such as concentration and column performance for each peak.
- [Data]: Displays a chromatogram and peak table for each data set.



[File name] : Summary1

3 Set up the summary report.

- 1 Enter [Summary Start] in the first data line to be included in the summary report.
Enter [Summary Run] in all of the subsequent data lines to be included in the summary report.
Enter [Summary End] in the last data line to be included in the summary report.

Folder: C:\LabSolutions\Data\Project1

Analysis	Level#	Inj. Volume	Report Output	Report Format File	Data Comment	Summary Type	Summary Report Format File
1	1	1				Summary Start	Summary1.lsr
2	2	1				Summary Run	
3	3	1				None	
4	4	1				None	
5	0	1				Summary End	

- 2 Enter a file name in the Summary Report Format File column.



If [Summary Type] and [Summary Report Format File] are not displayed in the Batch Table, use the right-click menu to select [Table Style] and enable display of these items.

4 Start realtime batch processing.

Realtime Analysis (Instrument1-System Administrator) - [Realtime Batch - Untitled (LCMS)]

File Edit View Instrument Batch Tools Window Help

Folder: C:\LabSolutions\Data\Project1

Analysis	Level#	Tray Name	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	Level#	Inj.
1	1	1			1-Standard (I)		Method1.lcm	Std01.lcd	1	
2	2	1			1-Standard		Method1.lcm	Std02.lcd	2	
3	3	1			1-Standard		Method1.lcm	Std03.lcd	3	
4	4	1			1-Standard		Method1.lcm	Std04.lcd	4	
5	5	1			0-Unknown		Method1.lcm	Unk01.lcd	0	

1 Start Realtime Batch

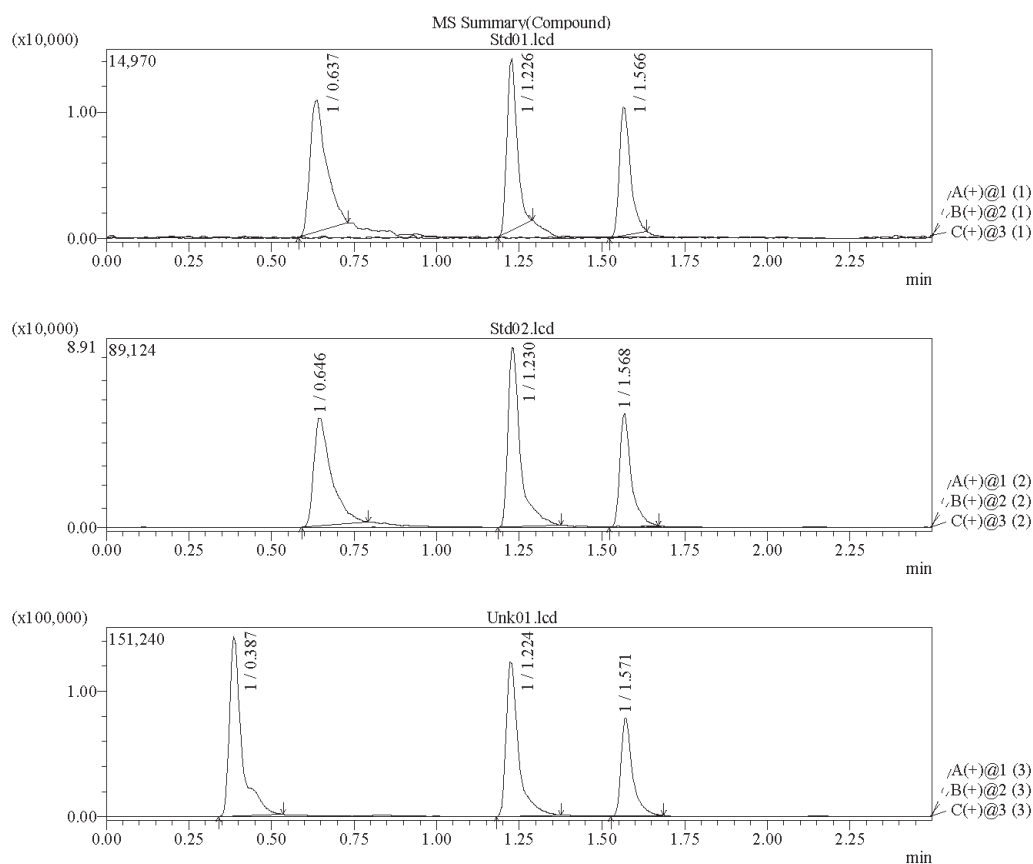
LC MS Ready Ready

Detail...

Item	Value	Setting	Units
Pump System A Isocratic flo			MPa
Pump A Pressur	0.1		MPa
Pump B Pressur	0.1		MPa
Pump System A	0.0500	0.0500	mL/min
Pump System B	0.0500	0.0500	mL/min
Pump A Degass	Not Conne		kPa
Pump B Degass	54		kPa
Oven Temperature	40.0	40	C
Temperature Li	105	105	C
Overlap Mode		Off	
Injection Vol			
Injection Volum			
Pump System B			%
Pump System B			%
Pump System B			%
Nebulizing Gas		3.0	L/min
Drying Gas Flo		15.0	L/min
Heating Gas Flo		15.0	L/min
Interface	IonFocus		
Interface Voltage		0.0	kV
Interface Current	0.0		uA
Interface Temp	42	300	C
Desolvation Te	42	526	C
DL Temperatur	42	250	C

The specified summary report is printed when the batch processing is complete.

Summary Report Printout Example



ID#1 Compound Name: A

Title	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Std01.lcd			0.637	35904	10454	0.009
Std02.lcd			0.646	186026	50731	0.045
Unk01.lcd			0.387	371763	142787	0.089
Average			0.557	197897	67991	0.048
%RSD			26.366	85.016	99.770	83.399
Maximum			0.646	371763	142787	0.089
Minimum			0.387	35904	10454	0.009
Standard Deviation			0.147	168244	67834	0.040

ID#2 Compound Name: B

Title	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Std01.lcd			1.226	28590	13560	0.008
Std02.lcd			1.230	219416	84130	0.049
Unk01.lcd			1.224	318970	123206	0.069
Average			1.227	188992	73632	0.042
%RSD			0.229	78.078	75.472	74.140
Maximum			1.230	318970	123206	0.069
Minimum			1.224	28590	13560	0.008
Standard Deviation			0.003	147561	55572	0.031

ID#3 Compound Name: C

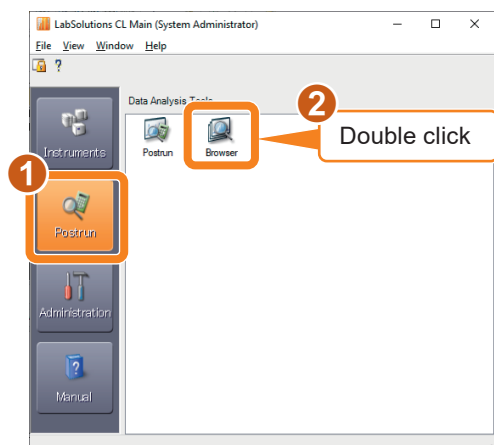
Title	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Std01.lcd			1.566	23534	10163	0.009
Std02.lcd			1.568	127900	53366	0.049
Unk01.lcd			1.571	186467	78613	0.073
Average			1.568	112634	47381	0.044
%RSD			0.164	73.275	73.058	73.335
Maximum			1.571	186467	78613	0.073
Minimum			1.566	23534	10163	0.009
Standard Deviation			0.003	82532	34616	0.032

Chapter 8. Quantitative Data Analysis

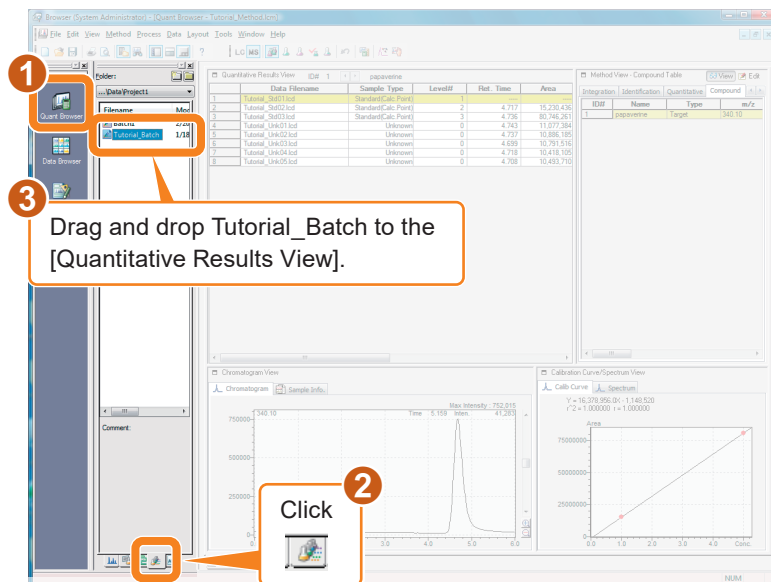
8.1 Confirm Quantitative Results in the [Quant Browser] Window

Use the [Quant Browser] window to easily apply quantitative calculation to multiple data sets.

1 Start the [Browser] program.



2 Load the sample data.



Sample data (Tutorial_Std01.lcd to Tutorial_Std03.lcd and Tutorial_Unk01.lcd to Tutorial_Unk05.lcd) registered in the batch file are opened.

You can select multiple data files in the [Data Explorer] sub-window and drag-and-drop them simultaneously.

3 Confirm quantitative results.

2

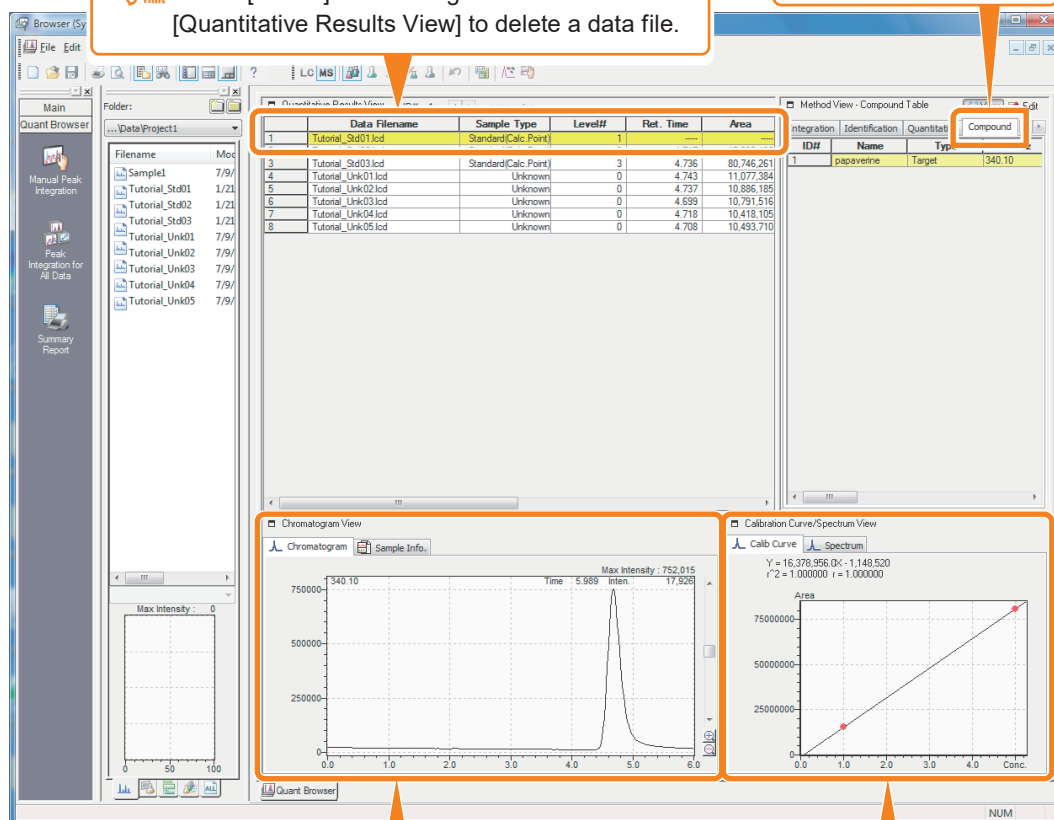
The quantitative results and calibration curve of the compound on the row selected at 1 are displayed.



Select [Delete] from the right-click menu of the [Quantitative Results View] to delete a data file.

1

Click the compound to be confirmed on the [Compound] tab.



3

Confirm the chromatogram.

The chromatogram of the selected data in the [Quantitative Results View] is displayed.

4

Confirm the calibration curve.

The calibration curve of the selected compound in the [Method View] is displayed.

8.2 Edit Integration Parameters and Re-Integrate

The sample data on the previous page is quantitative data for a three-point absolute calibration curve. However, if the area value for the first line of data (Tutorial_Std01.lcd) in the [Quantitative Results View] is found to be “----”, or if confirming the [Chromatogram View] reveals that peak integration was not performed, edit the peak integration parameters to obtain a suitable calibration curve.

1 Edit the quantitative parameters.



“10.3 Postrun Analysis of Multiple Data” in *Operators Guide for LCMS/MS system*.

Quant Browser (System Administrator) - [Quant Browser - Tutorial_Method.lcm]

Method View - Peak Integration Parameters

Integration Identification Quantitative Compound Performance Spectrum Custom QC Check

Integration

MaxPeak: 5 Width: 5 sec Slope: 100 Drift: 1000 min I. DBL: 0 Min. Area/Height: 0 counts Calculated by: Area Height

Quantitative Results View

Data Filename	Sample Name
Tutorial_Std01.lcd	Standard(Calc Point)
Tutorial_Std02.lcd	Standard(Calc Point)
Tutorial_Std03.lcd	Standard(Calc Point)
Tutorial_Unk01.lcd	Unknown
Tutorial_Unk02.lcd	Unknown
Tutorial_Unk03.lcd	Unknown
Tutorial_Unk04.lcd	Unknown
Tutorial_Unk05.lcd	Unknown

Chromatogram View

Chromatogram Sample Info

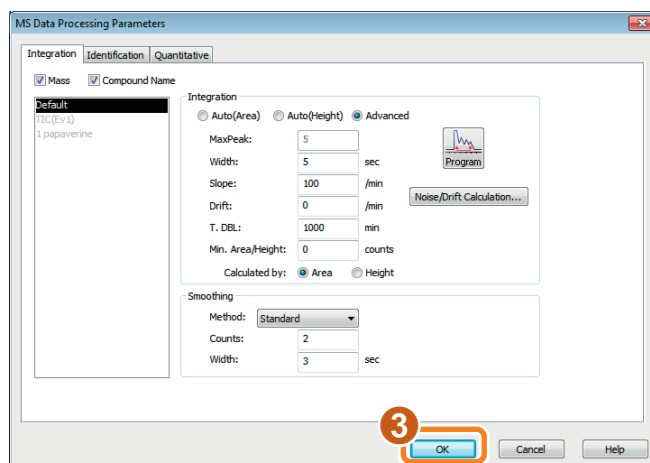
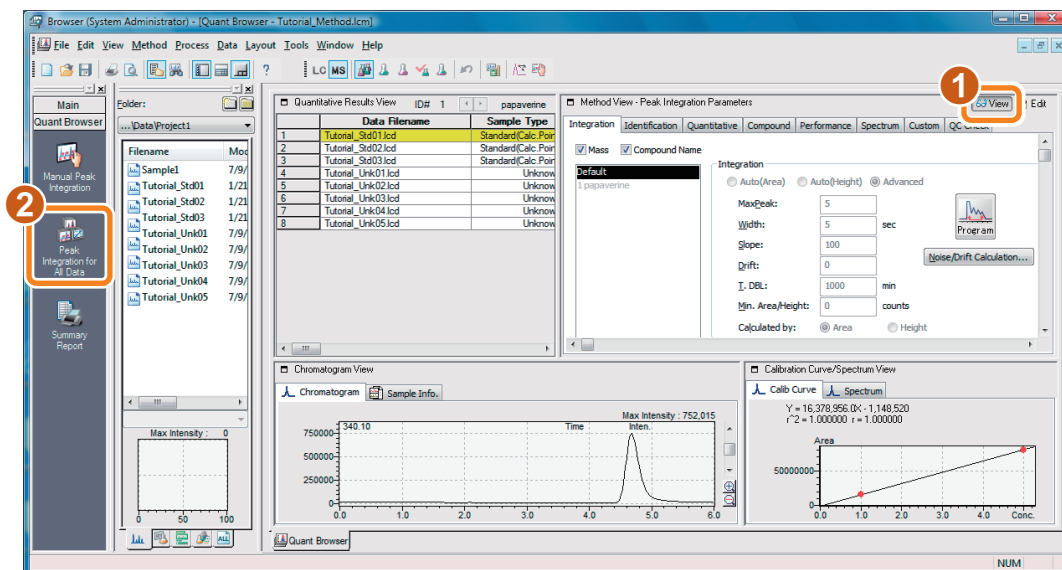
Max Intensity: 752,015

Time: 4.550 min. 229,844

Quant Browser

NUM

2 Re-integrate



Original Results

	Data Filename	Sample Type	Level#	Area	Conc. (ppm)	Std. Conc.
1	Tutorial_Std01.lcd	Standard(Calc. Point)	1	15,230.4	1.000	0.500
2	Tutorial_Std02.lcd	Standard(Calc. Point)	2	80,746.2	5.000	1.000
3	Tutorial_Std03.lcd	Standard(Calc. Point)	3	11,077.3	0.746	5.000
4	Tutorial_Unk01.lcd	Unknown	0	10,886.1	0.735	-----
5	Tutorial_Unk02.lcd	Unknown	0	10,791.5	0.729	-----
6	Tutorial_Unk03.lcd	Unknown	0	10,418.1	0.706	-----
7	Tutorial_Unk04.lcd	Unknown	0	10,493.7	0.711	-----

Edited Results

	Data Filename	Sample Type	Level#	Area	Conc. (ppm)	Std. Conc.
1	Tutorial_Std01.lcd	Standard(Calc. Point)	1	11,591.4	0.518	0.500
2	Tutorial_Std02.lcd	Standard(Calc. Point)	2	19,447.0	0.980	1.000
3	Tutorial_Std03.lcd	Standard(Calc. Point)	3	87,729.7	5.002	5.000
4	Tutorial_Unk01.lcd	Unknown	0	14,816.1	0.707	-----
5	Tutorial_Unk02.lcd	Unknown	0	14,840.6	0.709	-----
6	Tutorial_Unk03.lcd	Unknown	0	14,803.8	0.707	-----
7	Tutorial_Unk04.lcd	Unknown	0	14,238.4	0.673	-----
8	Tutorial_Unk05.lcd	Unknown	0	14,084.3	0.664	-----



When the standard sample data is integrated, the calibration curve is recreated and quantitative calculation is performed on all data.



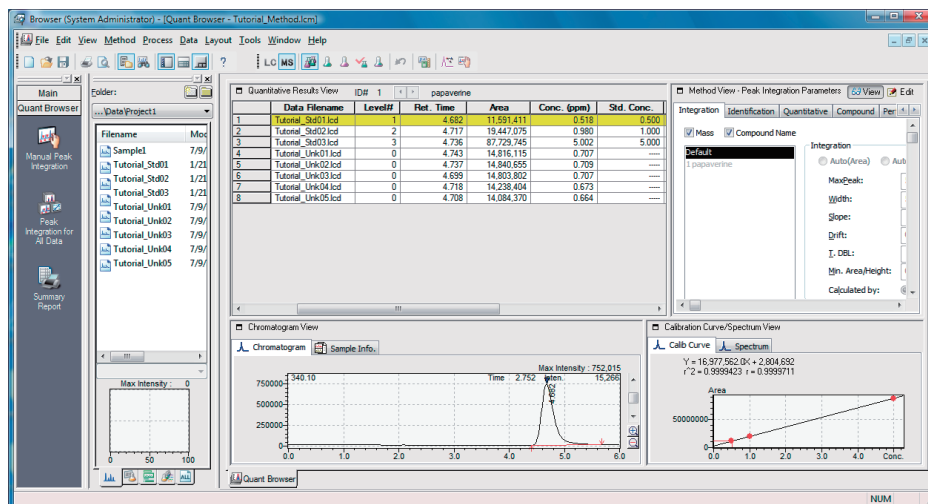
Integration can be initiated manually in the [Chromatogram View]. Select [Manual Integration Bar] from the right-click menu.



“5.5.6 Manual Quantitative Peak Integration” in *Operators Guide for LCMS/MS system*.

The peak is detected.

The 3-point calibration curve is displayed, and the correct quantitative value is determined.



■ Invalidate a Calibration Point

If a standard sample cannot be analyzed properly, the calibration point can be invalidated.

Remove the [Cal. Point] checkmark from the [Quantitative Results View] to invalidate the calibration point. The results are immediately recalculated.

You can enable/disable the calibration point for each compound registered in the [Compound Table].

	Data Filename	Conc. (ppm)	Std. Conc.	Accuracy%	Cal. Point
1	Tutorial_Std01.lcd	0.518	0.500	103	<input checked="" type="checkbox"/>
2	Tutorial_Std02.lcd	0.980	1.000	98	<input checked="" type="checkbox"/>
3	Tutorial_Std03.lcd	5.002	5.000	100	<input checked="" type="checkbox"/>
4	Tutorial_Unk01.lcd	0.707	-----	-----	<input type="checkbox"/>
5	Tutorial_Unk02.lcd	0.709	-----	-----	<input type="checkbox"/>
6	Tutorial_Unk03.lcd	0.707	-----	-----	<input type="checkbox"/>
7	Tutorial_Unk04.lcd	0.673	-----	-----	<input type="checkbox"/>
8	Tutorial_Unk05.lcd	0.664	-----	-----	<input type="checkbox"/>

■ Modify the Level Number

The level number assigned to a sample during analysis can be changed in the [Quantitative Results View].

When changes are applied and a different cell is selected, quantitative results are immediately recalculated.



The [Level#] can be edited regardless of the [Sample Type].

1

Select the cell of the [Level#] to be changed, and enter a new number.

	Data Filename	Sample Type	Level#	Ret. Time	Area	Conc. (ppm)
1	Tutorial_Std01.lcd	Standard(Calc. Point)	1	4.682	11,591.411	0.518
2	Tutorial_Std02.lcd	Standard(Calc. Point)	2	4.717	19,447.075	0.980
3	Tutorial_Std03.lcd	Standard(Calc. Point)	3	4.736	87,729.745	5.002
4	Tutorial_Unk01.lcd	Unknown	0	4.743	14,816.115	0.707
5	Tutorial_Unk02.lcd	Unknown	0	4.737	14,840.655	0.709
6	Tutorial_Unk03.lcd	Unknown	0	4.699	14,803.802	0.707
7	Tutorial_Unk04.lcd	Unknown	0	4.718	14,238.404	0.673
8	Tutorial_Unk05.lcd	Unknown	0	4.708	14,084.370	0.664

■ Change the Sample Type

The [Sample Type] assigned to a sample during analysis can be changed in the [Quantitative Results View].

When changes are applied, quantitative results are immediately recalculated.



Changes to the [Sample Type] are reflected in the files when saved.

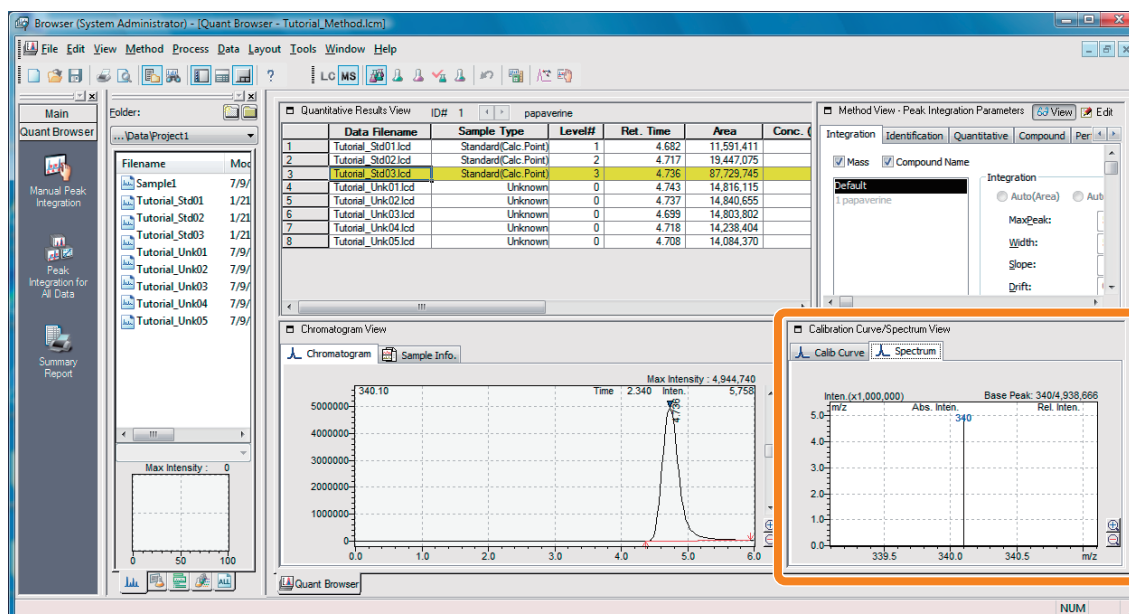
1

Select the [Sample Type] of the sample to be changed, and select the appropriate type from the drop-down list.

	Data Filename	Sample Type	Level#	Ret. Time	Area
1	Tutorial_Std01.lcd	Standard(Calc. Point)	1	4.682	11,591.411
2	Tutorial_Std02.lcd	Standard(Calc. Point)	2	4.717	19,447.075
3	Tutorial_Std03.lcd	Standard(Calc. Point)	3	4.736	87,729.745
4	Tutorial_Unk01.lcd	Unknown	0	4.743	14,816.115
5	Tutorial_Unk02.lcd	Standard(Calc. Point)	0	4.737	14,840.655
6	Tutorial_Unk03.lcd	Standard(No Calc. Point)	0	4.699	14,803.802
7	Tutorial_Unk04.lcd	Control	0	4.718	14,238.404
8	Tutorial_Unk05.lcd	Unspiked Spiked	0	4.708	14,084.370

Verify a Spectrum

Double-click the MS chromatogram in the [Chromatogram View] to display the MS spectrum at the clicked position in the [Calibration Curve/Spectrum View].



▼ Tips

Files Handled in the [Quant Browser] Window

The [Quant Browser] window is an application for editing a single method file, and performing postrun analysis on multiple loaded data sets using the data processing parameters of that method.

Files are loaded according to the following rules.

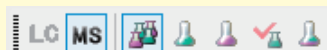
Method File

Load from the [Method] tab of the [Data Explorer] sub-window. If no method file is specified, the method file used for processing the first loaded data file is automatically loaded.

When the loaded Method file has calibration information, the data files of the standard sample used to create its calibration curve are also loaded.

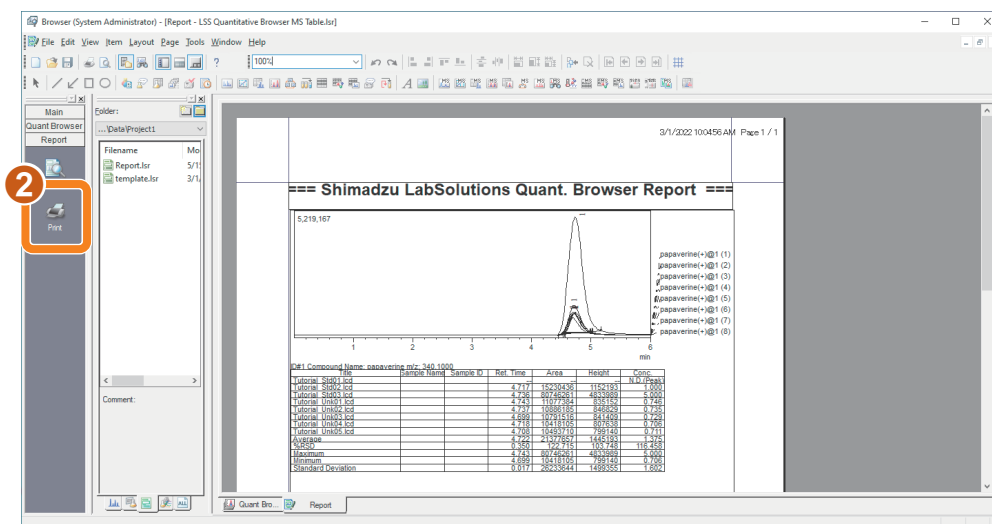
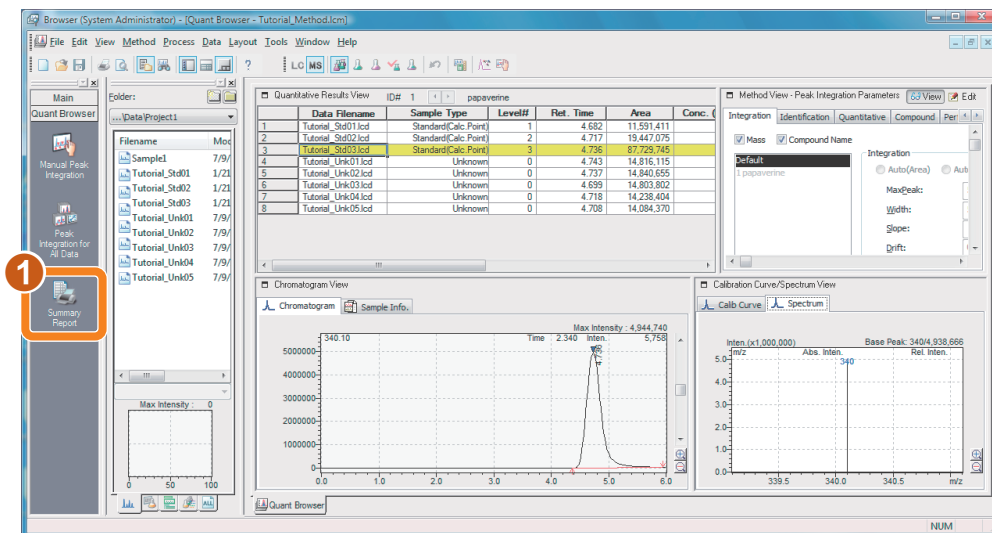
Data Files

Load from the [Data] tab of the [Data Explorer] sub-window. (Multiple data sets can be loaded.) Select the toolbar buttons to determine which sample type is to be displayed.



8.3 Print a Summary Report from the [Quant Browser] Window

The [Quant Browser] window has a Summary Report function for creating a combined report from multiple loaded data sets.



Information associated with each compound is printed in the report.

Chapter 9. Qualitative Data Analysis

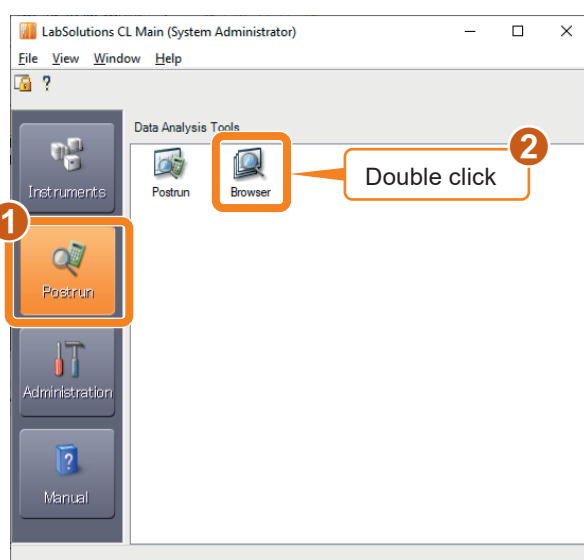
9.1 Display Data Files in the [Data Browser] Window

The [Data Browser] window can be used to display chromatograms, spectra and multiple data file information from different detectors.

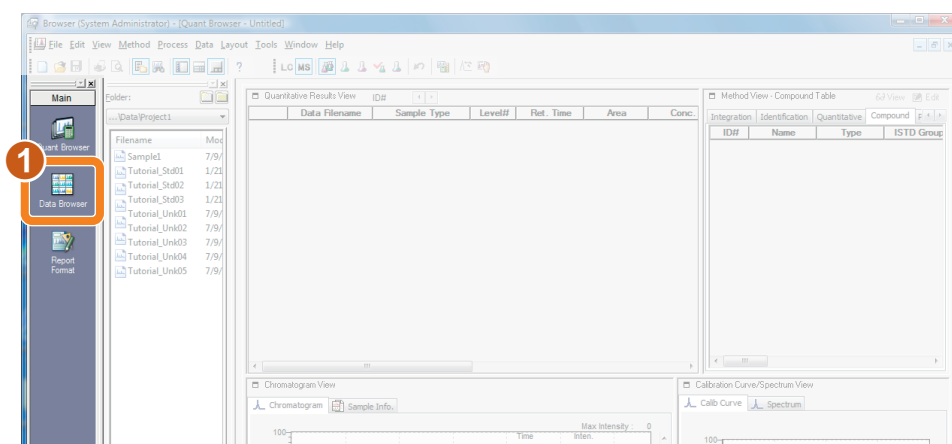


“11.4 Compare Data” in *Operators Guide for LCMS/MS system*.

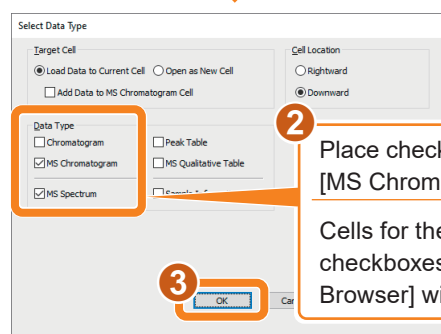
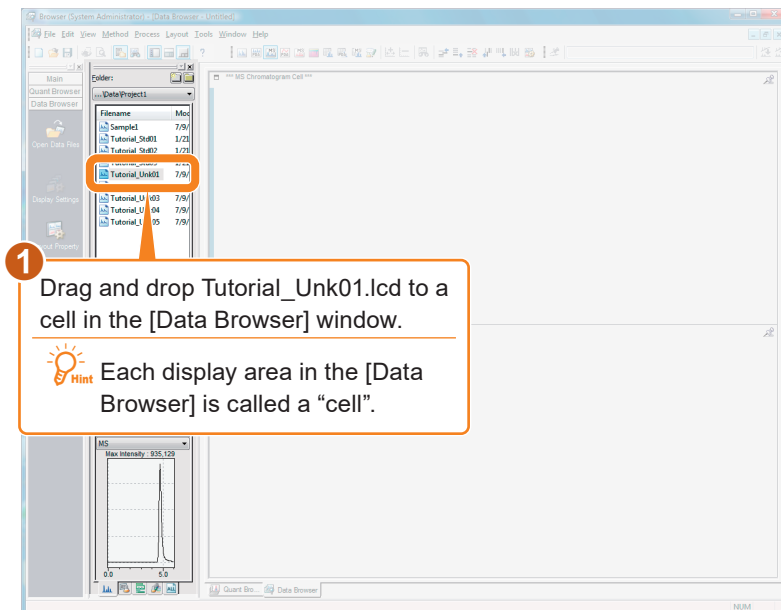
1 Start the [Browser] program.



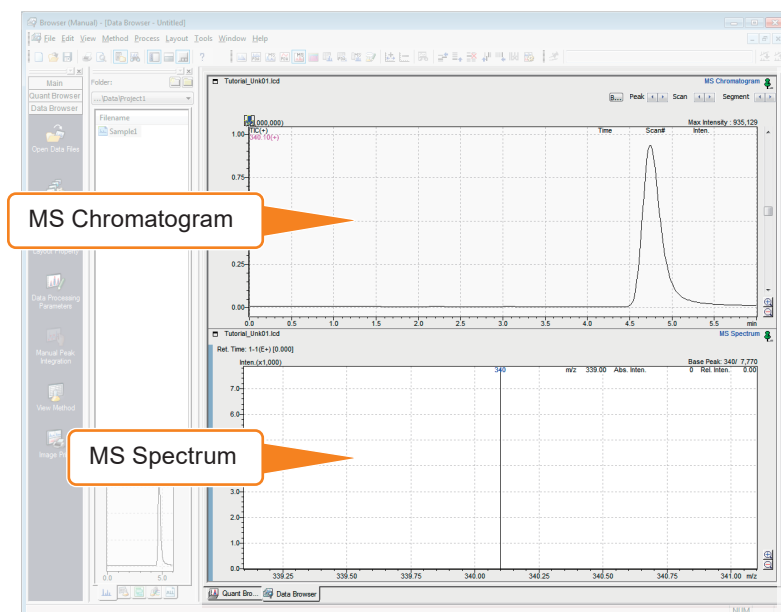
2 Open the [Data Browser] window.



3 Select a data file.



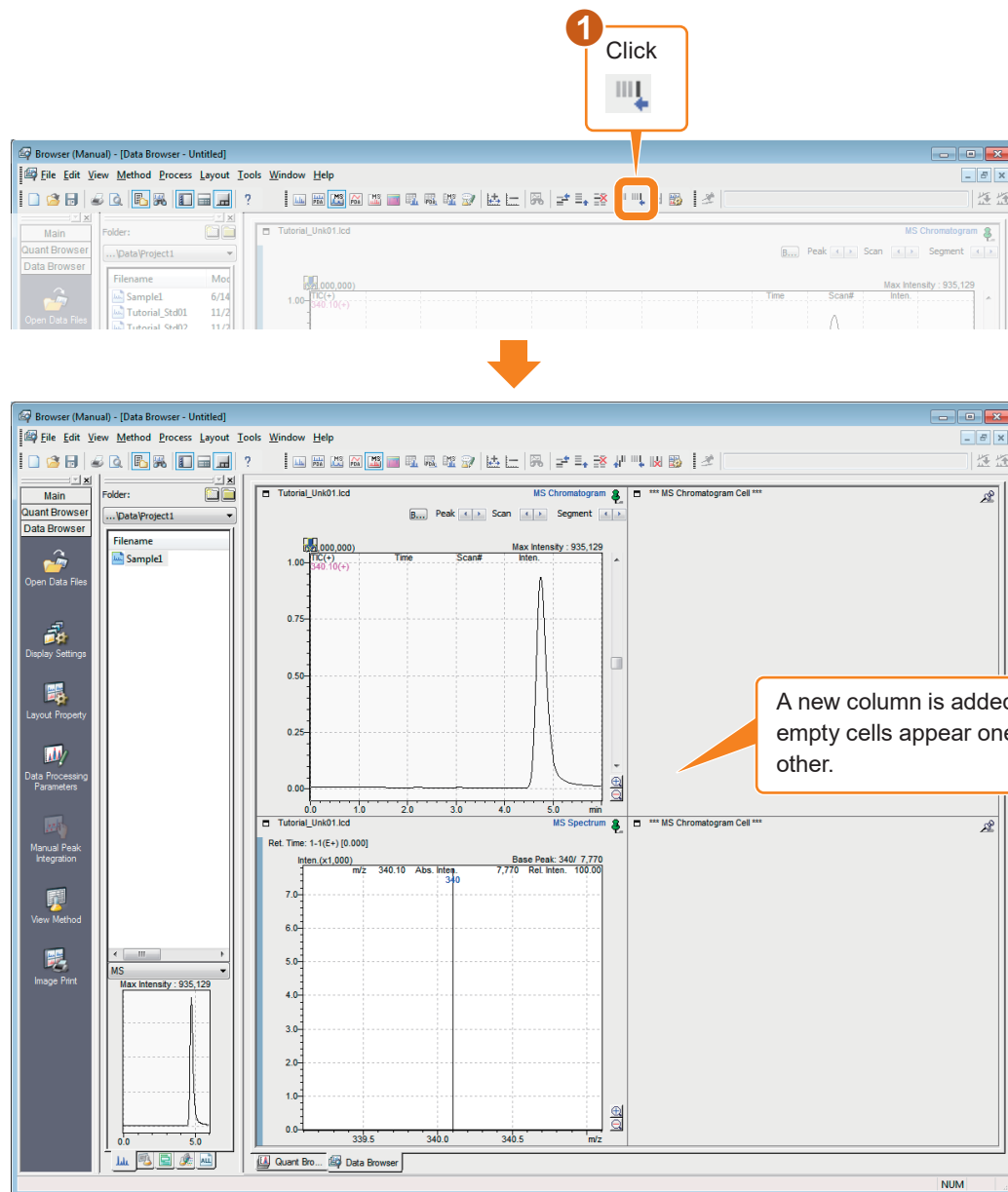
The MS chromatogram and MS spectrum are displayed.
Double click a point on the MS chromatogram to display the MS spectrum at that point.



9.2 Change the Display Layout Settings

1 Add a column

The number of cells can be increased by adding rows or columns to the [Data Browser] window. The procedure to add a column is described here.



2 Copy and paste cell contents

You can copy information from one cell to another.

The screenshot shows the software interface with two context menus open. The first menu, on the left, is open over a source cell and has the 'Copy Cell' option highlighted. The second menu, on the right, is open over a destination cell and has the 'Paste Cell' option highlighted. Two callout boxes with numbered circles (1 and 2) provide instructions for each step. A hint box with a lightbulb icon is also present.

1 Right-click on the copy source cell and click [Copy Cell].

Hint Use this on any cell you want to copy.

2 Right-click on the copy destination cell and click [Paste Cell].

The copy of the MS chromatogram of the source cell now appears in the destination cell.

9.3 Compare Different Types of Chromatograms

1 Compare the data for different chromatograms.

The chromatograms of different data files can be displayed in an [MS Chromatogram] cell.

1 Drag-and-drop Tutorial_Std02.lcd and Tutorial_Std03.lcd from the [Data Explorer] sub-window to the empty cell at the lower right.

Hint Multiple files can be selected by holding the Ctrl or Shift key during selection.

2 Select [Load Data to Current Cell] and [Add Data to MS Chromatogram Cell].

3 Select [MS Chromatogram].

4 Click [OK].

The names of the open files are displayed.

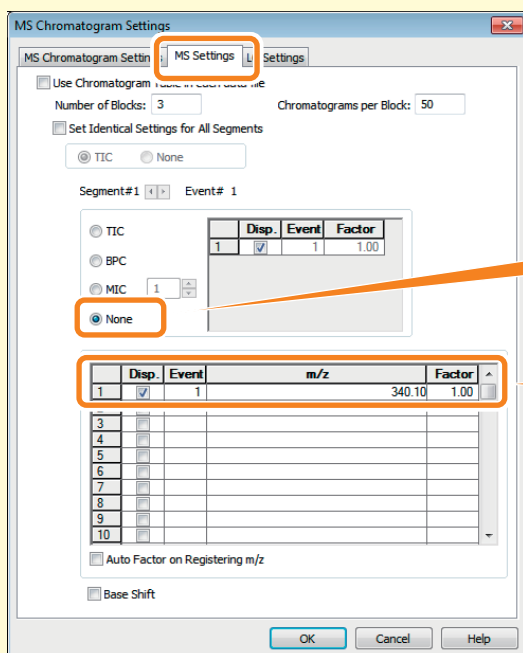
The final MS Chromatogram Cell displays the following data:

File Name	Time (min)	Scan#	Intensity
Tutorial_Std02.lcd	0.093	7	1,797
Tutorial_Std03.lcd	0.093	7	1,797
Tutorial_Std02.lcd	0.093	7	1,797
Tutorial_Std03.lcd	0.093	7	1,797

▼ Tips

Change the MS Chromatogram

To change the m/z of the MS chromatogram to be displayed in the [MS Chromatogram] cell, use the [MS Chromatogram Settings] sub-window.



When [None] is selected, only MC is displayed.

Enter the m/z to be displayed and select the [Disp.] checkbox.




In the case of SIM or MRM analysis data, select m/z from the pull-down list opened by clicking the [m/z] column.

9.4 Use the Cell Fixed Function

1 Assign cell numbers.

Using the Cell Fixed Function, the same data may be opened in different cells that have been assigned the same cell number.

1 Click 

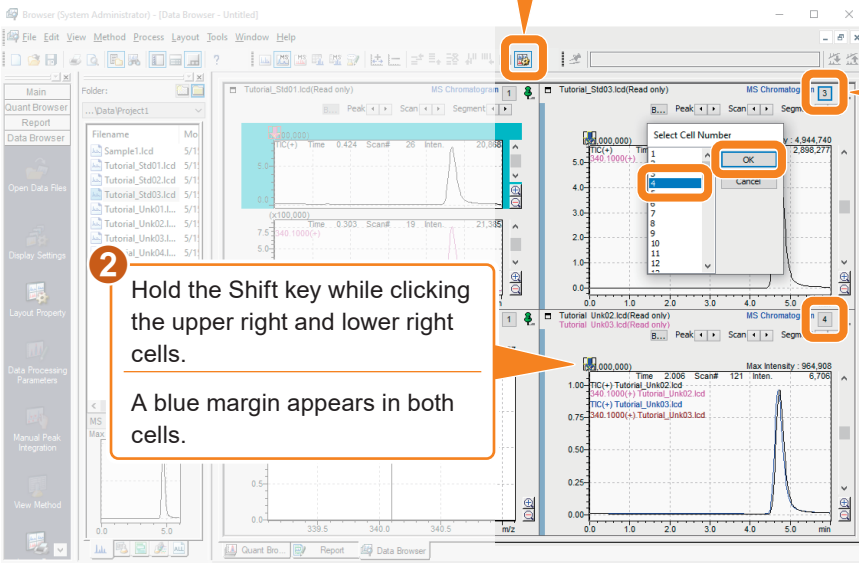
The entire [Data Browser] window enters the [Cell Fix] mode with [Cell Number] displayed at the top right of each cell.

2 Hold the Shift key while clicking the upper right and lower right cells.

A blue margin appears in both cells.

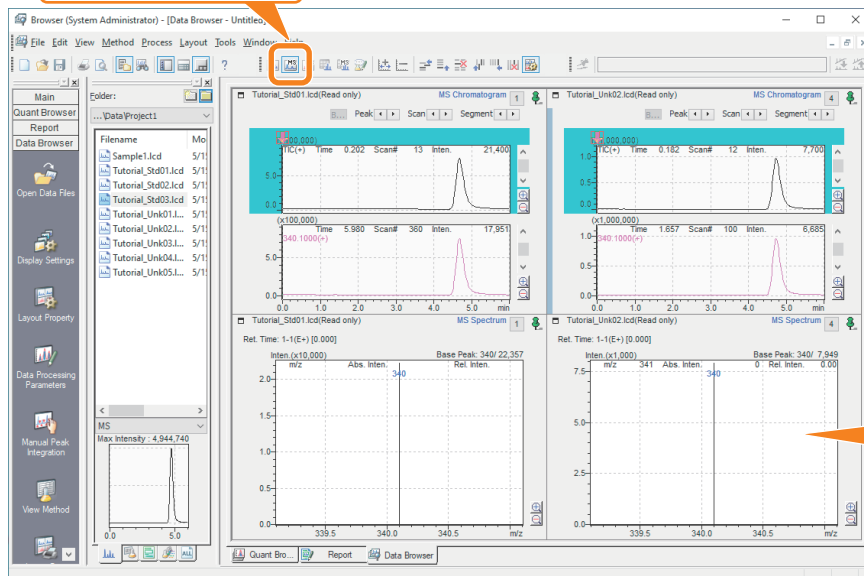
3 Click [Cell Number] with the [Shift] key held down, select cell number 4 and click [OK].

The cell numbers of two cells are both changed to 4.



2 Display an MS chromatogram and MS spectrum.

1 Click  (MS Chromatogram)



2 Hold the Shift key while clicking the lower two cells.



When both cells are active, they can be selected at the same time using the toolbar buttons.

At the left side, the cell numbers of the two cells are both 1, and the same data file (Tutorial_Unk01.lcd) is displayed in both. At the right side, the numbers of the two cells are both 4, and the same data file (Tutorial_Std01.lcd) is displayed in both. When the Cell Fixed mode is enabled, the same data file is displayed in all cells having the same cell number.

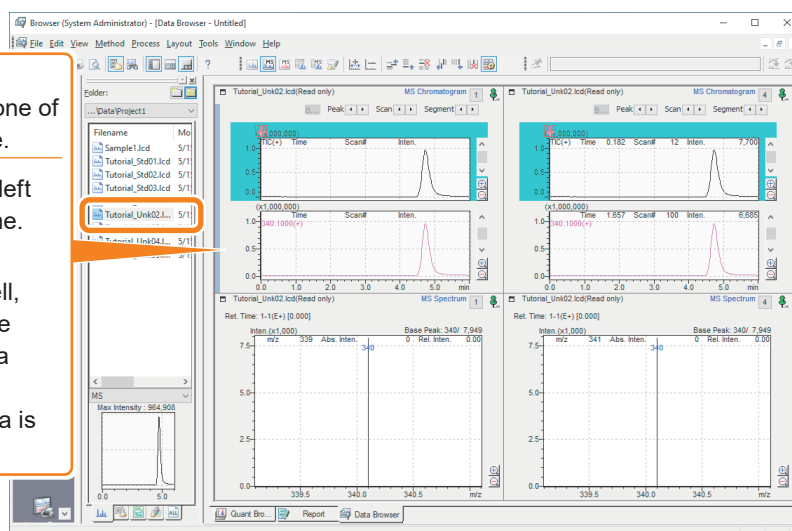
3 Confirm while comparing data.

In this state, data files can be switched for easy data comparison.

1 Drag and drop Tutorial_Unk02.lcd to one of the cells at the left side.

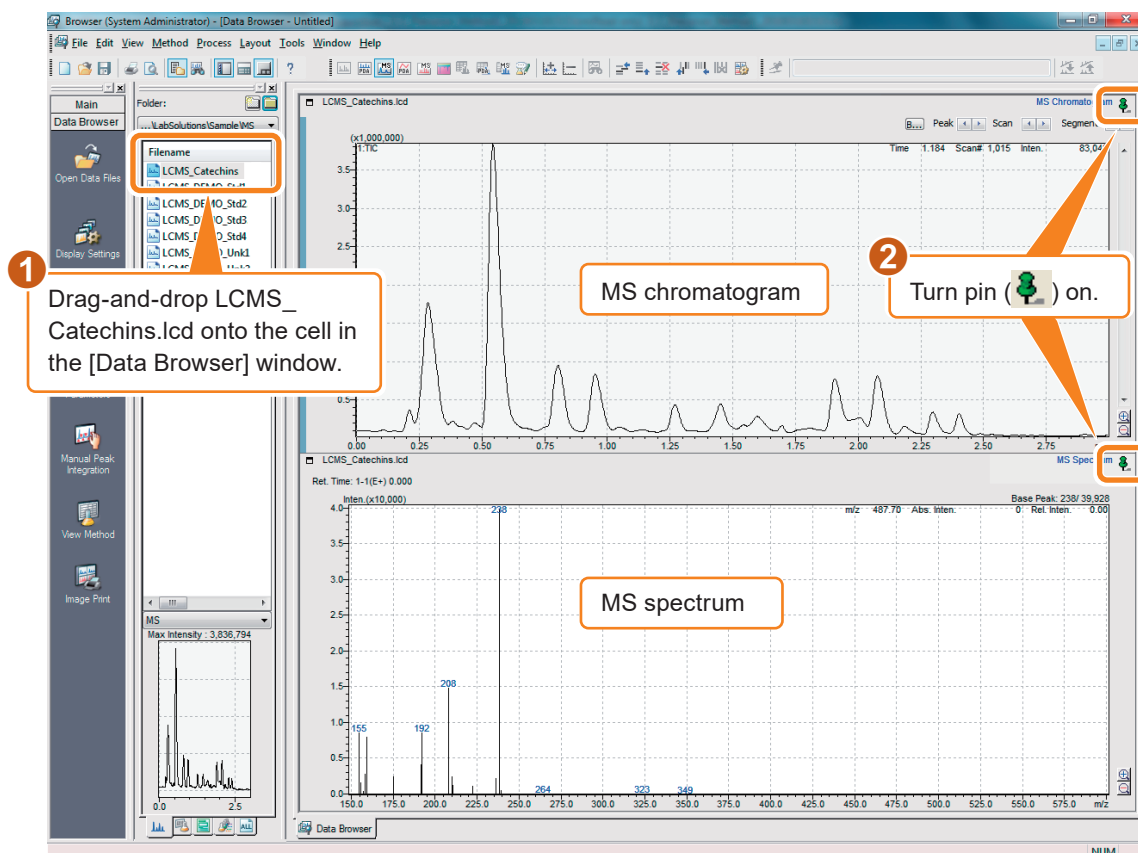
Both of the cells at the left change at the same time.

When dropping to the [MS Chromatogram] cell, a confirmation message appears before the data is added or changed. Select [No] and the data is changed.



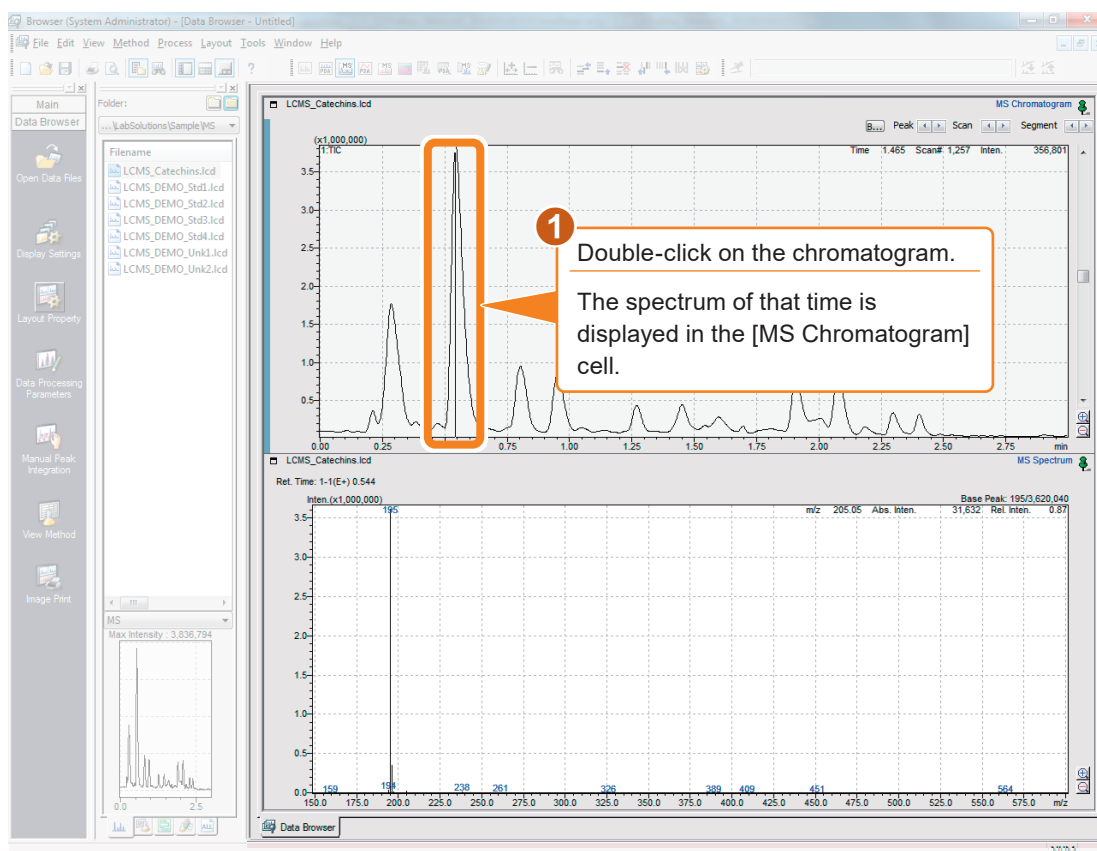
9.5 Qualitative Processing in the [Data Browser] Window

1 Load the data file.



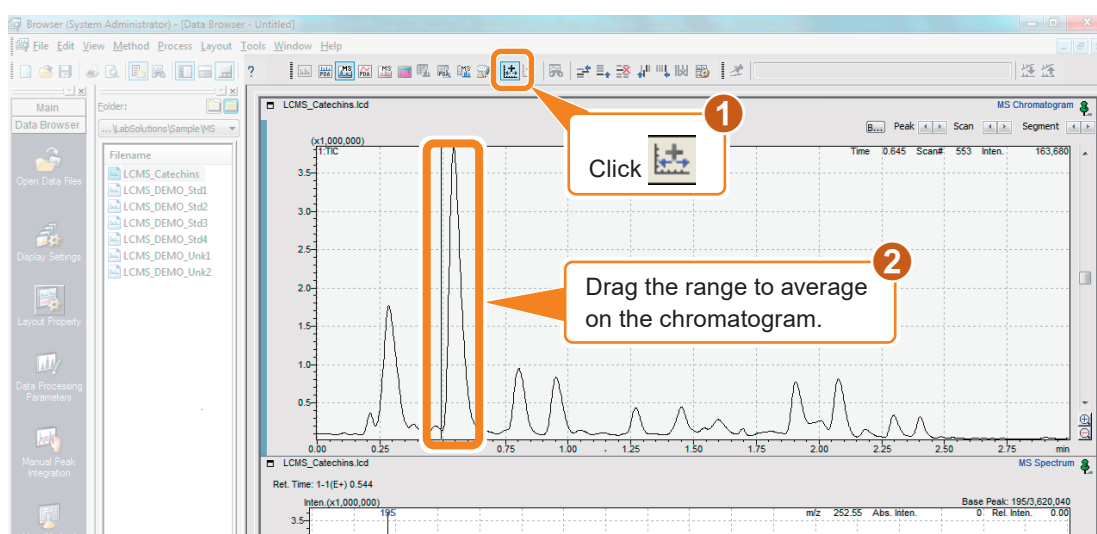
Clicking the pin switches toggles it on and off. Cells are interlocked when the pin is on. Browser functions applied to one pinned cell are executed in all of the pinned cells.

2 Display the MS spectrum.



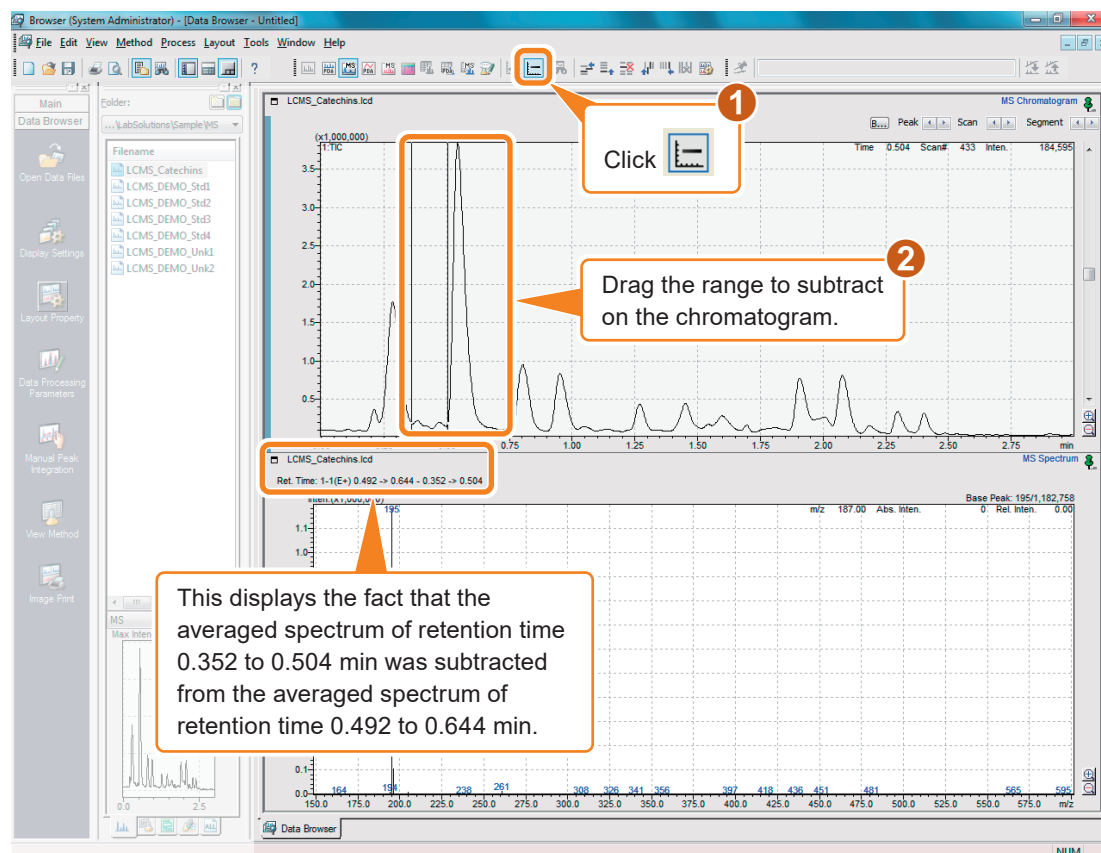
3 Average the MS spectrum.

A stable spectrum can be displayed by totaling and averaging the spectra within a certain time range.



4 Perform subtraction on the MS spectra.

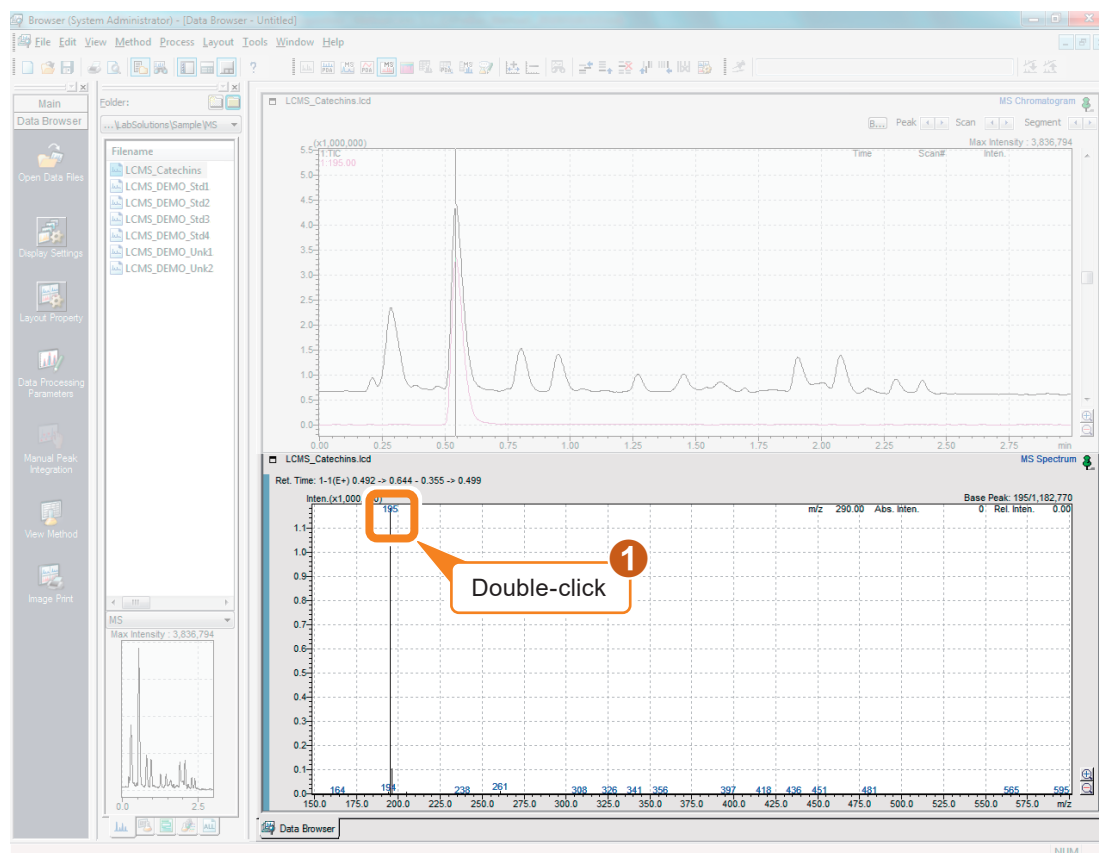
A cleaner-looking spectrum can be displayed by subtracting the background MS spectrum from the averaged spectrum.



Hint After the subtract button is selected, double-clicking on the chromatogram subtracts the spectrum at that clicked position.

5 Display the MS chromatogram.

Double-click the MS spectrum peak. The chromatogram of the m/z at the position double-clicked in the [MS Chromatogram] cell is added to the display.

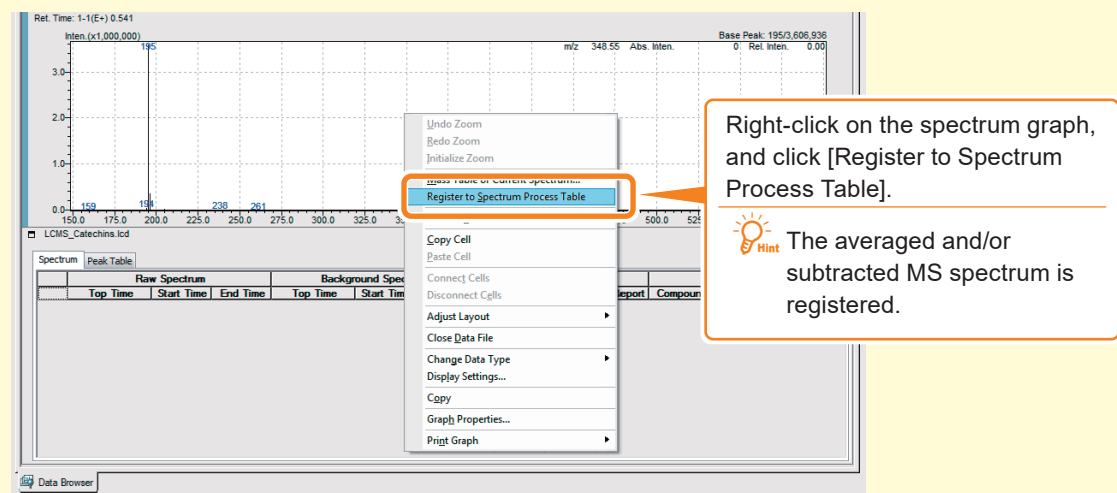


▼ Tips

Register an Averaged/Calculated Spectrum in the Spectrum Process Table

When a spectrum has been subjected to averaging/calculation, the results can be registered in the Spectrum Process Table for easy recall of the calculated spectrum at a later time.

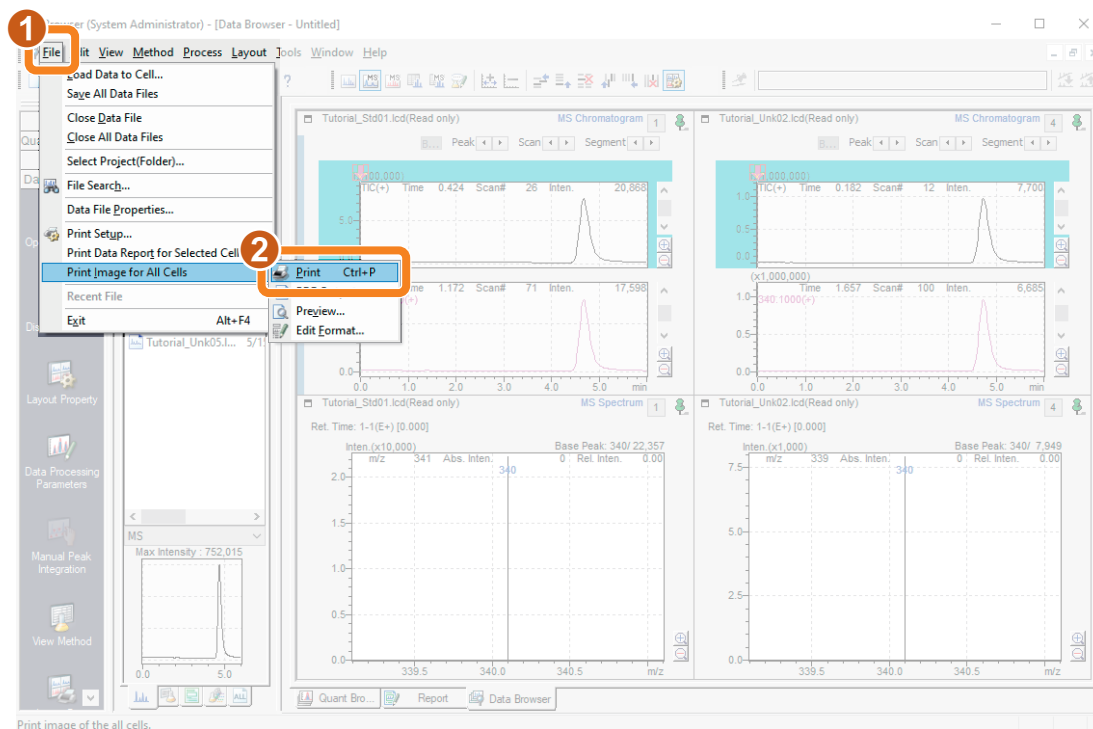
The spectrum can also be printed in the [Report] window.



9.6 Print from the [Data Browser] Window

1 Print an image of the display.

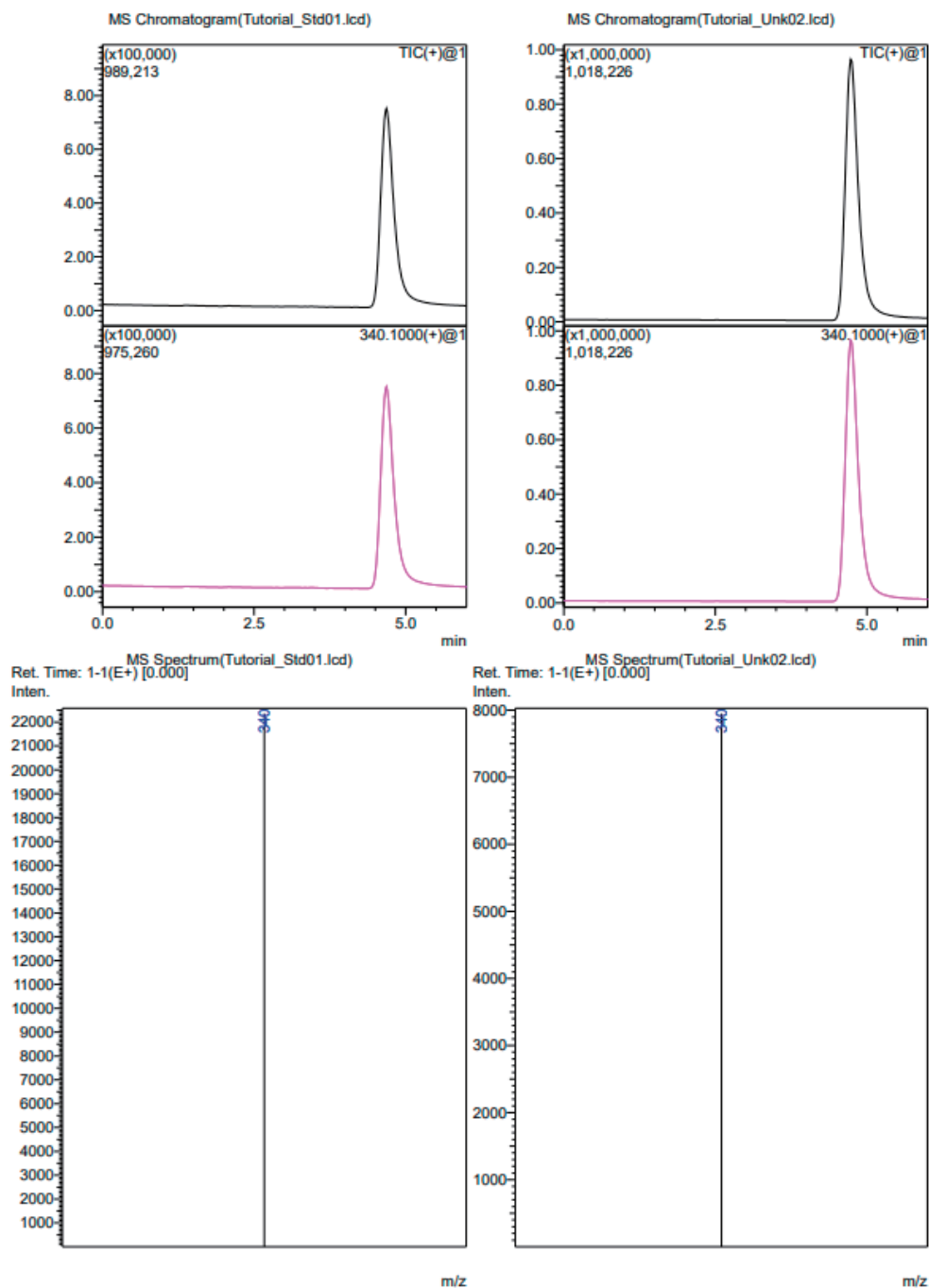
The cells displayed in the [Data Browser] window can be printed in their current displayed format.



Hint

Select [Print Data Report for Selected Cell] from the [File] menu to print using the report format saved in the data file.

==== Shimadzu LabSolutions Browser Report ====



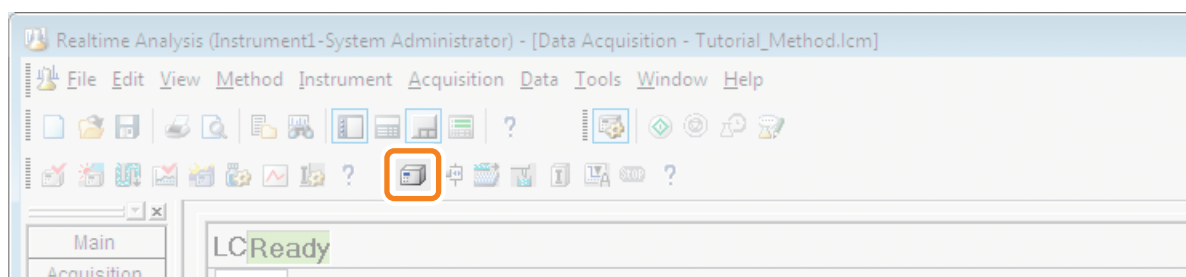
Chapter 10. Shutdown (LC)

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

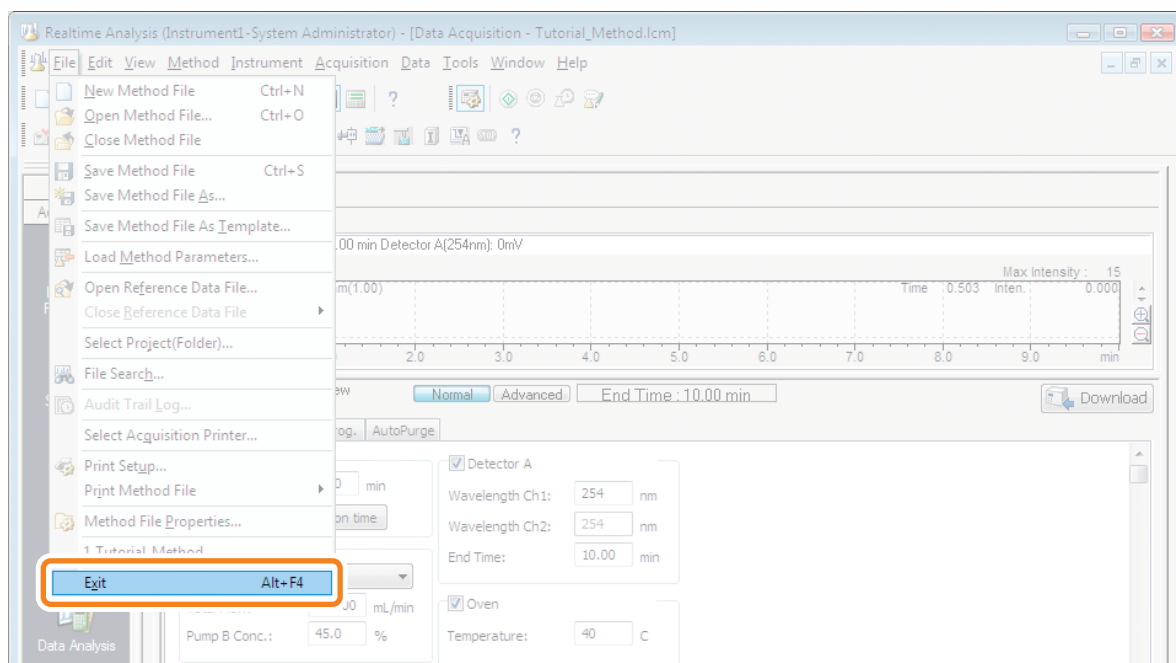
1 Stop instrument operation.

Stop pump solvent delivery and heating of the column oven.

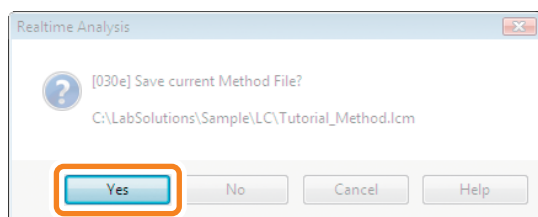
2 Set to OFF.



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



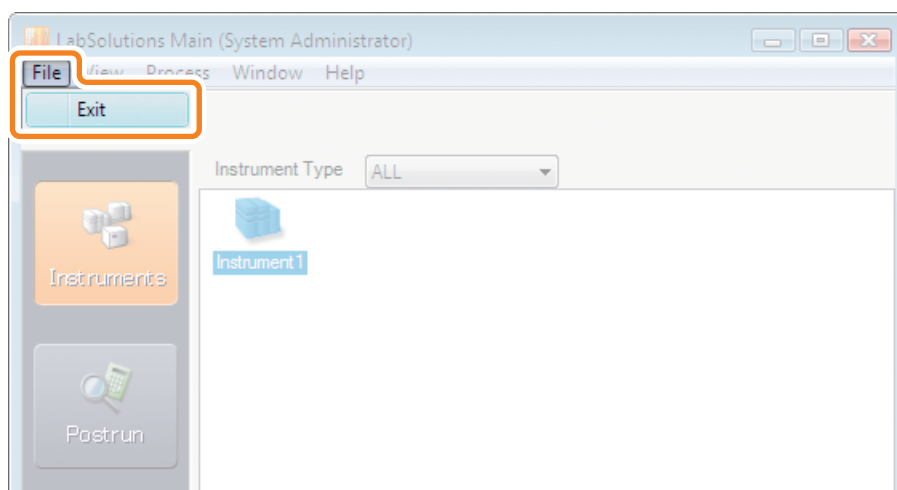
4 Click [Yes].



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.

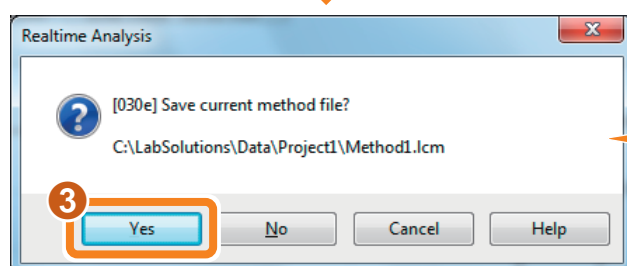
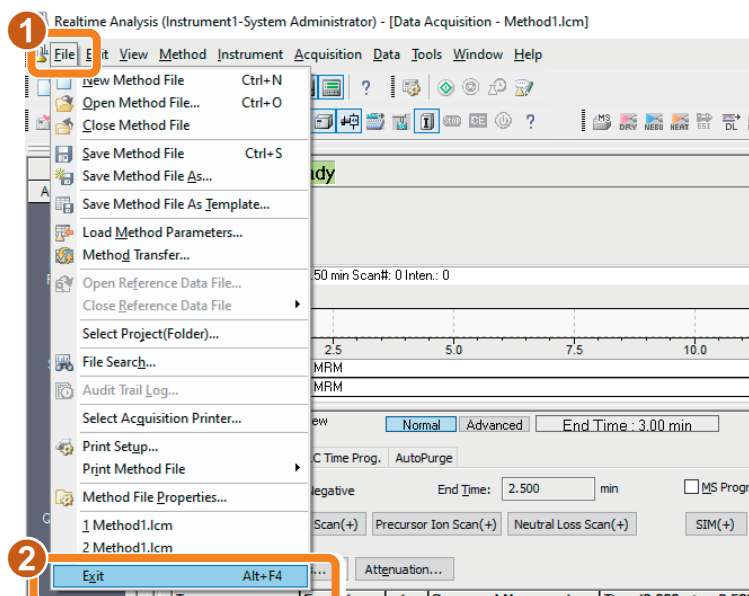



6 Shutdown Windows, and turn the PC and printer off.

7 Turn each instrument off.

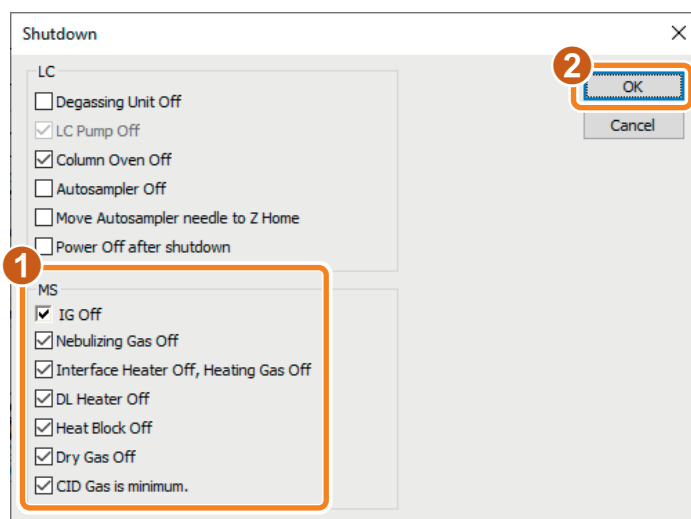
Chapter 11. Shutdown (LCMS)

1 Close any open windows.

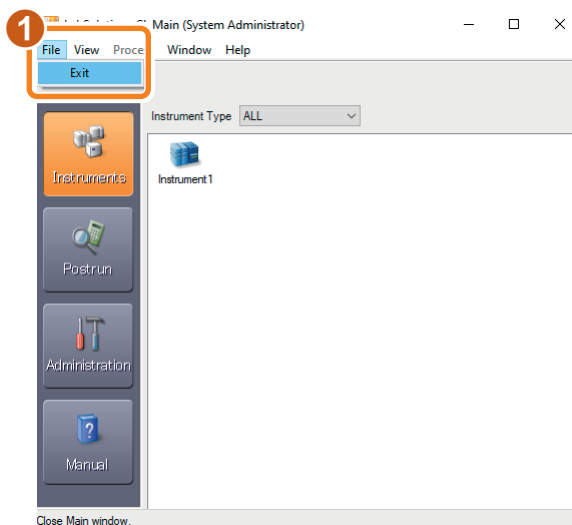


 **Hint** This sub-window appears if there are any unsaved files.

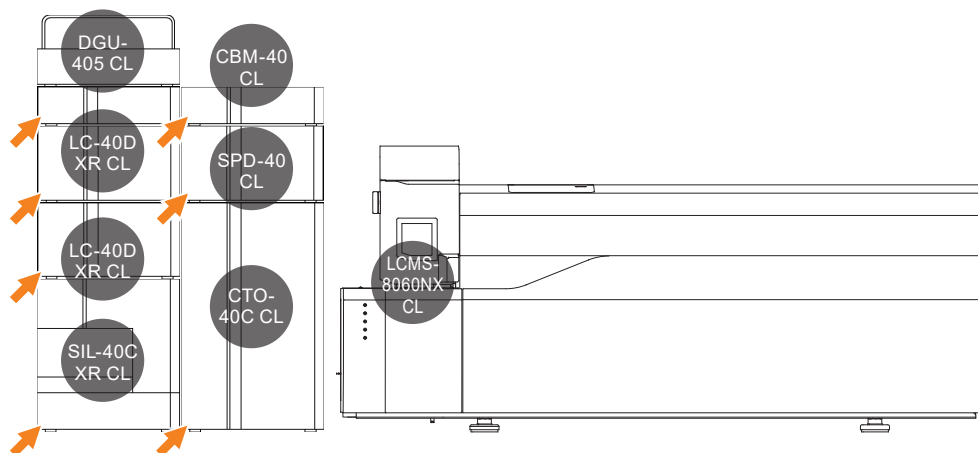
2 Stop the LC pumps, gas flows and heaters from the [Shutdown] sub-window.



3 Exit LabSolutions.



4 Turn off the power to the LC modules.



During routine operation, the LCMS-8060NX is not turned off.

5 Stop supplying nitrogen gas and plug DL with DL plug.