

LabSolutions LCMS

Getting Started Guide

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- Original version is approved in English.

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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.

■ Installation & Maintenance Guide

This manual describes installation and maintenance of the LabSolutions software.

■ 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:

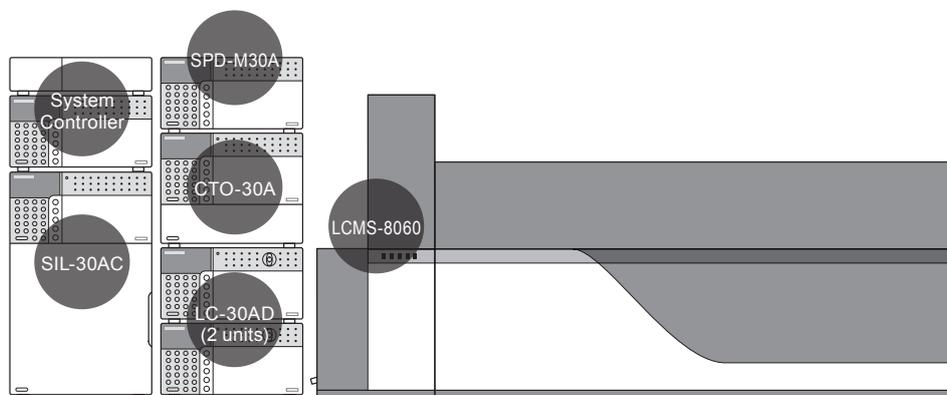
- Data acquisition and control of analytical instruments
- Data analysis and viewing of data
- Creation and printing of various customizable reports

System Structure

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

High-pressure gradient LCMS + PDA system

- System Controller ... CBM-20A
- Column Oven CTO-30A
- Autosampler SIL-30AC
- Pump LC-30AD (2 units)
- Detector SPD-M30A
- MS Detector LCMS-8060



Acquisition Conditions

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

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.

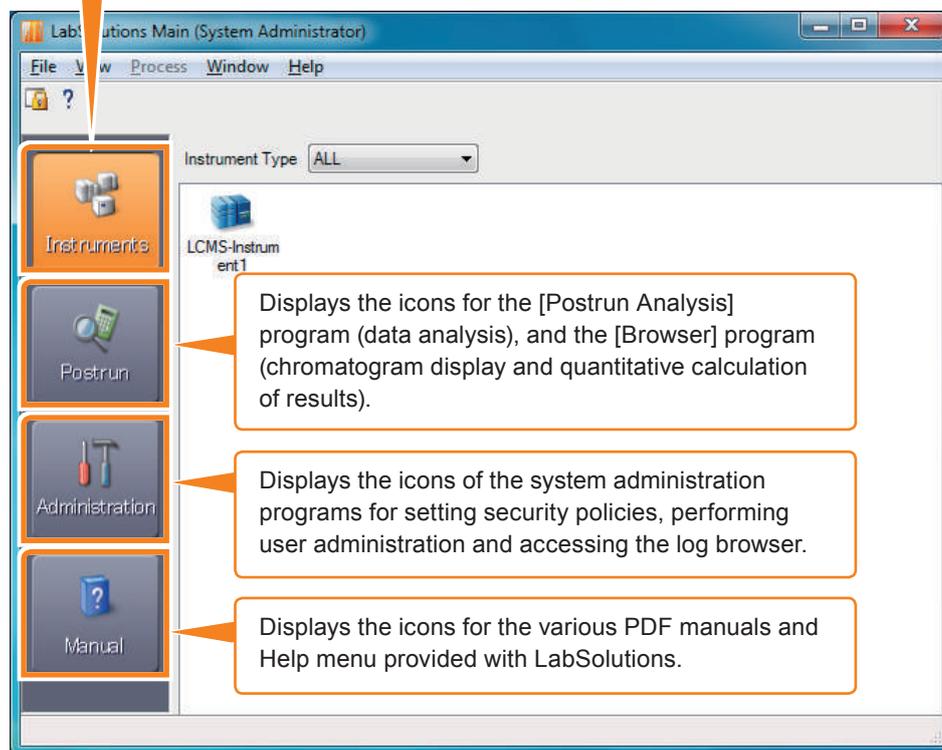
Report format file (.lsr)

This file is used to print data acquisition results.

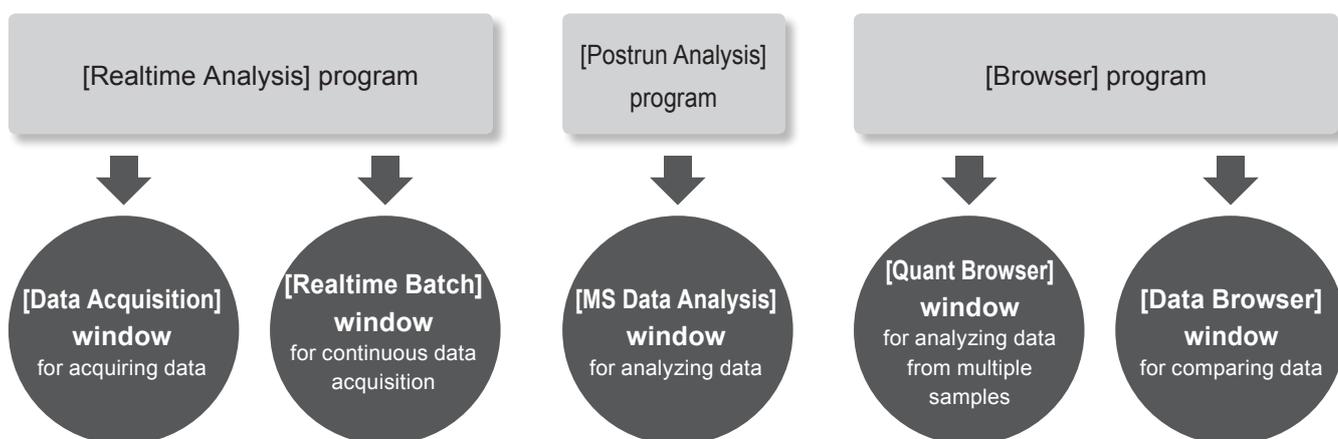
LabSolutions Main Window

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.

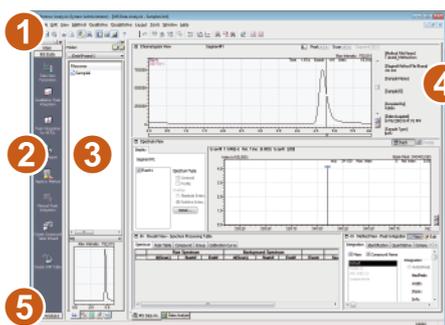


LabSolutions Main Programs and Main Windows



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], [PDA 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	System Adm.
MS 8 is the exchange time of the oil of a rotary pump.		2/19/2008	7:57:20 AM	0x7306	System Adm.

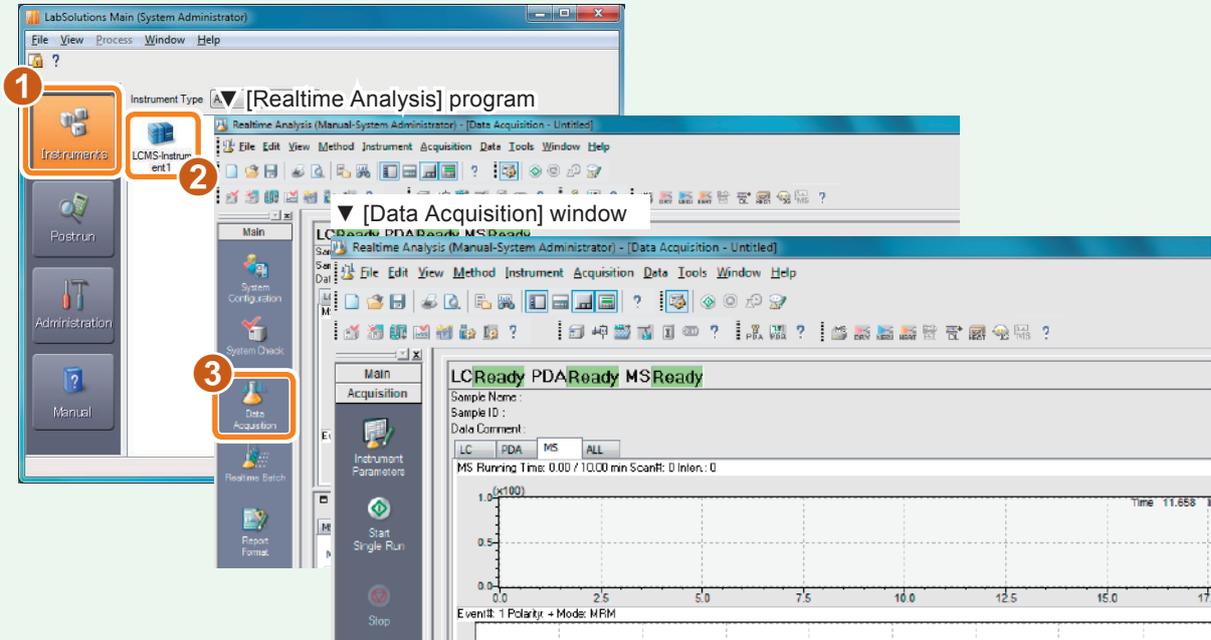
How to Open Windows

Set the Data Acquisition Parameters and Execute a Single Run

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

 Reference 2. Single Run

▼ Main window



1 Instruments

2 LCMS-Instrument1

3 Data Acquisition

▼ [Data Acquisition] window

LCReady PDAReady MSReady

Sample Name:
Sample ID:
Data Comment:

MS Running Time: 0.00 / 10.00 min Scan#: 0 Inlet: 0

1.0 (x100)

Time 11.655

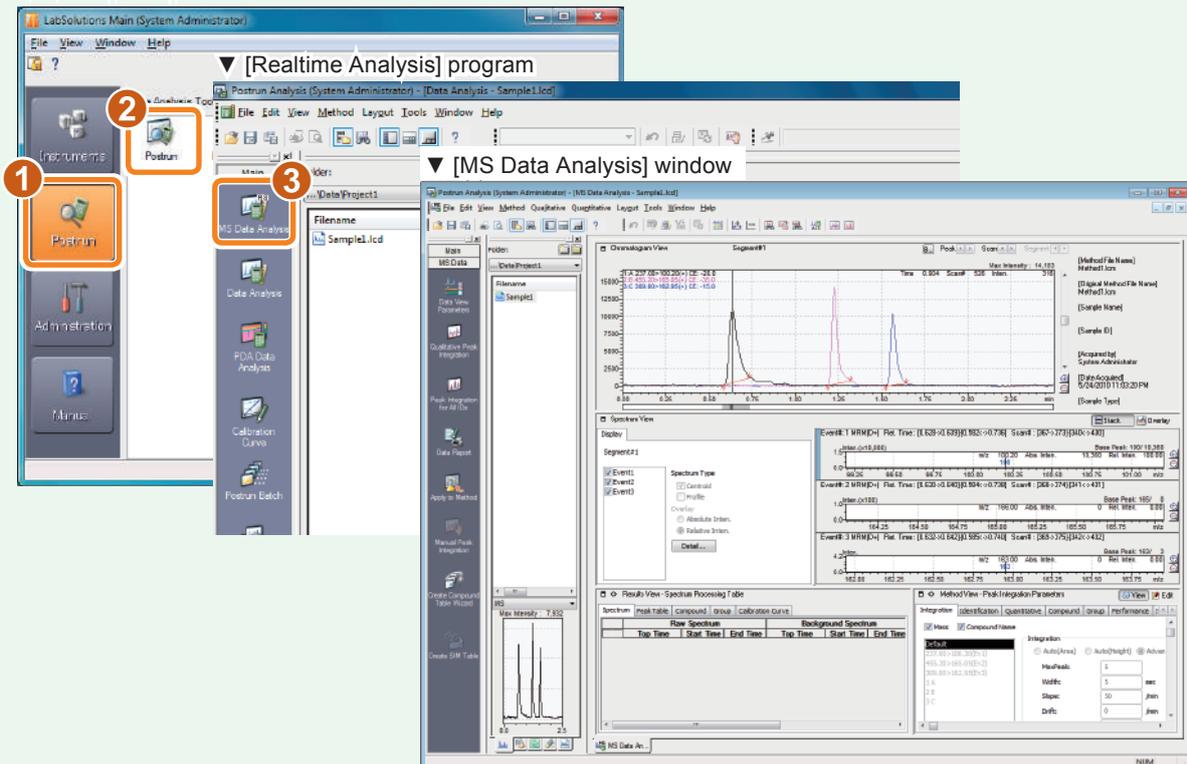
Event#: 1 Polarity: + Mode: MRM

Data Analysis and Qualitative Calculations

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

 Reference 3. Confirm Single Run Results

▼ Main window



1 Postrun

2 MS Data Analysis

3 MS Data Analysis

▼ [MS Data Analysis] window

Chromatogram View

Event#: 1 WRMID-4 Peak Time: [1.628-0.639][8.882-0.738] Scan#: [865-777][840-943]

Event	Time	Area	Height	Width	Retention	Integration
1	1.628	100.00	100.00	100.00	1.628	100.00
2	8.882	100.00	100.00	100.00	8.882	100.00
3	8.882	100.00	100.00	100.00	8.882	100.00

Results View - Spectrum Processing Table

Raw Spectrum	Background Spectrum
Time	Time
1.628	1.628
8.882	8.882
8.882	8.882

Method View - Peak Integration Parameters

Integration

AutoHeight: Active

Height: 5

Width: 1

Slope: 30

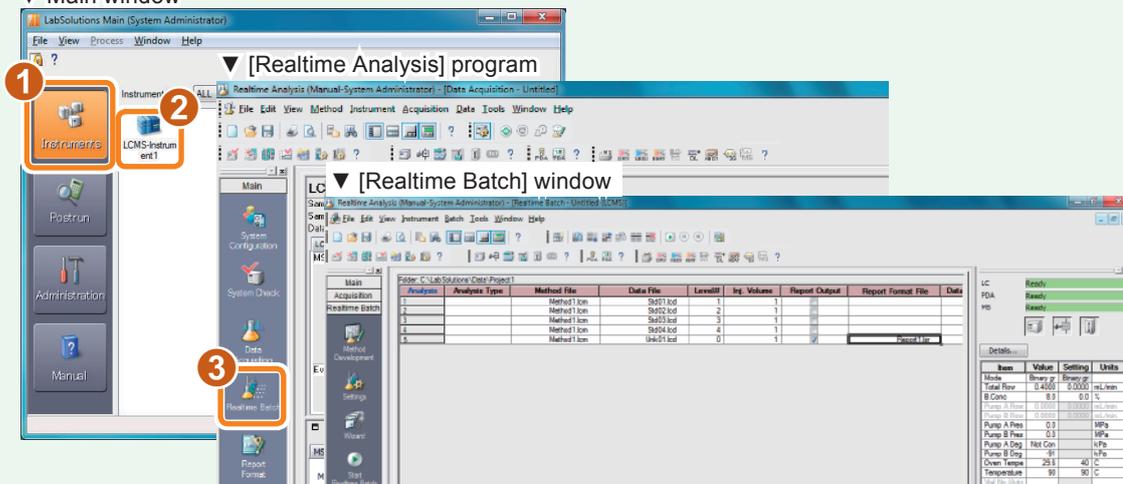
Delta: 0

Continuous Data Acquisition of Sequential Samples

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

 Reference 4. Realtme Batch

▼ Main window

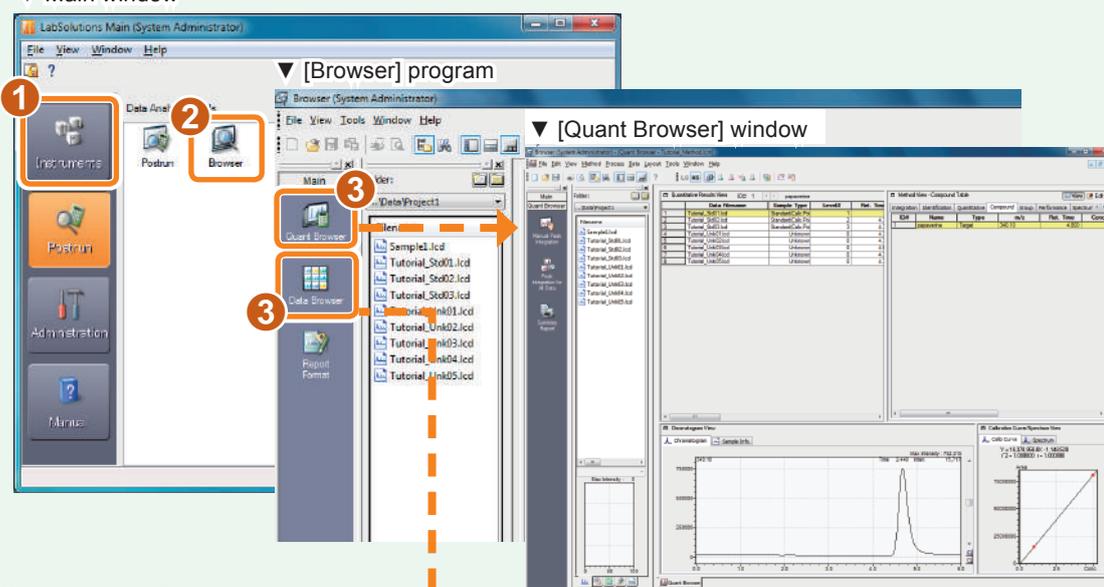


Confirm Quantitative Results

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

 Reference 5. Quantitative Data Analysis

▼ Main window

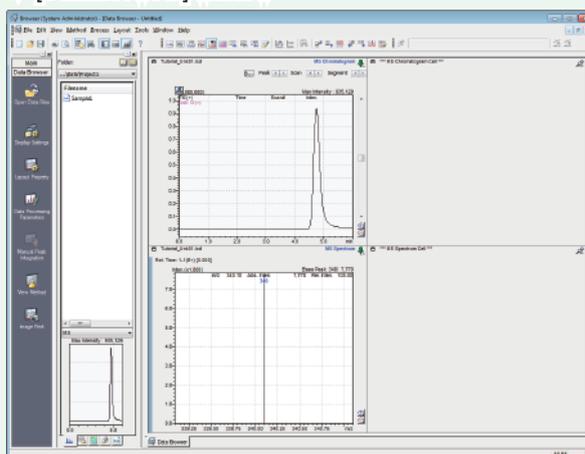


Compare Data

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

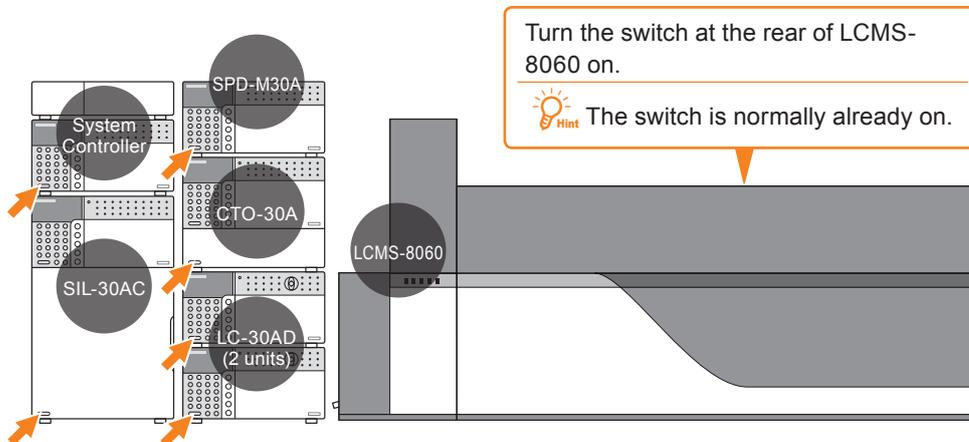
 Reference 6. Qualitative Data Analysis

▼ [Data Browser] window



Chapter 1. Startup

1 Turn ON all of the instruments.



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

3 Start the PC.

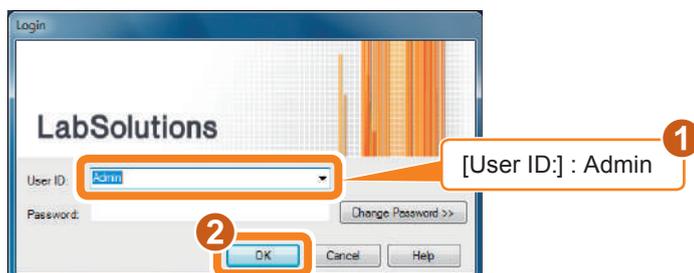
4 Verify that the [LabSolutions Service] icon in the system tray on the Taskbar is green.



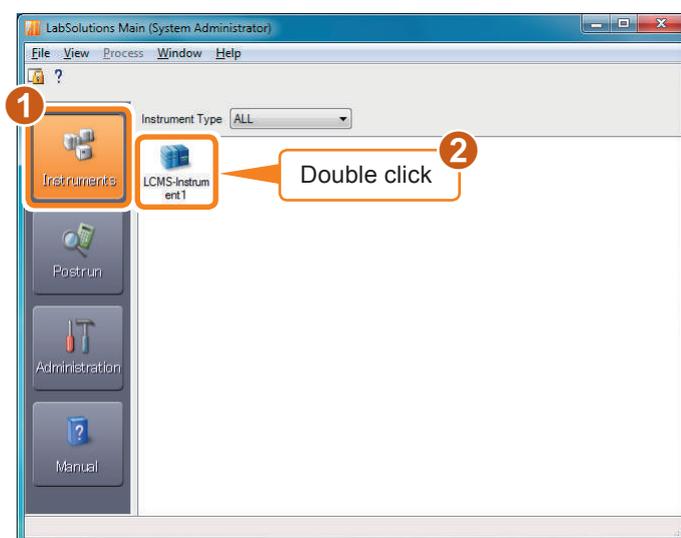
Icon Color	LabSolutions Status	Operation
Green	Normal	
Yellow	Starting up	Please wait
Red	Error	Please restart the PC.

5 Double-click on the desktop.

6 Log in.



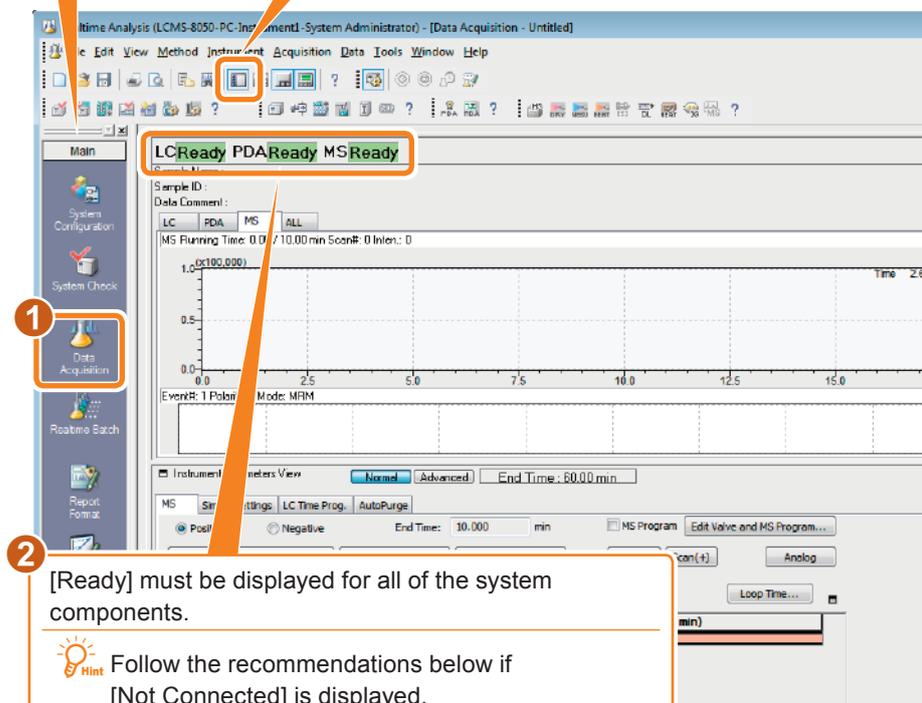
7 Start the [Realtime Analysis] program.



8 Open the [Data Acquisition] window.

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

 **Hint** Click  if the assistant bar is not displayed.



Chapter 2. Single Run

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

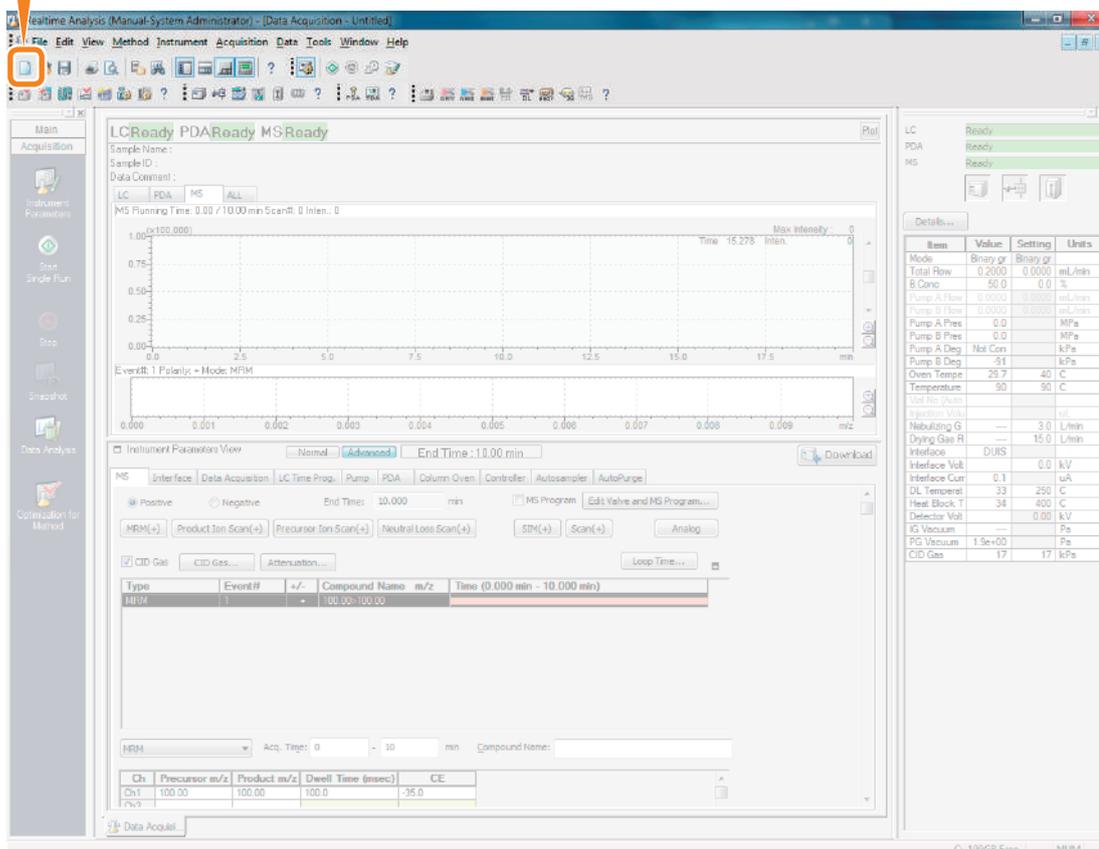
2.1 Create a Method File

1 Click [New] on the toolbar.

Click 



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



The screenshot shows the 'Data Acquisition' window of the LCMS software. The 'New' icon on the toolbar is highlighted with a red box. The interface displays instrument status (LC Ready, PDA Ready, MS Ready), a chromatogram, and instrument parameters.

Item	Value	Setting	Units
Mode	Binary	Binary	g
Total Flow	0.2000	0.0000	mL/min
B Conc	50.0	0.0	%
Pump A Flow	0.0000	0.0000	mL/min
Pump B Flow	0.0000	0.0000	mL/min
Pump A Pres	0.0	0.0	MPa
Pump B Pres	0.0	0.0	MPa
Pump A Deg	Npl Con		kPa
Pump B Deg	-91		kPa
Oven Tempe	25.7	40	C
Temperature	90	90	C
Injection Vol			µL
Neubuting G		3.0	L/min
Drying Gas R		15.0	L/min
Interface	DUIS		
Interface Volt		0.0	kV
Interface Curr	0.1		µA
DL Temperat	33	250	C
Heat Block T	34	400	C
Detector Volt		0.00	kV
IG Vacuum			Pa
PG Vacuum	1.5e+00		Pa
CID Gas	17	17	kPa

2.2 Prepare for Method Optimization

MRM (Multiple Reaction Monitoring) measurement on the LCMS-8030/8040/8045/8050/8060 enables high-sensitivity quantitative data acquisition.

The optimum conditions for MRM data acquisition can automatically be determined by executing method optimization.

In this example, we enter the 3-component precursor m/z to be used for quantitative data acquisition, and set the parameters for executing flow injection analysis (FIA) in preparation for executing the method optimization.



Reference "11 Method Optimization" in *Operators Guide*.

1 Remove the column.

Remove the column if it is installed on the CTO-30A.

2 Detect the type of autosampler rack.

Item	Value	Setting	Units
Mode	Isocratic	Isocratic	
Total Flow	0.1000	0.1000	mL/min
Pump A Flow	0.0000	0.0000	mL/min
Pump B Flow	0.1000	0.0000	mL/min
Pump A Pres	0.0		MPa
Pump B Pres	0.0		MPa
Pump A Deg	Not Conn		kPa
Pump B Deg	91		kPa
Oven Tempe	29.8	40	C
Temperature	90	90	C
Valv Pos (Auto)			
Injection Vol			µL
Rebuilding G	---	1.5	L/min
Drying Gas R	---	15.0	L/min
Interface	DUIS		
Interface Volt		0.0	kV
Interface Cur		0.1	µA
DL Temperl		130	250
Heat Block T		219	400
Detector Volt		0.00	kV
IG Vacuum	---		Pa
PG Vacuum	1.5e+00		Pa
CID Gas	17	17	kPa

3 Set the LC instrument parameters.

3 [LC Stop Time] : 0.5

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

1 [Advanced]

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

5 [End Time] : 0.5

6 [Download]

▼ 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 130 MPa, as an example.

1 [Advanced]

2 [Pump]

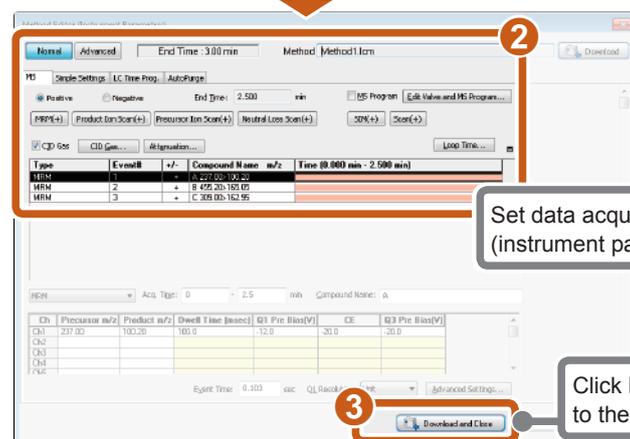
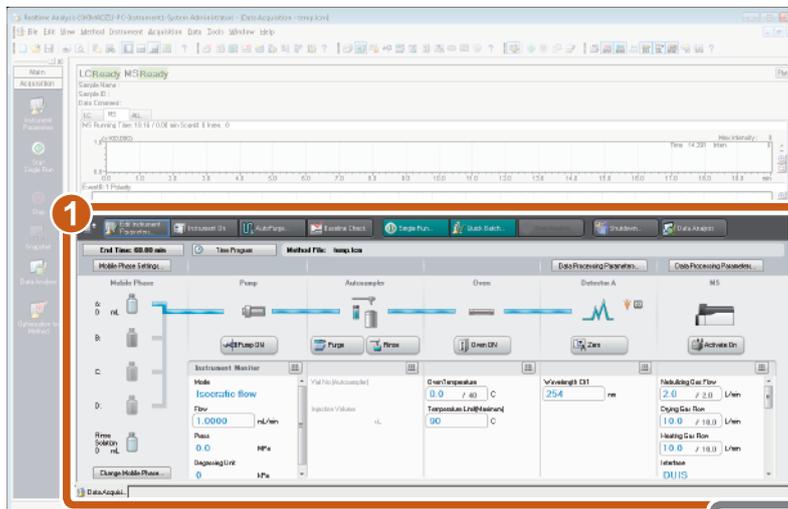
3 [Maximum] : 130

LabSolutions



Control Panel

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



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

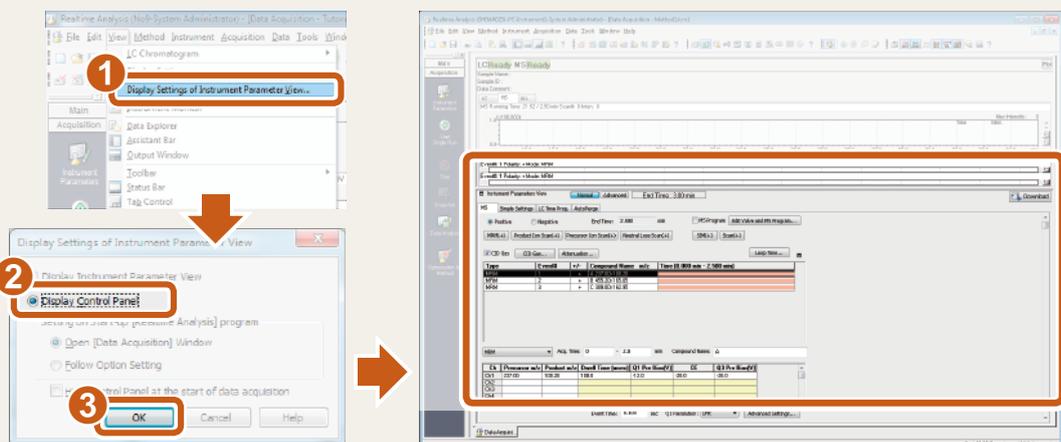
Set data acquisition conditions (instrument parameters).

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



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.



2.3 Instrument Control

1 Take control of the instrument.

The DL plug must be removed before starting analysis.

The screenshot shows the Realtime Analysis software interface. Two callouts with numbered arrows point to specific icons in the top toolbar:

- 1** Click To start operation of the LC instrument
- 2** Click To start operation of the MS instrument

The interface also displays the Instrument Parameters View, a chromatogram, and a status panel on the right showing 'LC Ready', 'PDA Ready', and 'MS Ready'.

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.

The screenshot shows the Instrument Parameters View with the 'Advanced' tab selected. The 'Interface' sub-tab is active, displaying the following settings:

- Interface: ESI
- Nebulizing Gas Flow: 3 L/min
- Heating Gas Flow: 10 L/min
- Interface Temperature: 300 C
- DL Temperature: 250 C
- Heat Block Temperature: 400 C
- Drying Gas Flow: 10 L/min

Callouts 1, 2, and 3 highlight the 'Advanced' tab, the 'Interface' sub-tab, and the gas flow/temperature settings respectively.

2.4 Execute Method Optimization

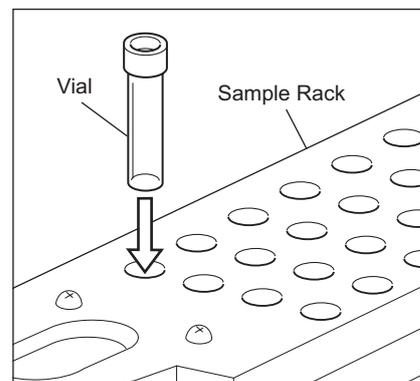
Determine the optimum parameters for MRM data acquisition of each sample by executing method optimization.



"11 Method Optimization" in *Operators Guide*.

1 Place the samples in the autosampler.

- Vial 1, sample A 0.5 ng/ μ L solution
- Vial 2, sample B 0.5 ng/ μ L solution
- Vial 3, sample C 0.5 ng/ μ L solution

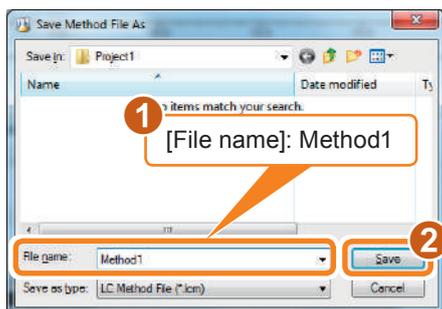


2 Click [Optimization for Method] on the [Acquisition] assistant bar.

The screenshot shows the Realtime Analysis software interface. The 'Acquisition' assistant bar on the left has a red circle and the number '1' around the 'Optimization for Method' button. The main window displays a chromatogram with a peak at 14.118 minutes. The 'Instrument Parameters View' is set to 'Advanced' and shows the following parameters:

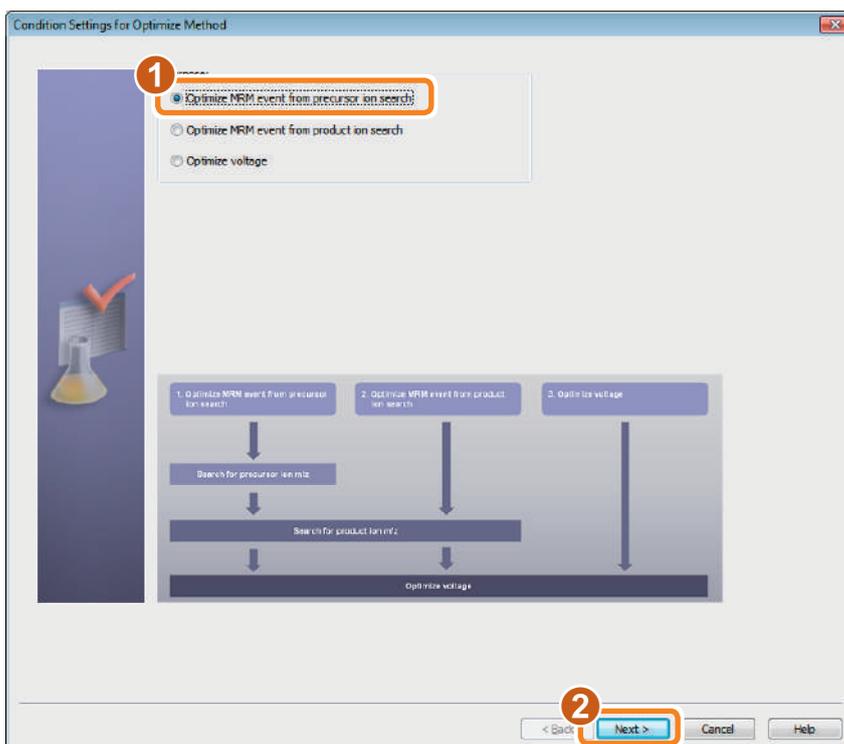
Item	Value	Setting	Units
Mode	Binary gr	Binary gr	
Total Flow	0.2000	0.0000	mL/min
B Conc	50.0	0.0	%
Pump A Flow	0.0000	0.0000	mL/min
Pump B Flow	0.0000	0.0000	mL/min
Pump A Pres	0.0	0.0	MPa
Pump B Pres	0.0	0.0	MPa
Pump A Deg	Not Conn		kPa
Pump B Deg	91		kPa
Oven Temp	25.7	40	C
Temperature	50	50	C
Vial No (Auto)			
Injection Vol			μ L
Nebulizing G	3.0	3.0	L/min
Drying Gas R	15.0	15.0	L/min
Interface	DUIS		
Interface Vol		0.0	kV
Interface Cur	0.1		μ A
DL Temperat	251	250	C
Heat Block T	400	400	C
Detector Vol		0.00	kV
IG Vacuum	5.2e-004		Pa
PG Vacuum	1.3e+00		Pa
CID Gas	17	17	kPa

3 Save the method file.

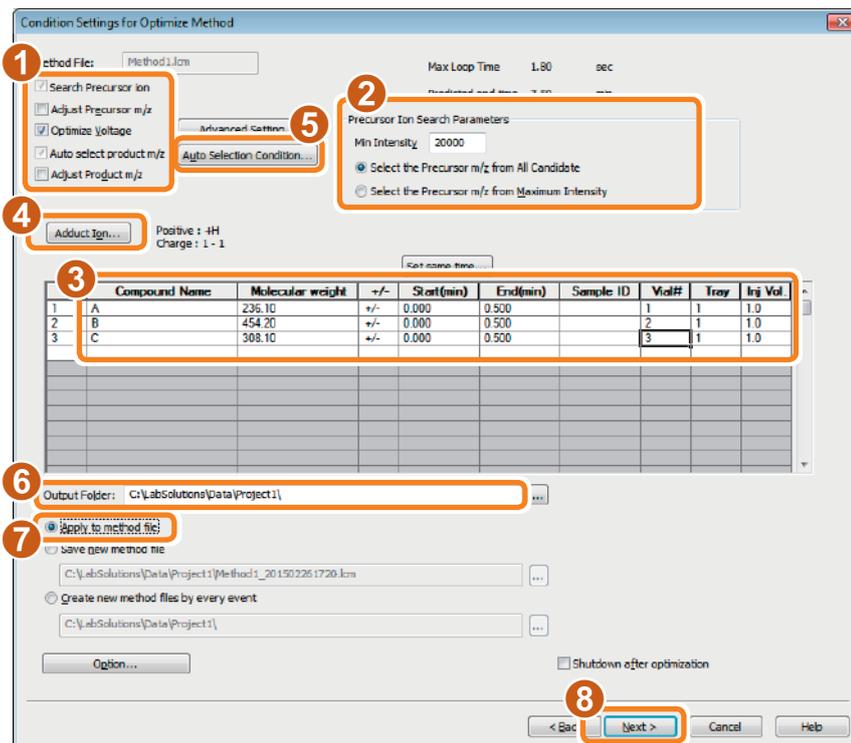


This sub-window is not displayed when a method file is already saved.

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



5 Set the parameters.



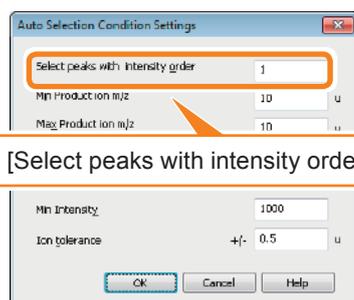
- 1 Check [Optimize Voltage].
- 2 Set the parameters for selecting precursor ions.
- 3 Set the information of compounds to be searched for.

	#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

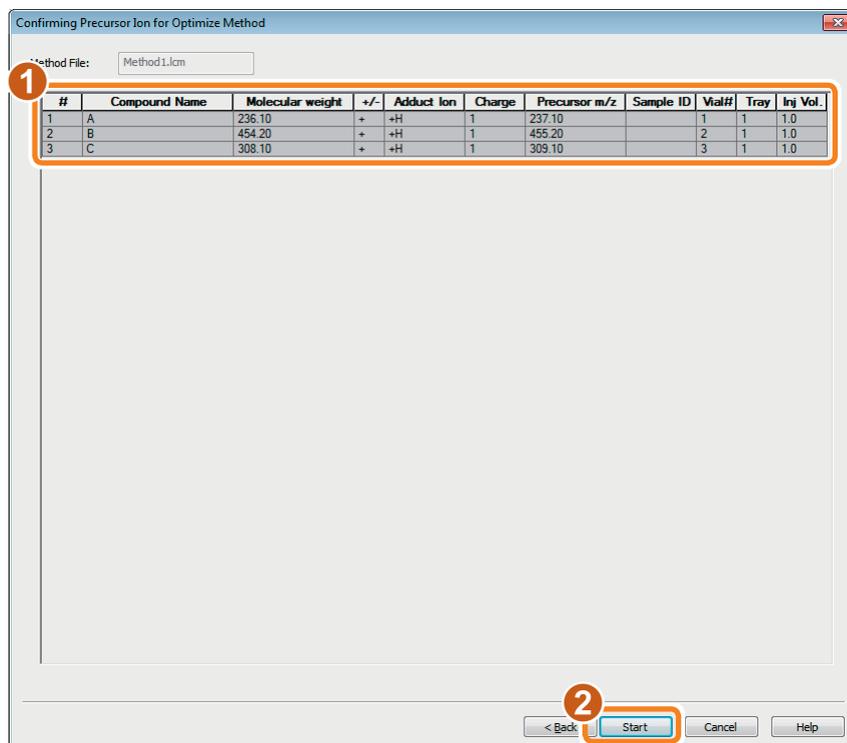
- 6 A subfolder is created under the folder specified here. The name of the subfolder is determined by the date and time. The files automatically created during the optimization are output in this folder.



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.

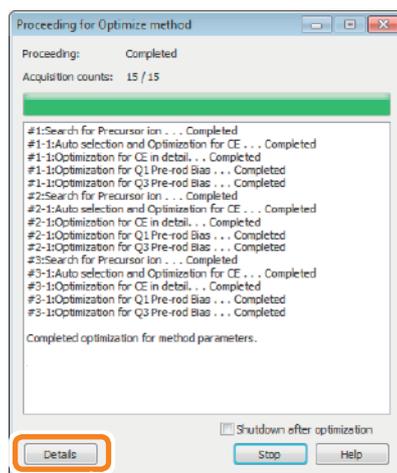
6 Confirm the calculated precursor m/z and start the method optimization.



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

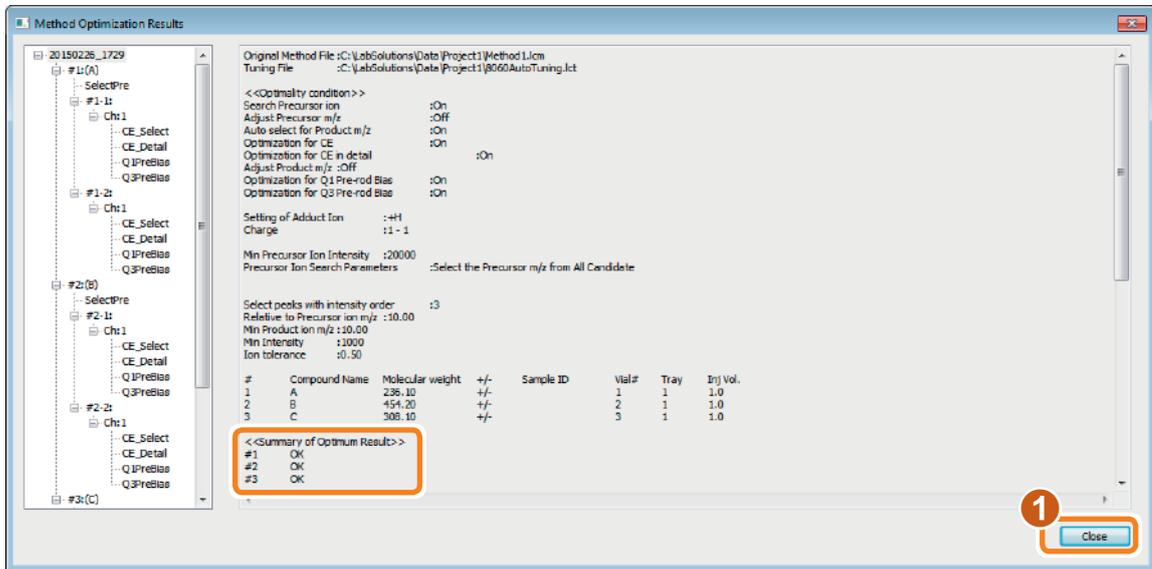


After the method optimization is completed, the word "Completed" is displayed on the window.

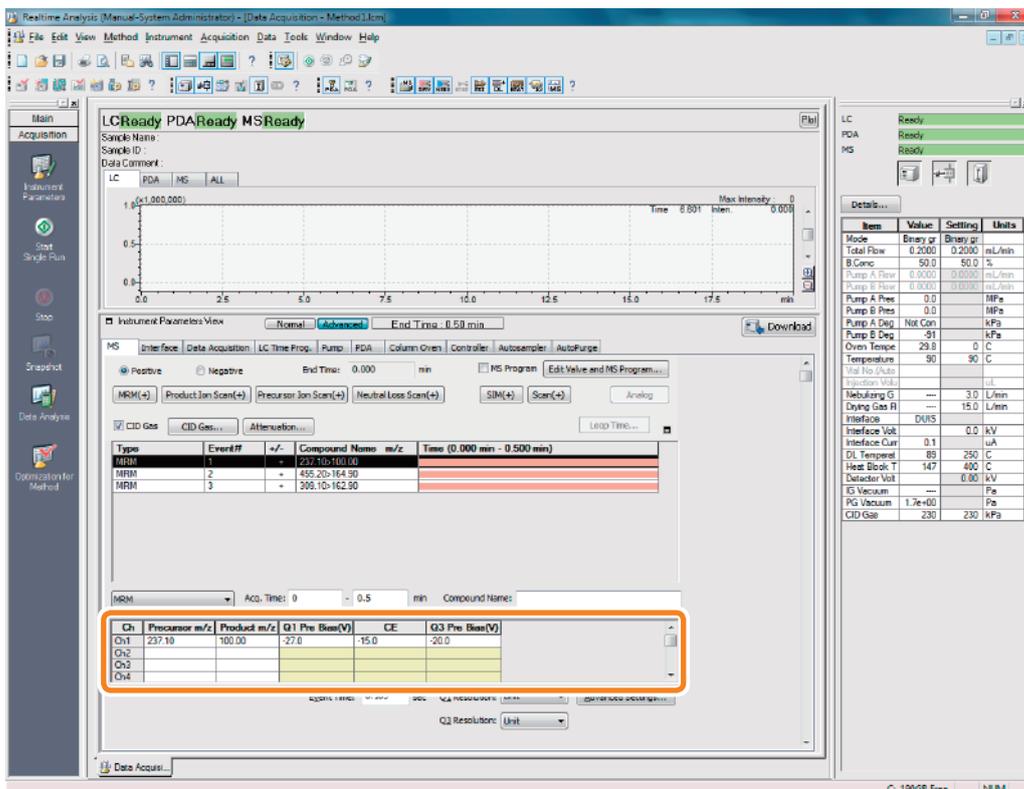


3 To check optimization results, click [Details].

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

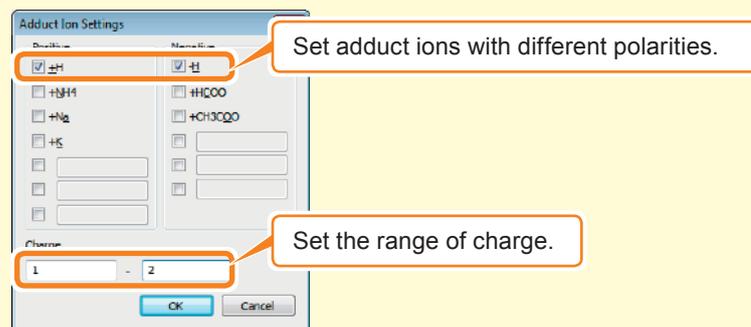
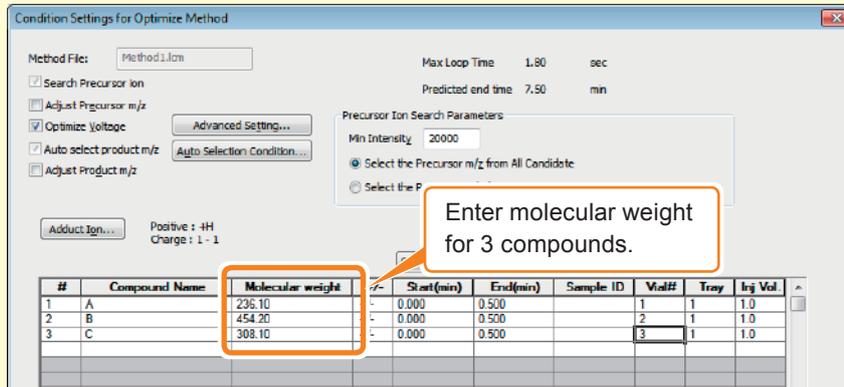


The results reflected in the method parameters.



▼ 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.



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

#	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

2.5 Set the Parameters for Single Run

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

1 Install the column.

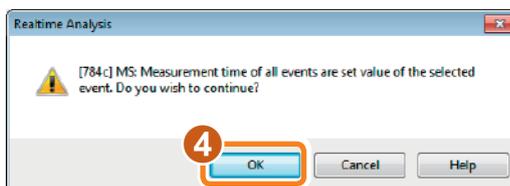
Open the CTO-30A door, and install the column.

2 Set the MS instrument parameters.

The screenshot shows the Realtime Analysis software interface. The main window displays a chromatogram plot with a peak at 2.385 minutes. The 'Instrument Parameters View' window is open, showing the 'MS' tab. A table lists events with columns for Type, Event #, +/-, Compound Name, m/z, and Time. Event #1 is selected, and a right-click context menu is open over it, with 'Set same measurement time' highlighted. Callout boxes provide instructions: 1. Enter the acquisition time of event #1. [Acq. Time]: 0 - 2.5. 2. Select event #1 and display the right-click menu. 3. Select [Set same measurement time].

Type	Event #	+/-	Compound Name	m/z	Time (0.000 min - 2.500 min)
MS1	1	+	237.10210100		
MS1	1.3	+	1456.20162 G1		
MS1	1.3	+	1453.10176 G2		

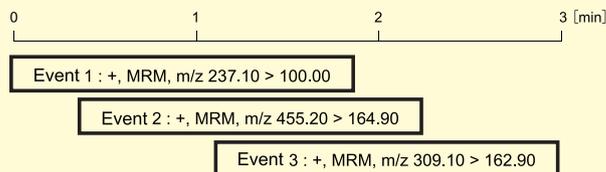
m/z	Product m/z	Q1 Pre Bias(V)	CE	Q3 Pre Bias(V)
100.00	-27.0	-15.0	-20.0	



▼ Tips

Switch the Polarity for Each Event

On the LCMS-8030/8040/8045/8050/8060, 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 - 0.500 min)
MRM	1	+	237.10	100.00	0.000 - 0.500
MRM	2	+	455.20	164.90	0.500 - 1.000
MRM	3	+	309.10	162.90	1.000 - 1.500

Ch	Precursor m/z	Product m/z	Q1 Pre Bias(V)	CE	Q3 Pre Bias(V)
Ch1	237.10	100.00	27.0	-15.0	-20.0
Ch2					
Ch3					
Ch4					

Hint "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].

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

Hint Ch1 is used for the quantitative calculation.

Reference "2 Data Acquisition" in *Operators Guide*.

▼ Tips

Check the loop time

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

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

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

3 Set the LC instrument parameters.

1. End Time: 3.00 min

2. LC Stop Time: 3.00 min

3. [LC Stop Time] : 3.0

4. [Mode] : Binary gradient
[Total Flow] : 0.4
[Pump B Conc.] : 8

5. [End Time] : 3
[Temperature] : 40

6. Download

Item	Value	Setting	Units
Mode	Binary gr	Binary gr	
Total Flow	0.2000	0.0000	mL/min
B Conc	50.0	0.0	%
Pump A Flow	0.0000	0.0000	mL/min
Pump B Flow	0.0000	0.0000	mL/min
Pump A Pres	1.7		MPa
Pump B Pres	1.7		MPa
Pump A Deg	Not Con		kPa
Pump B Deg	Not Con		kPa
Oven Temp	30.11	40	C
Temperature	30	30	C
Use File (Auto)			
Injection Valve			
Heating G	3.0	3.0	L/min
Drying Gas F	15.0	15.0	L/min
Interface	DUIS-E		
Interface Volt		0.0	kV
Interface Curr	0.0		uA
DL Temp	250	250	C
Heat Block T	401	400	C
Detector Volt		0.00	kV
IG Vacuum	5.4e-004		Pa
PG Vacuum	1.2e+00		Pa
CID Gas	17	17	kPa

4 Set the Gradient conditions.

Change the mobile phase mixture ratio.

1. LC Time Prog.

2. Set the [Time], [Module], [Command] and [Value] as shown.

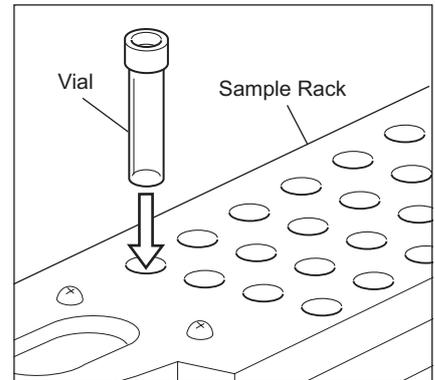
Time	Module	Command	Value
1	Pumps	Pump B Conc.	90
2	Pumps	Pump B Conc.	90
3	Pumps	Pump B Conc.	8
4	Controller	Stop	
5	0.00		
6	0.00		
7	0.00		
8	0.00		
9	0.00		
10	0.00		
11	0.00		

3. Draw curve

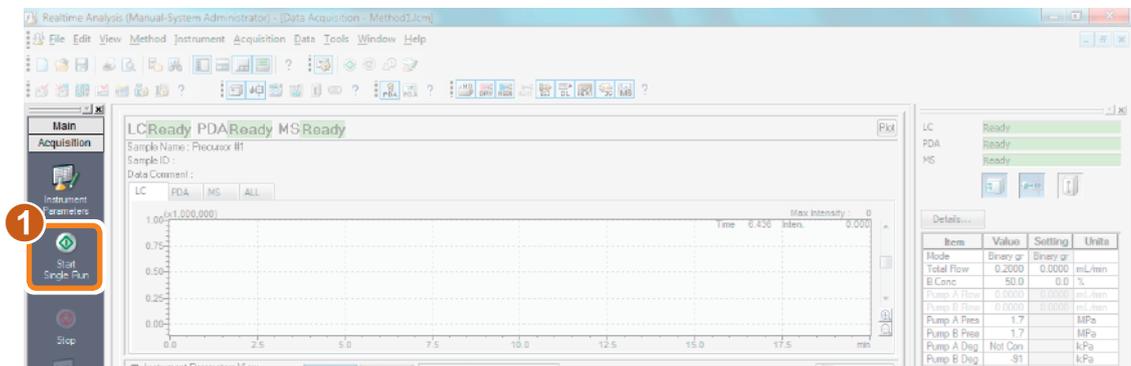
2.6 Execute Single Run to Determine Retention Time

1 Place the samples in the autosampler.

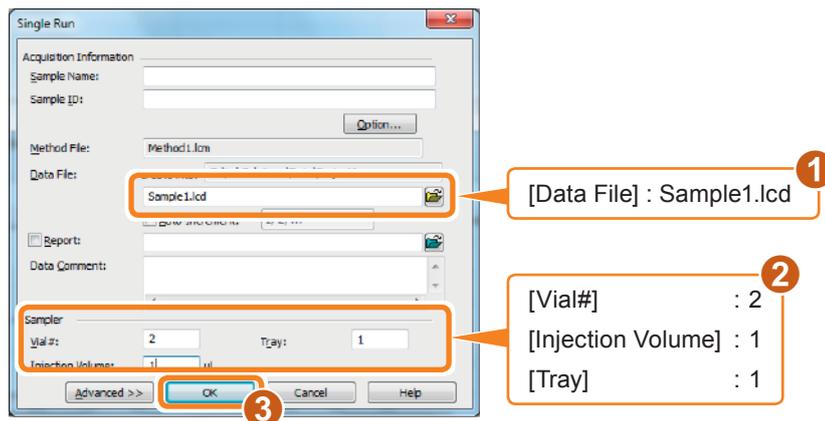
Vial 2, analytes A, B, C 0.05 ng/ μ L mixture



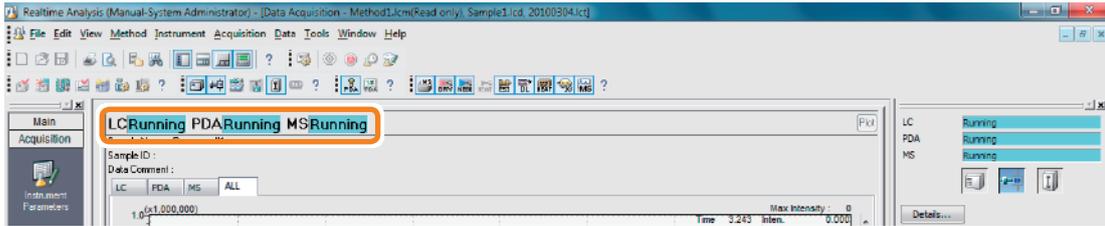
2 Open the [Single Run] sub-window.



3 Set the conditions for a single run.



3 Click [OK] to start the acquisition.

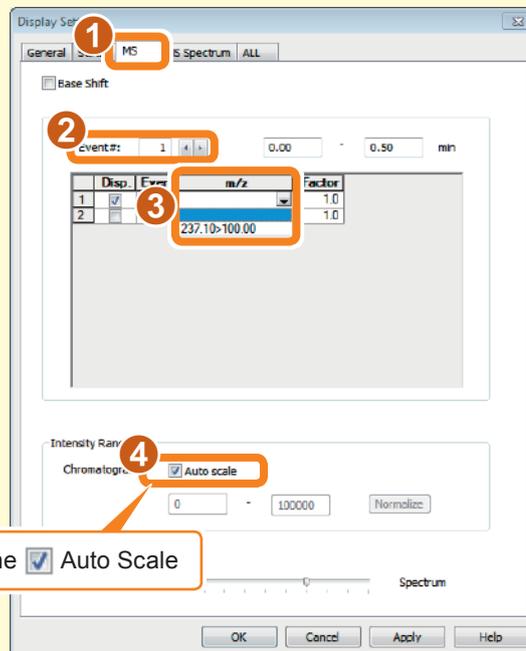


Data acquisition ends automatically when the [Acquisition Time] set in the method file has elapsed.

▼ 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].

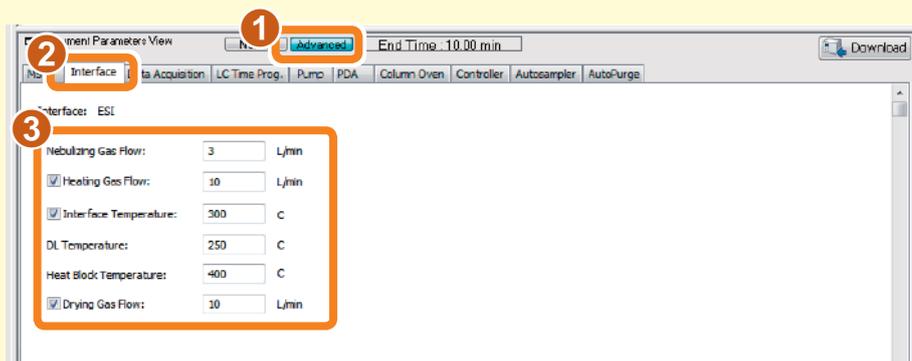


Select in the Auto Scale

▼ Tips

Set the interface temperature and the gas flow

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

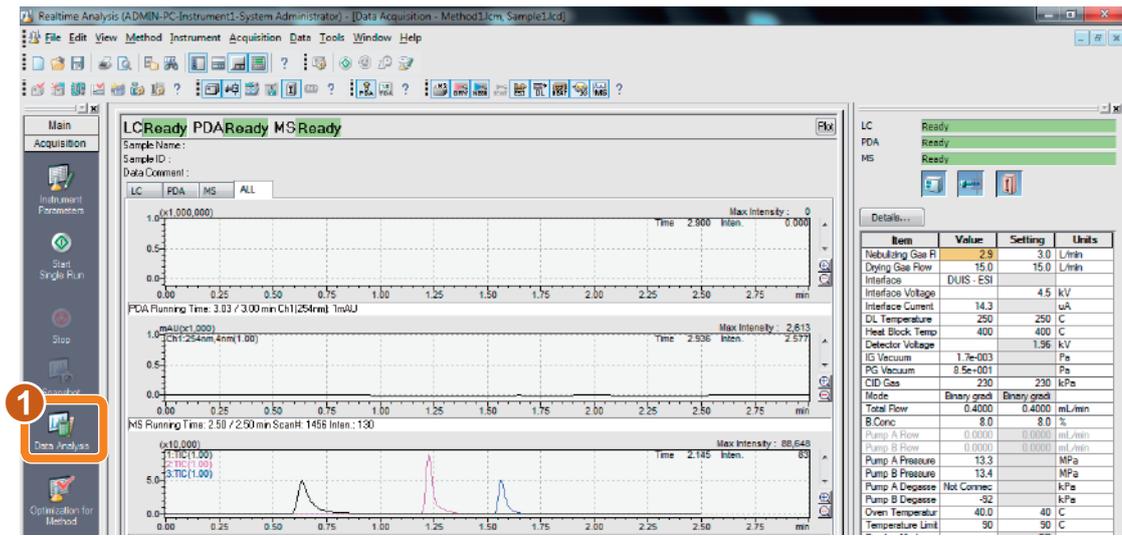


Chapter 3. Confirm Single Run Results

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

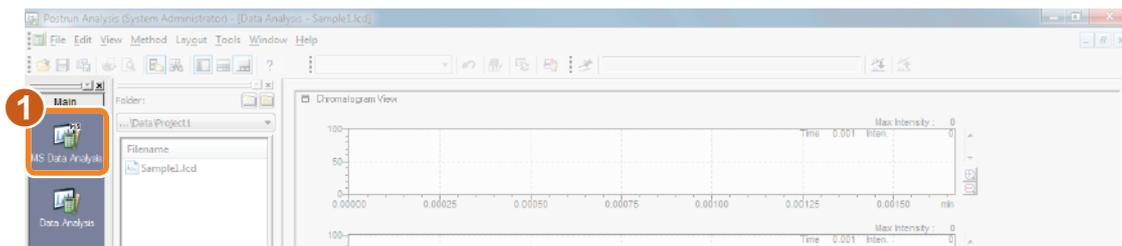
Display the results of single run in the [MS Data Analysis] window, and set the parameters for quantitative data acquisition.

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

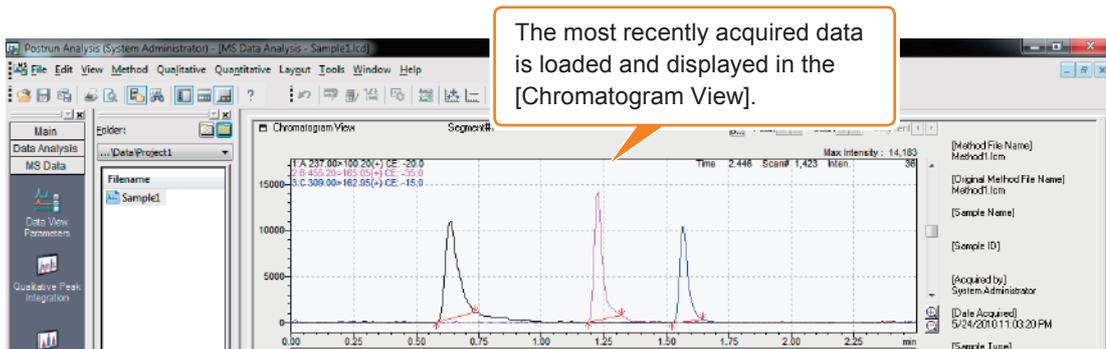


The [Postrun Analysis] program starts.

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



The [MS Data Analysis] window opens.

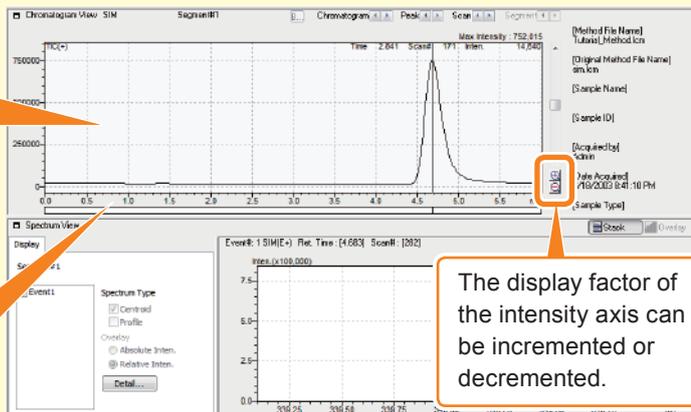


▼ Tips

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.

3.2 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].

4 [Slope] : 100

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

1 Edit

2 Integration

3 Advanced

Integration

Auto(Area) Auto(Height) Advanced

MaxPeak: 5

T. DBL: 1000 min

Min. Area/Height: 0 counts

Calculated by: Area Height

Smoothing

Method: Standard

Counts: 1

Width: 1 sec

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.

1 **Quantitative Method**: External Standard

2 **# of Calib. Levels**: 4

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

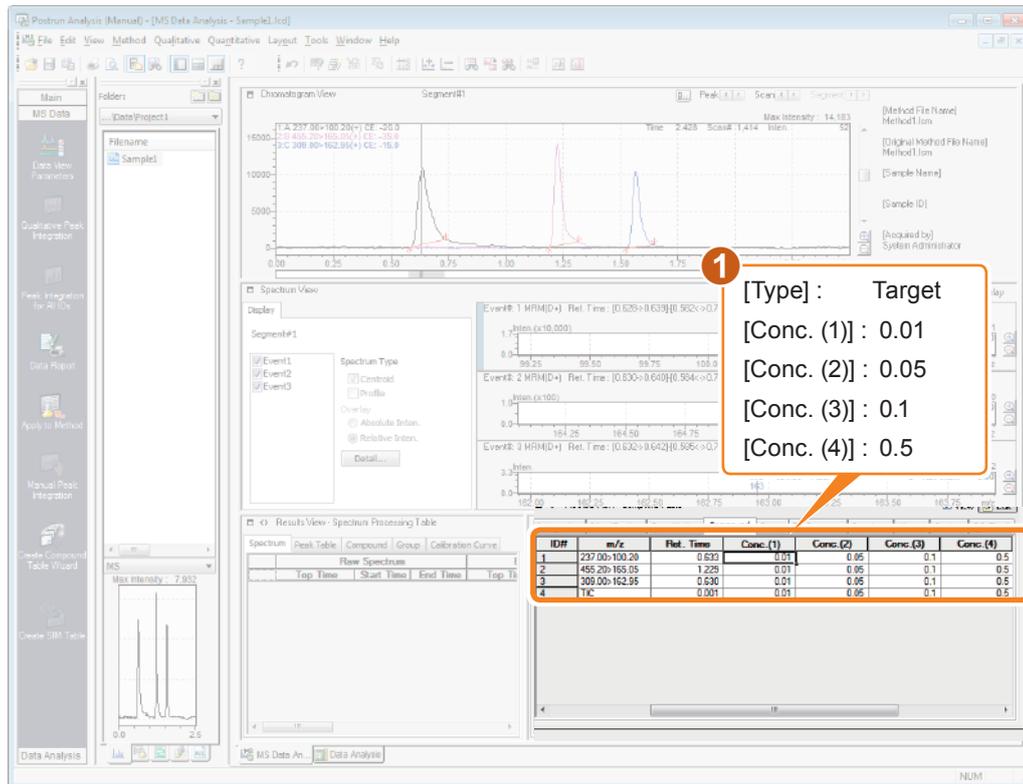
3 Click the peak in [Chromatogram View].

2 Click

4 The time is automatically entered.

ID#	Name	Type	Ret. Time	Conc. (1)	Conc. (2)
1	A	Target	237.00>100.20<>0.633	0.01	0.0
2	B	Target	455.20>165.0<>0.633	0.01	0.0
3	C	Target	309.00>162.95<>0.630	0.01	0.0
4		Target	TIC	0.001	0.0

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



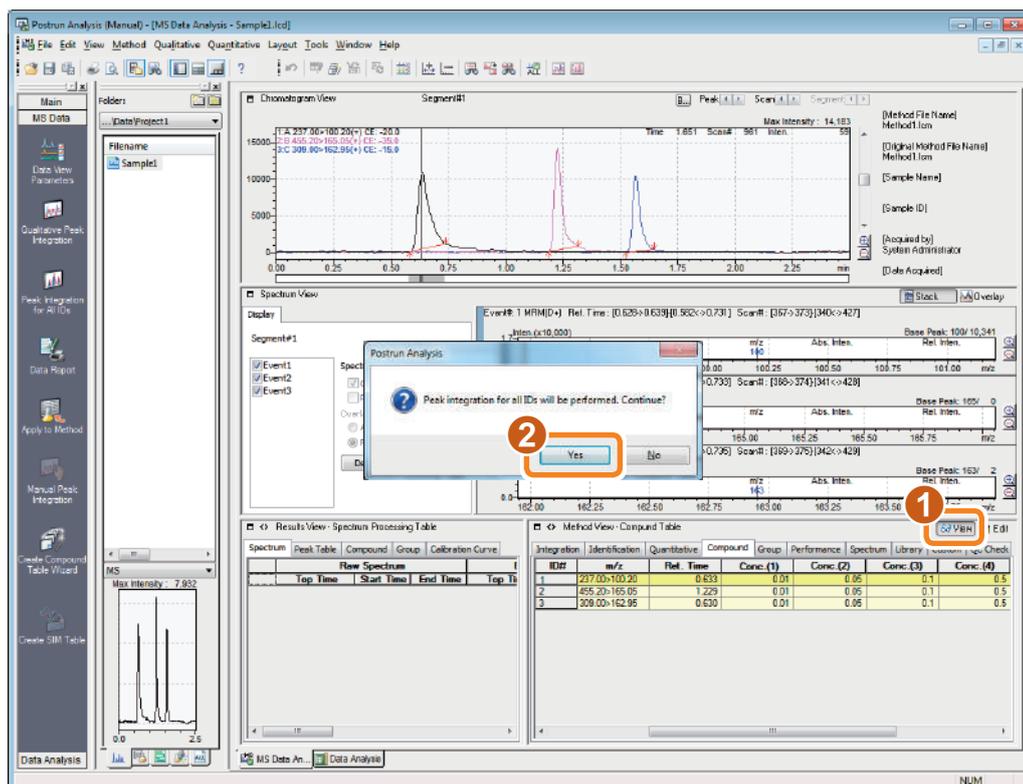
The screenshot shows the Postrun Analysis software interface. The 'Results View - Spectrum Processing Table' is visible, showing a table with columns for ID#, m/z, Ret. Time, and concentrations (Conc. (1) through Conc. (4)). A callout box labeled '1' points to the concentration values for the four peaks.

ID#	m/z	Ret. Time	Conc. (1)	Conc. (2)	Conc. (3)	Conc. (4)
1	237.00>100.20	0.630	0.01	0.05	0.1	0.5
2	455.20>165.05	1.225	0.01	0.05	0.1	0.5
3	309.00>162.95	0.630	0.01	0.05	0.1	0.5
4	116	0.001	0.01	0.05	0.1	0.5

Callout box content:

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

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



The screenshot shows the Postrun Analysis software interface. A dialog box is displayed over the 'Results View - Spectrum Processing Table'. The dialog box contains the text: "Peak integration for all IDs will be performed. Continue?". The 'Yes' button is highlighted with a callout box labeled '2'. The 'View' button in the bottom right corner of the software window is highlighted with a callout box labeled '1'.

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	0.630	0.01	0.05	0.1	0.5		
2	455.20>165.05	1.225	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.

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

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

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

Spectrum	Peak	Compound	Group
1	A	0.637	0.010
2	B	1.226	0.009
3	C	1.566	0.010

Integration	Identification	Quantitative	Compound	Group
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	

4 Confirm that "Method1" is selected.

5 Click Save.

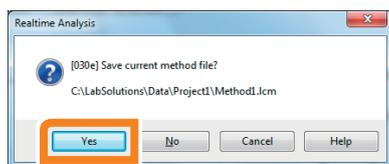
Hint If a peak is detected but not identified, check the retention time in the compound table and window width in the identification parameters.

6 Click OK.

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

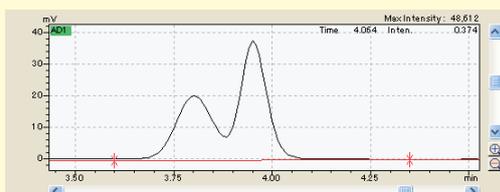
Simple Peak Integration Parameters

First set smaller values for the width and slope. Then double the values to confirm the peak detection status.

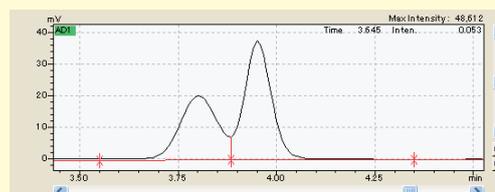
Setting a large width value prevents detection of peaks in background noise. Also, setting a large slope value prevents detection of peaks in slow baseline undulations.

Repeat the above setting adjustments until no unwanted peaks are detected, then use those settings as the peak integration parameters.

Width Setting Example

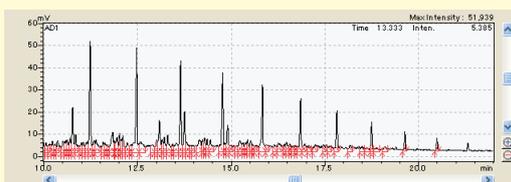


With the [Width] set to 30, the data is processed as one peak.

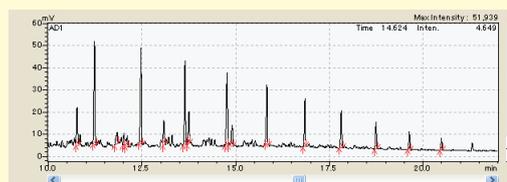


With the [Width] set to 10, the data is processed as two peaks.

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.

3.3 Print Results

Print the Information Displayed in the Window



The screenshot displays the Postrium Analysis software interface. The main window is titled "Postrium Analysis (Manual) - [MS Data Analysis - Sample1.Lcd]". The toolbar at the top includes a print icon, which is highlighted by a callout box labeled "1 Click". The interface is divided into several panels:

- Chromatogram View:** Shows a chromatogram with three peaks. The x-axis is labeled "Time" and ranges from 0.00 to 2.25 minutes. The y-axis is labeled "Intensity" and ranges from 0 to 15000. The peaks are labeled with their retention times: 1.237, 1.522, and 1.574 minutes.
- Spectrum View:** Displays three mass spectra corresponding to the peaks in the chromatogram. Each spectrum shows intensity versus m/z. The x-axis ranges from approximately 100 to 180 m/z. The y-axis is labeled "Intensity" and ranges from 0.0 to 1.0 (x1000).
- Results View - Spectrum Processing Table:** A table with columns for "Spectrum", "Peak Table", "Compound", "Group", "Calibration Curve", "Row Spectrum", and "Background Spectrum". The table is currently empty.
- Method View - Peak Integration Parameters:** A panel for configuring peak integration parameters. It includes fields for "MaxPeaks" (set to 5), "Width" (set to 5 sec), "Slopes" (set to 100 /min), "Drift" (set to 0 /min), "T. DBL" (set to 1000 min), and "Min. Area/Height" (set to 0 counts).

Graphic Image Printout Example

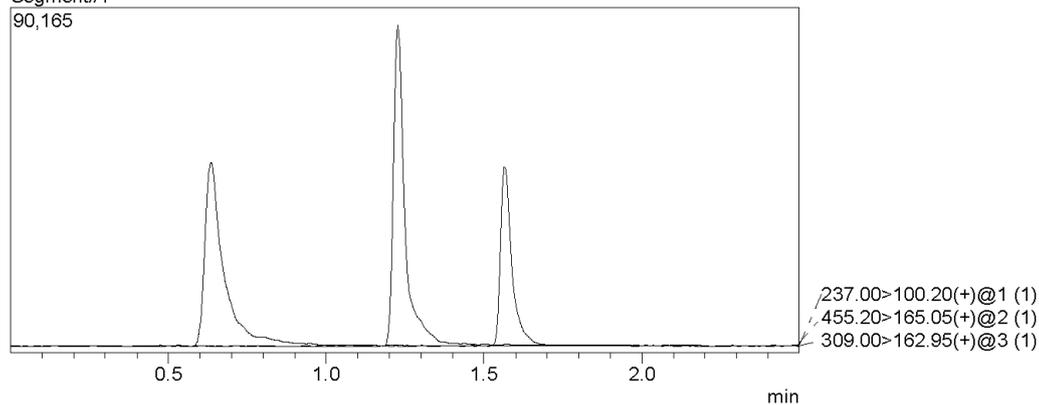
==== Shimadzu Labsolutions Data Report ====

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

<Chromatogram>

Segment#1

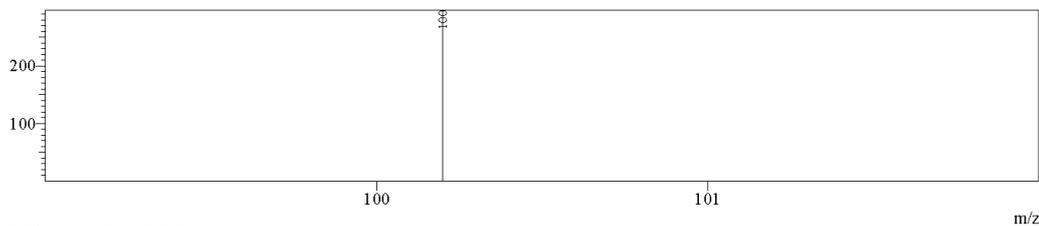
90,165



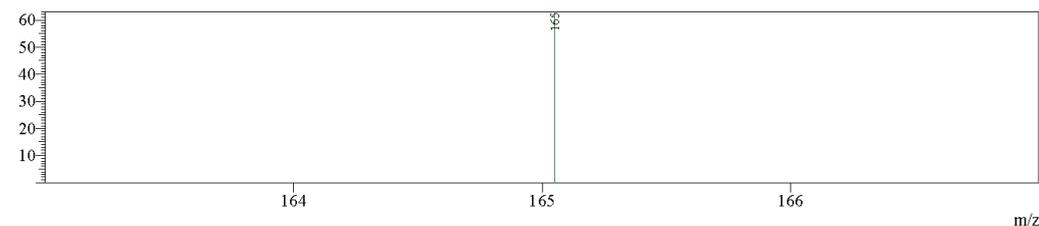
237.00>100.20(+>@1 (1)
455.20>165.05(+>@2 (1)
309.00>162.95(+>@3 (1)

<Spectrum>

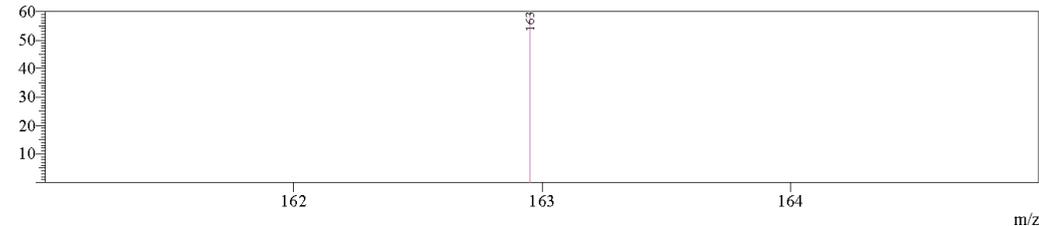
R.Time:0.999(Scan#:583)
MassPeaks:1 BasePeak:100(297)
Polarity:Positive Segment 1 - Event 1



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.

Click

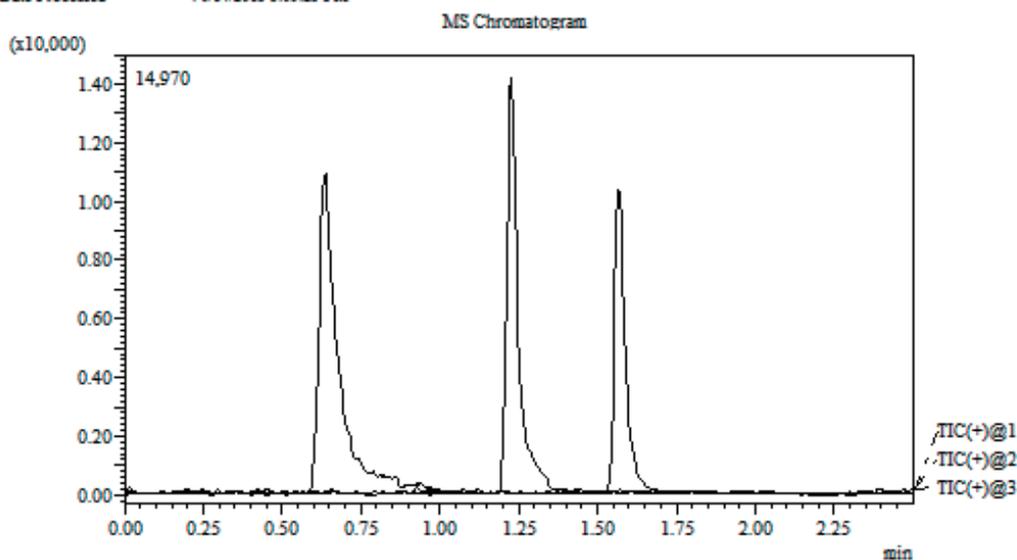
4

3 Drag and drop the file to the layout view frame at the right.

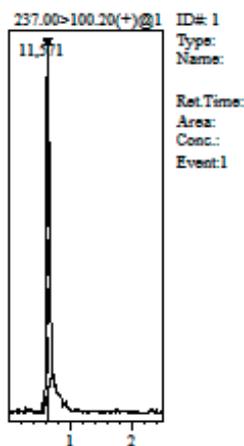
Report Format Printout Example

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.icd
 Method File : Method1.icm
 Original Method File : Method1.icm
 Report Format File : DEFAULT.rpt
 Tuning File : Tuning.txt
 Processed by : Manual
 Date Processed : 6/14/2013 3:09:25 PM

Sample Information

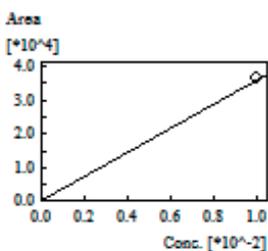


Mass Quant Graph



m/z: 237. ID# : 1 m/z : 237.00>
 Name : A
 Target Function : $f(x)=3.61950e+006*x+0$
 A $R^2=1.000000$ $R^2=1.000000$
 MeanRF: 3.619502e+006 RF SD: 0.000000e+000 RF %RSD: 0.000000
 FitType : Linear
 ZeroThrough : Not Through
 Weighted Regression : 1/C^2
 Quantitation Method : External Standard

Calibration Curve



#	Conc.(Ratio)
1	0.01

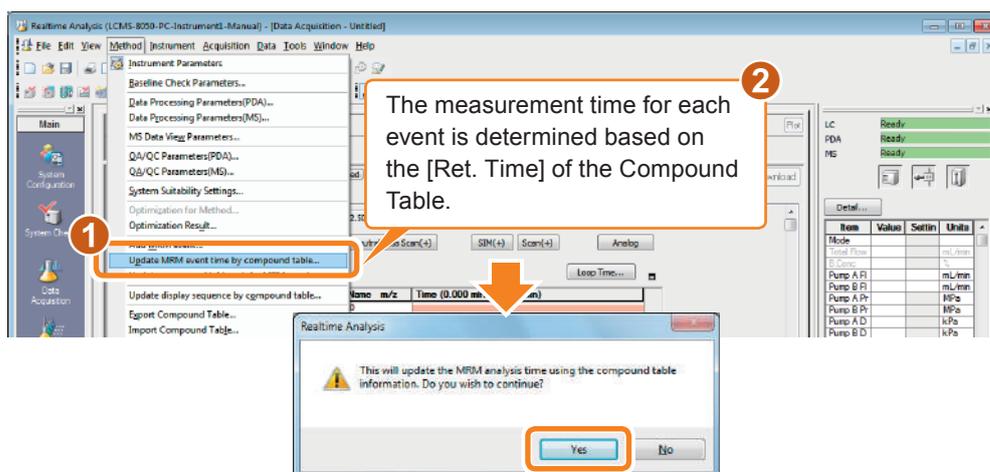
MeanArea	Area
36195	36195

Chapter 4. Realtime Batch

4.1 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.

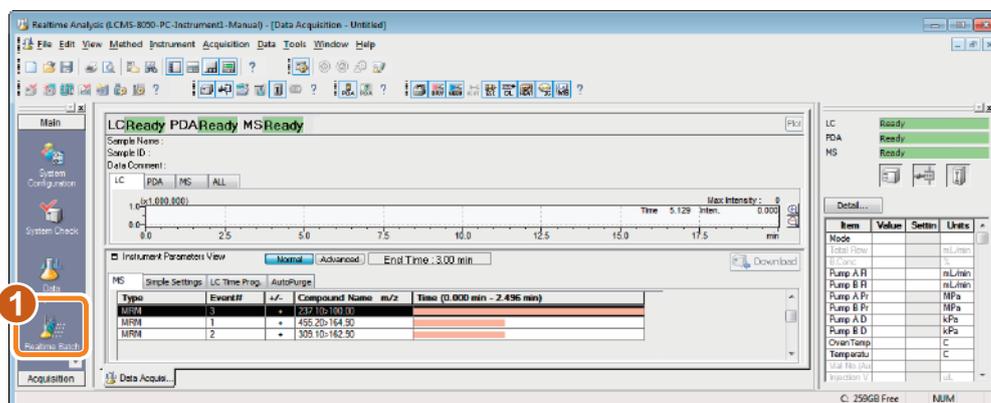
The start time of measurement = [Ret. Time]

- [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.



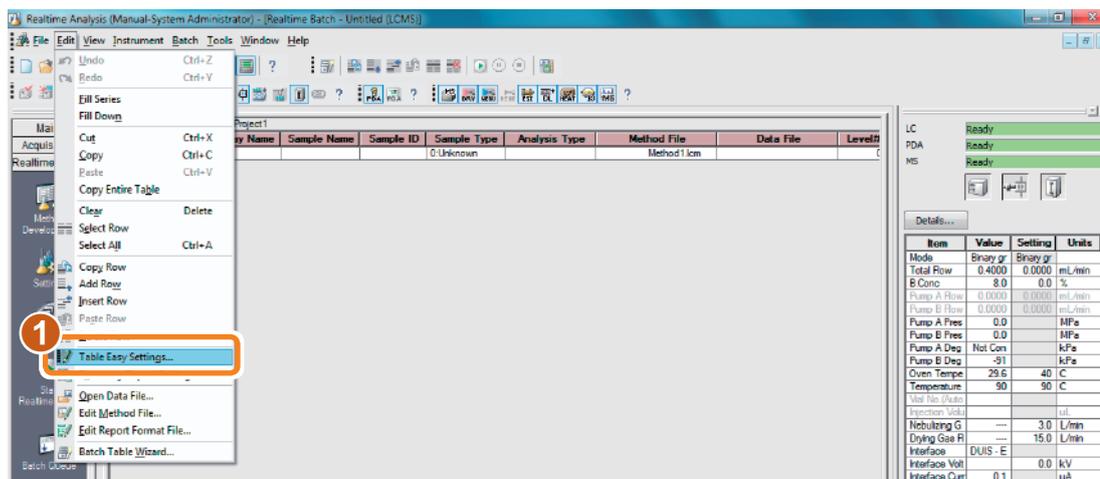
The [Batch Table] window is displayed.

Create the Batch Table using the following procedure.

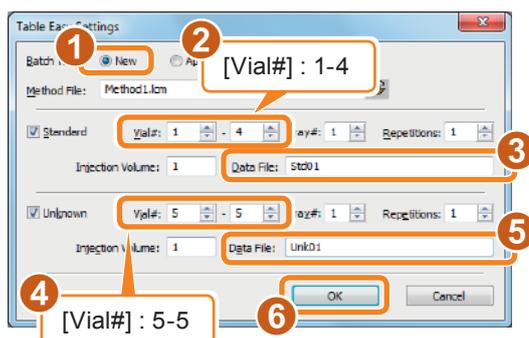
Use the first four rows for the standard sample and the

fifth row for the unknown sample.

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

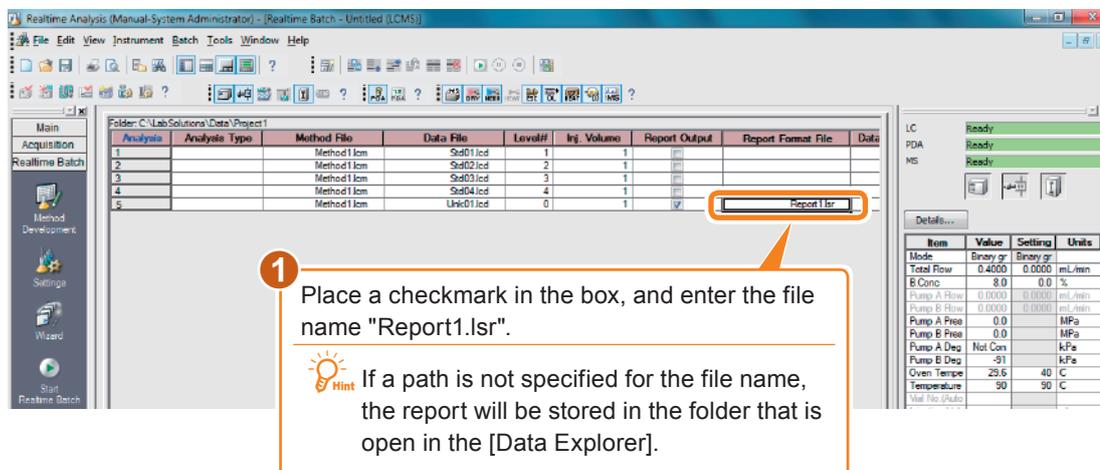


4 Make the following settings on the [Table Easy Settings] sub-window.

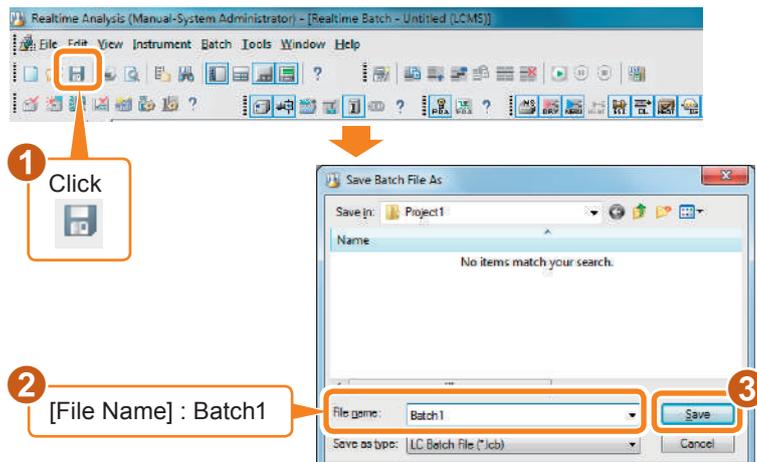


A five-row Batch Table is created.

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



6 Save the Batch Table settings.

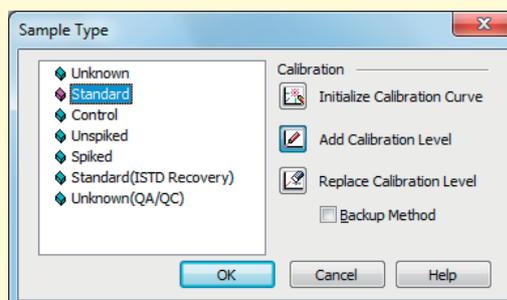


▼ Tips

Batch Table Settings

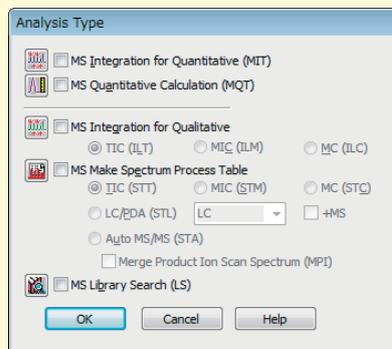
Sample Type

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 and PDA data.



Level Number

Enter a level number for all of the standard samples.

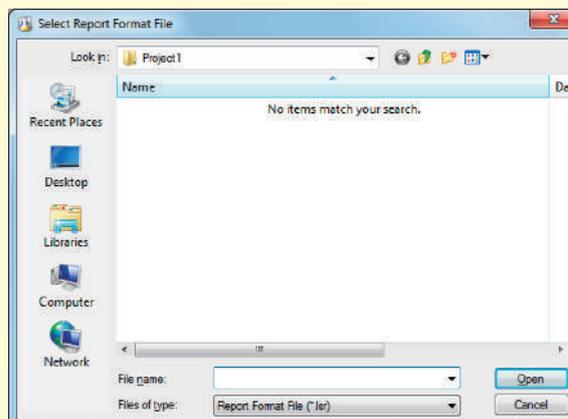
Report Output

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.



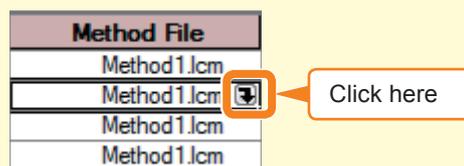
Help

▼ Tips

Table Entries

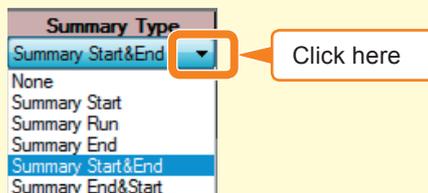
Popup Windows (for complex settings)

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.



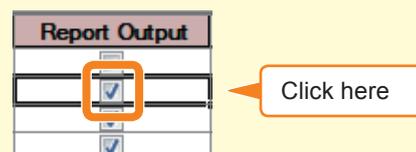
Drop-Down List (to select from a list of choices)

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)

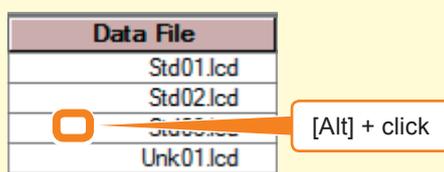
Click the displayed check box to select or clear a checkmark.



[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.

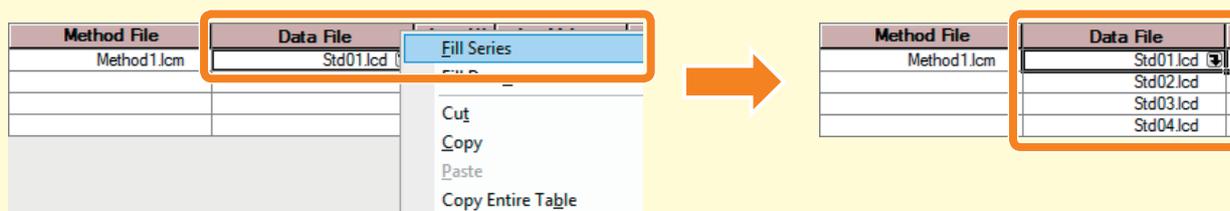


▼ Tips

Fill Series and Fill Down

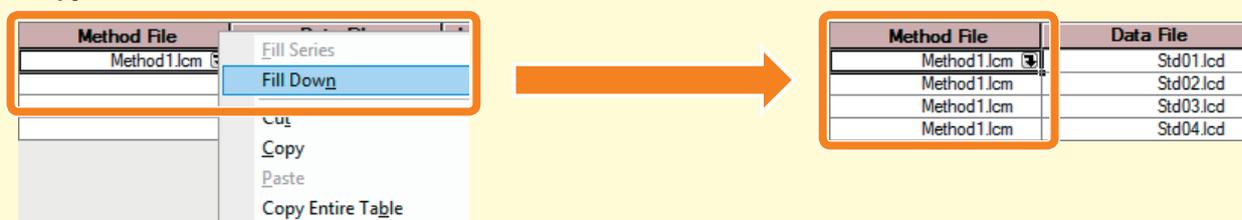
Use the right-click menu on the Batch Table to select [Fill Series] to enter a numbered series or [Fill Down] to copy a particular cell entry to the rest of the cells in the column.

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.

Create a Batch Table Using Quick Batch

You can also create a Batch Table using quick batch.

1 Click **Quick Batch...**

2 Enter the sample information.

3 Select a sample type and vials.

4 Click **Add Batch Table**

5 Start 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.

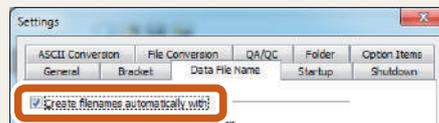
Editor	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	File	Date
				0	Unknown		(Auto)



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.



4.2 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/ μ L each (standard sample)

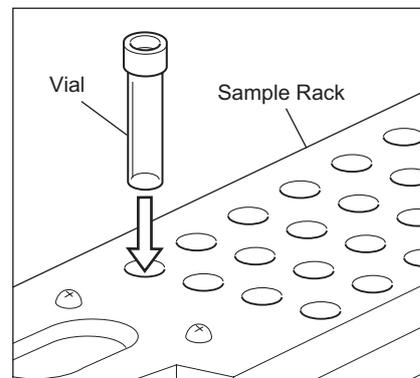
Vial 2, sample solution containing A, B, C at 0.05 ng/ μ L each (standard sample)

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

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

Vial 5, unknown (to be quantitated) sample

In this example, a sample solution containing A, B, C at 0.075 ng/ μ L 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.

Analysis	Analysis Type	Method File	Data File	Level#	Inj. Volume	Report Output	Report Format File	Data
1		Method1.lcm	Std01.lcd	1	1			
2		Method1.lcm	Std02.lcd	2	1			
3		Method1.lcm	Std03.lcd	3	1			
4		Method1.lcm	Std04.lcd	4	1			
5		Method1.lcm	Unk01.lcd	0	1		Report1.rpt	

Hint Click to stop batch processing.

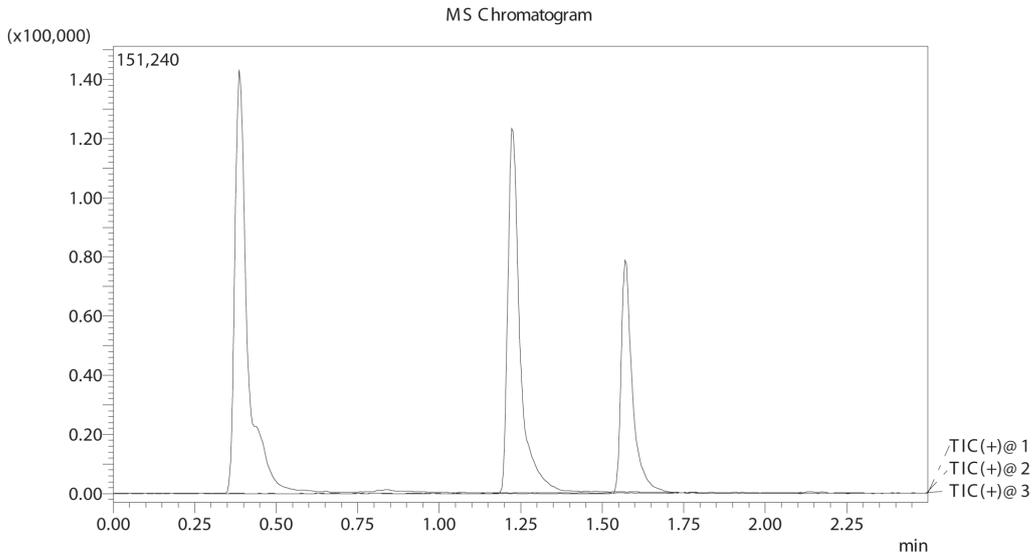
Hint By pausing the Batch Table, modifications can be made while measurements for the current analysis continue.

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

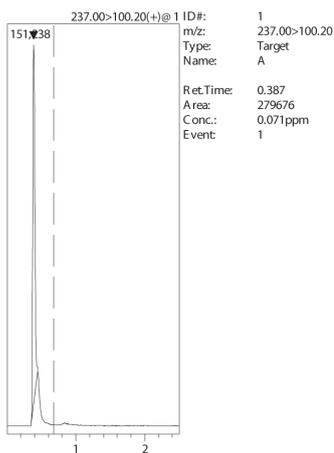
Realttime Batch Report Printout Example

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

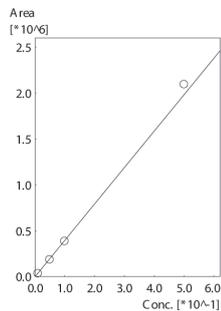


Mass Quant Graph

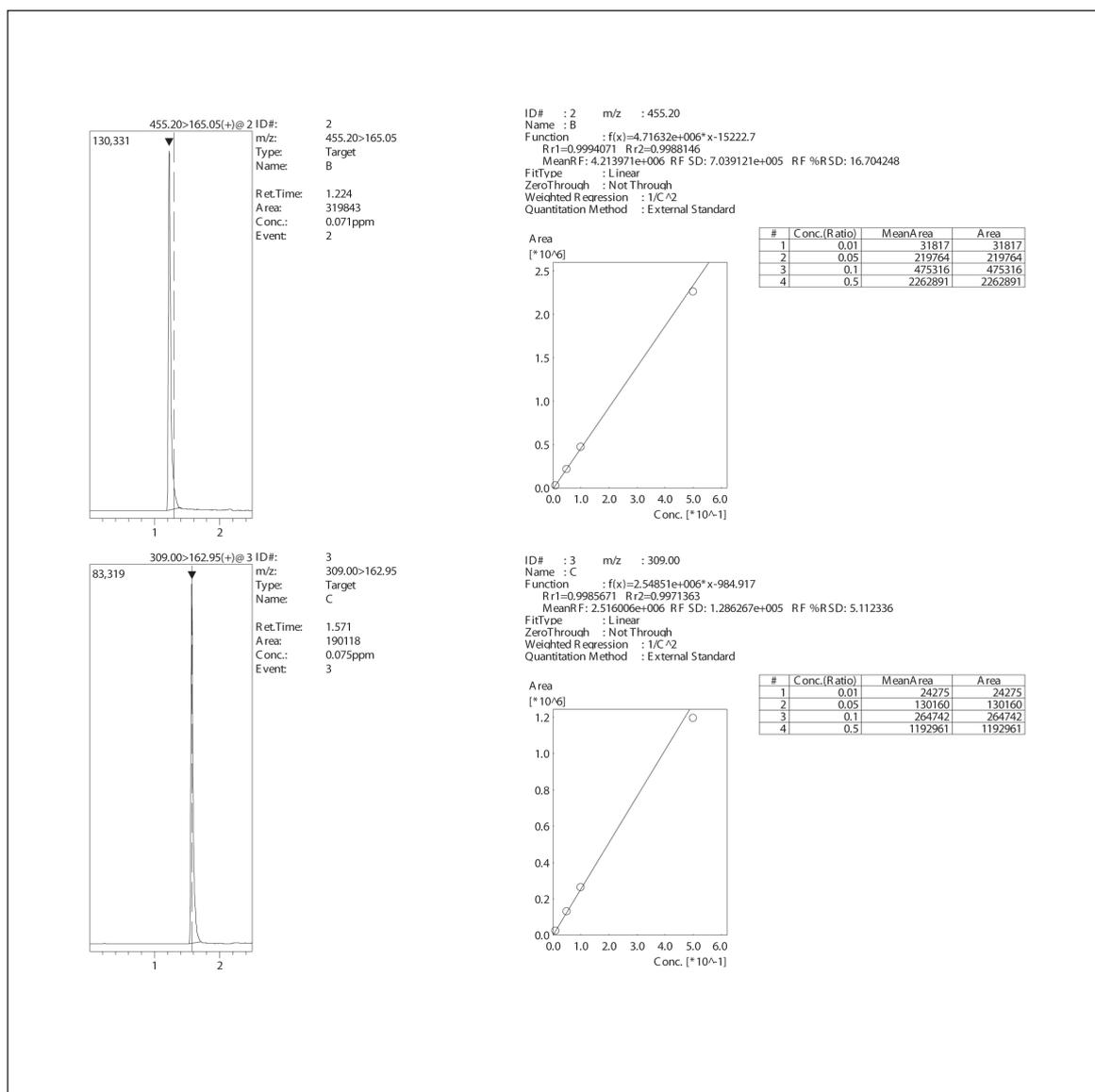


Calibration Curve

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



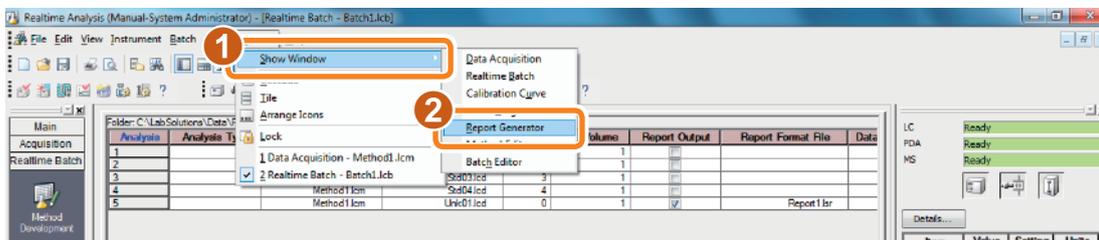
This example report for unknown sample (vial 5) shows the quantitated values for A, B and C. Also shown are the method calibration curves for A, B and C.

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

4.3 Print Batch Processing Reports

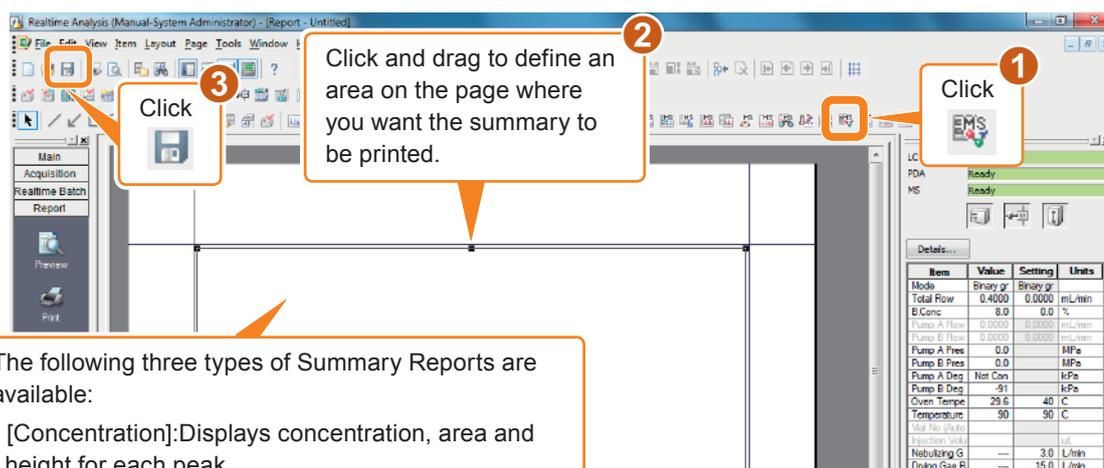
Prints a batch processing summary report (a simple combined report of two or more sets of analysis results).

1 Open the [Report] window.



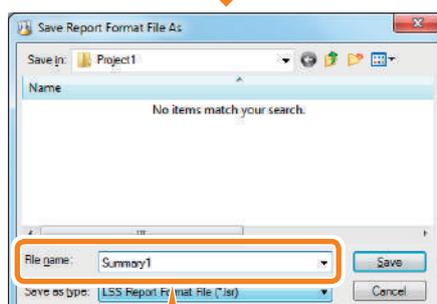
2 Create a summary report format with the [MS Summary (Compound)] report item.

Reference "8.4 Create a Report Format File" in *Operators Guide*.



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.



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.

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.

Hint 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.

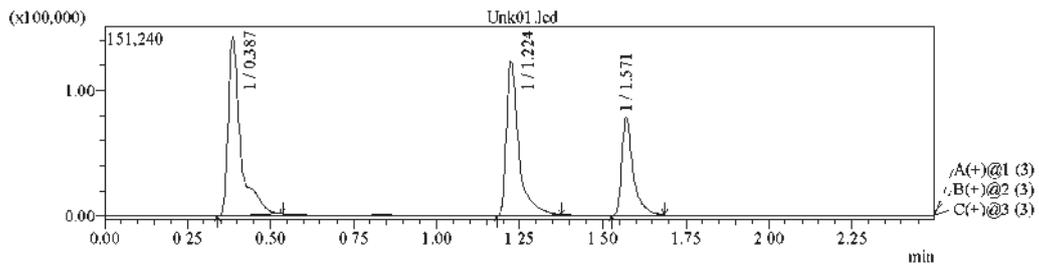
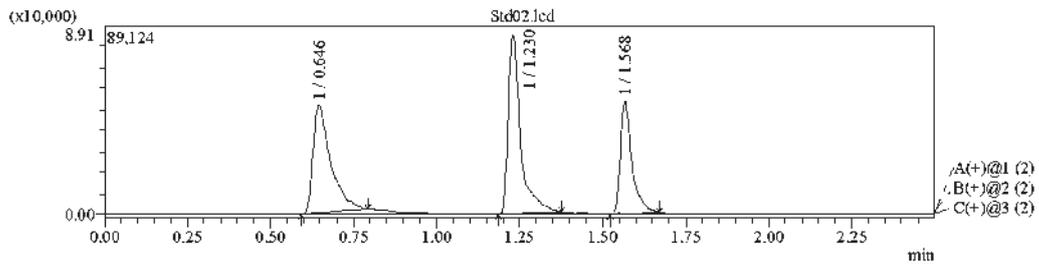
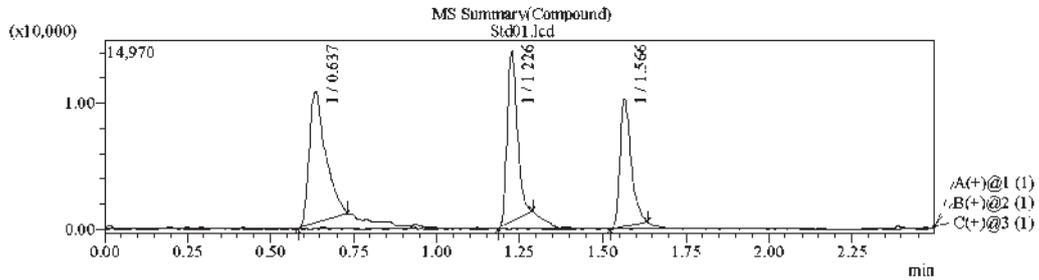
4 Start realtime batch processing.

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

Item	Value	Setting	Units
Mode	Binary gr	Binary gr	
Total Flow	0.2000	0.2000	mL/min
B.Conc	50.0	50.0	%
Pump A Flow	0.0000	0.0000	mL/min
Pump B Flow	0.0000	0.0000	mL/min
Pump A Pres	0.0		MPa
Pump B Pres	0.0		MPa
Pump A Deg	Not Con		kPa
Pump B Deg	-32		kPa
Oven Temp	29.4	0	C
Temperatur	90	90	C
Val No (Auto)			
Injection Volu			uL
Nebulizing G	---	3.0	L/min
Drying Gas Fl	---	15.0	L/min
Interface	DUIS - E		
Interface Volt	0.0		kV
Interface Curr	0.1		uA
DL Temperat	39	250	C
Heat Block T	45	400	C
Detector Volt	---	0.00	kV
IG Vacuum	---		Pa
PG Vacuum	1.9e+00		Pa
CID Gas	17	17	kPa

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

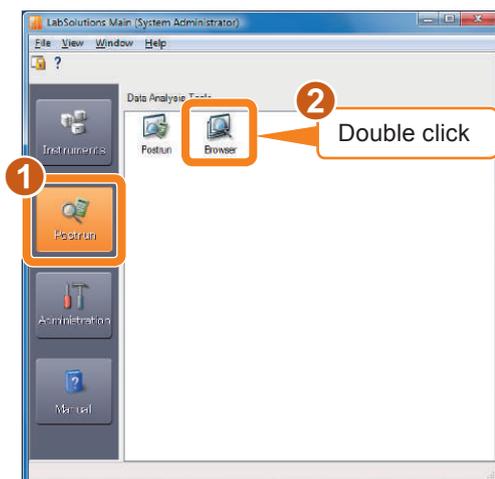
Title	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Std01.lcd			1.566	23534	10163	0.009
Std02.lcd			1.568	127900	53366	0.049
Unk01.lcd			1.571	186467	78613	0.073
Average			1.568	112634	47381	0.044
%RSD			0.164	73.275	73.058	73.335
Maximum			1.571	186467	78613	0.073
Minimum			1.566	23534	10163	0.009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

Chapter 5. Quantitative Data Analysis

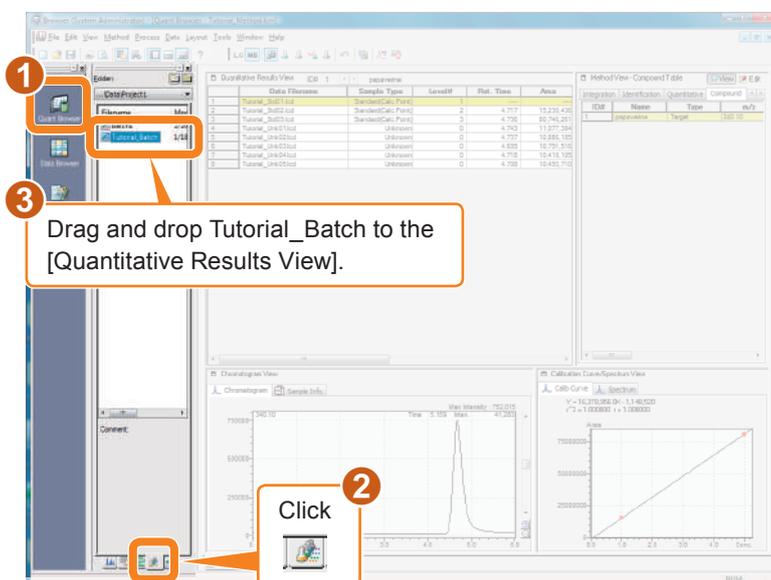
5.1 Confirm Quantitative Results in the [Quant Browser] Window

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

1 Start the [Browser] program.



2 Load the sample data.

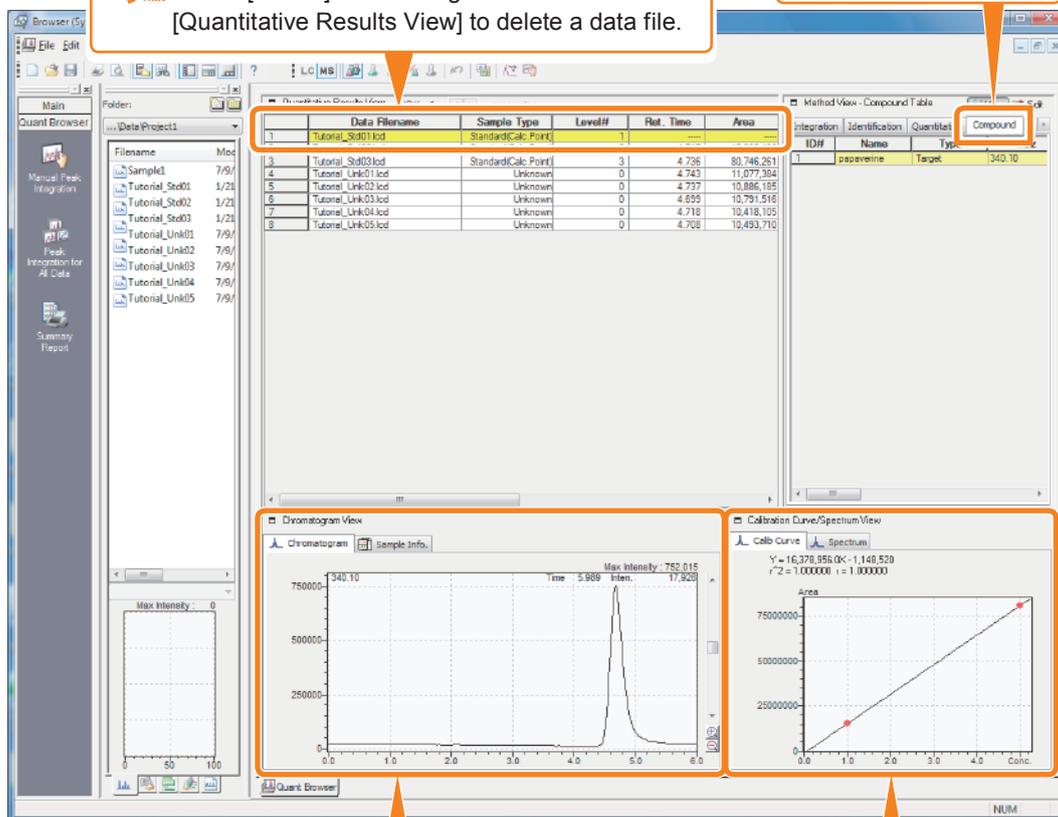


Sample data (Tutorial_Std01.lcd to Tutorial_Std03.lcd and Tutorial_Unk01.lcd to Tutorial_Unk05.lcd) registered in the batch file are opened.

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.
 -  **Hint** 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.

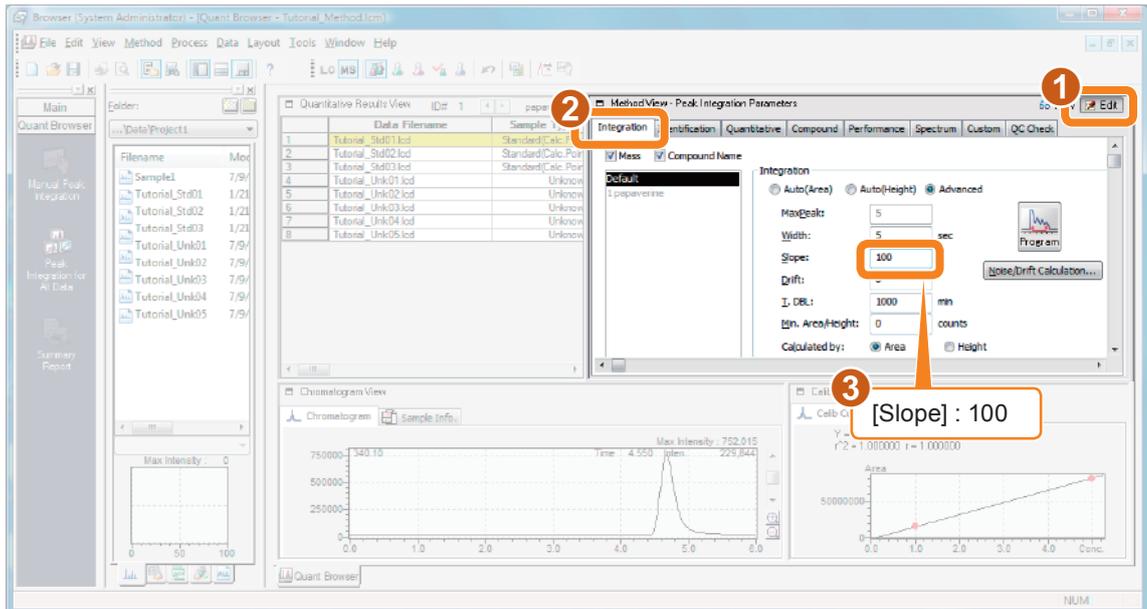
The calibration curve of the selected compound in the [Method View] is displayed.

5.2 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.

 **Reference** "13.3 Postrun Analysis of Multiple Data" in *Operators Guide*.



The screenshot displays the Quant Browser software interface. The 'Method View - Peak Integration Parameters' dialog box is open, showing the 'Integration' tab. The 'Slope' parameter is set to 100, which is highlighted with a red box and labeled '100'. A callout box points to the 'Slope' field with the text '[Slope] : 100'. The 'Integration' tab is selected, and the 'Advanced' radio button is chosen. The 'Quantitative Results View' shows a table of data points, and the 'Chromatogram View' shows a peak at 4.550 minutes.

ID#	Filename	Sample	Calc. P
1	Tutorial_Std01.lcd	Standard	Calc. P
2	Tutorial_Std02.lcd	Standard	Calc. P
3	Tutorial_Std03.lcd	Standard	Calc. P
4	Tutorial_Unk01.lcd	Unknown	
5	Tutorial_Unk02.lcd	Unknown	
6	Tutorial_Unk03.lcd	Unknown	
7	Tutorial_Unk04.lcd	Unknown	
8	Tutorial_Unk05.lcd	Unknown	

2 Re-integrate



Original 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	-----



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.



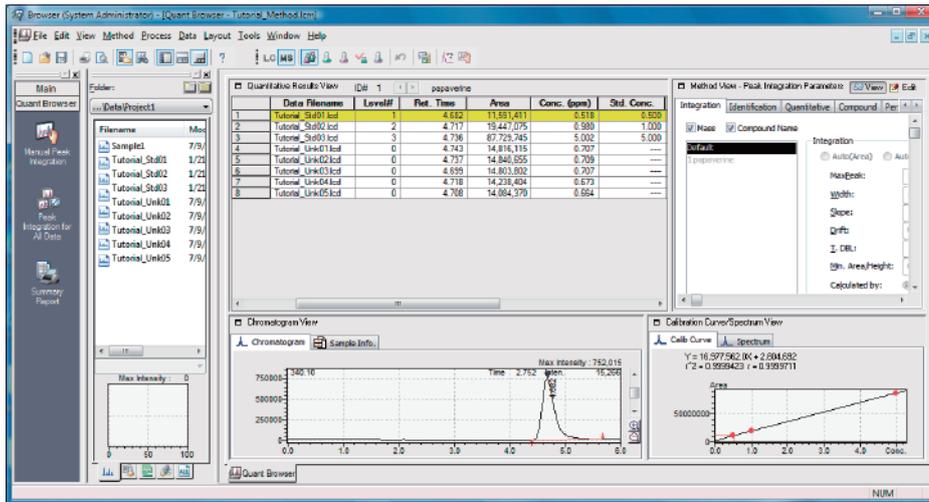
Integration can be initiated manually in the [Chromatogram View]. Select [Manual Integration Bar] from the right-click menu.



"7.5.6 Manual Quantitative Peak Integration" in *Operators Guide*.

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.

 **Hint** 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	0.51
2	Tutorial_Std02.lcd	Standard(Calc. Point)	2	4.717	19,447,075	0.98
3	Tutorial_Std03.lcd	Standard(Calc. Point)	3	4.736	87,725,745	5.01
4	Tutorial_Unk01.lcd	Unknown	0	4.743	14,816,115	0.71
5	Tutorial_Unk02.lcd	Unknown	0	4.737	14,840,655	0.71
6	Tutorial_Unk03.lcd	Unknown	0	4.699	14,803,802	0.71
7	Tutorial_Unk04.lcd	Unknown	0	4.718	14,238,404	0.67
8	Tutorial_Unk05.lcd	Unknown	0	4.708	14,084,370	0.66

■ 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.

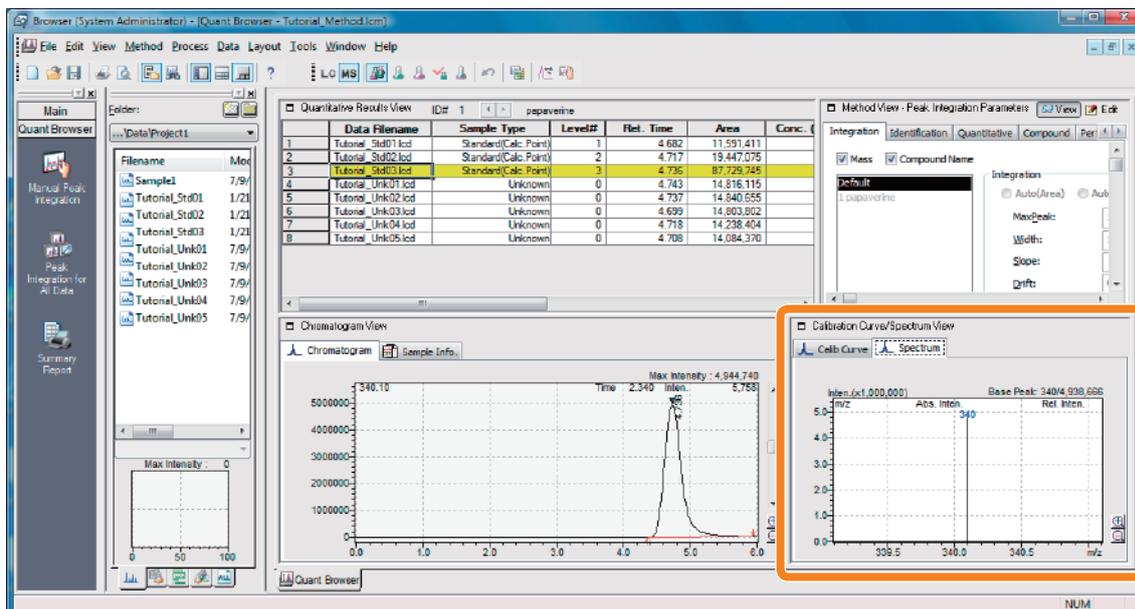
 **Hint** Changes to the [Sample Type] are reflected in the files when saved.

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	87,725,745
4	Tutorial_Unk01.lcd	Unknown	0	4.743	14,816,115
5	Tutorial_Unk02.lcd	Standard(No 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	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 post-run analysis on multiple loaded data sets using the data processing parameters of that method.

Files are loaded according to the following rules.

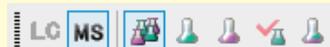
Method File

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.

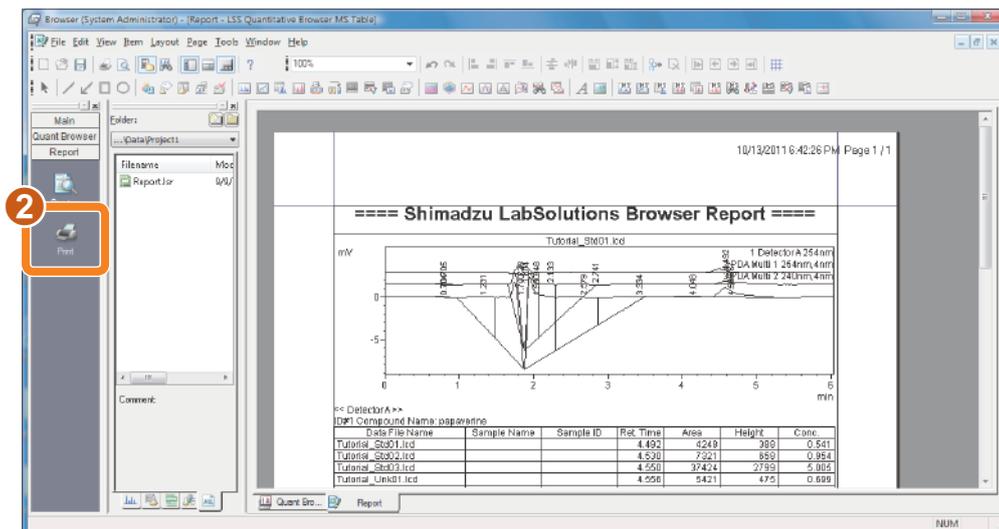
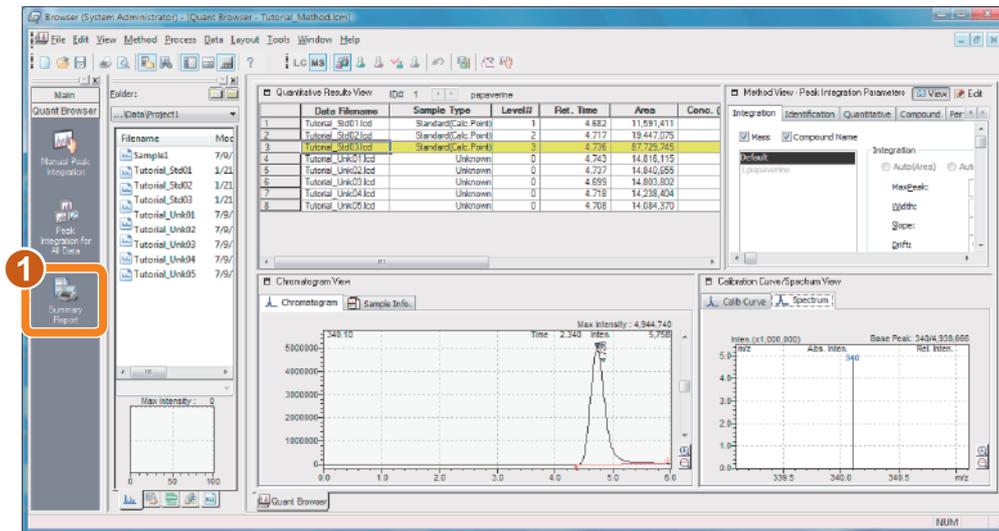
Data Files

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.



5.3 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 6. Qualitative Data Analysis

6.1 Display Data Files in the [Data Browser] Window

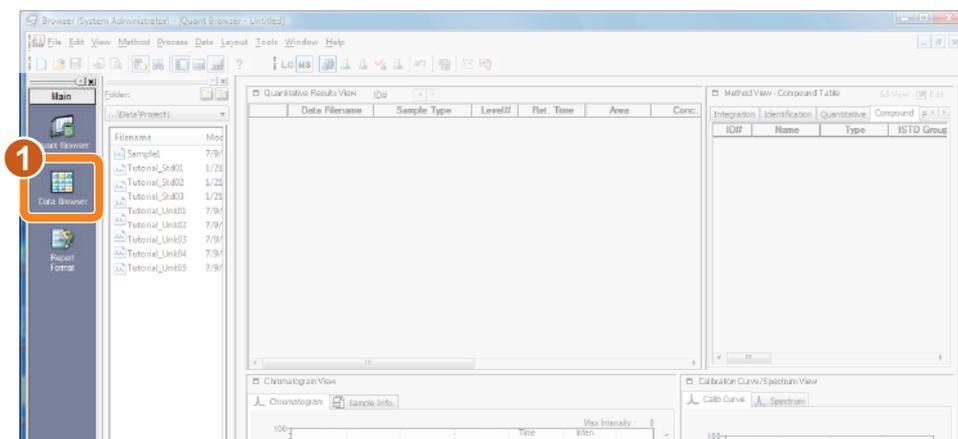
The [Data Browser] window can be used to display chromatograms, spectra and multiple data file information from different detectors, such as MS or PDA, in various formats.

 **Reference** "14.4 Compare Data" in *Operators Guide*.

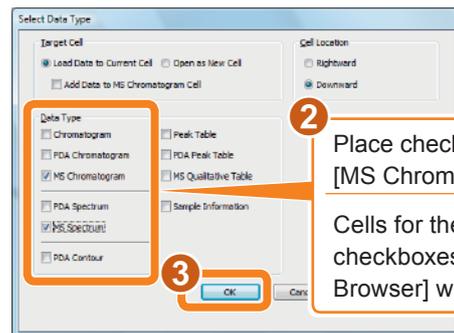
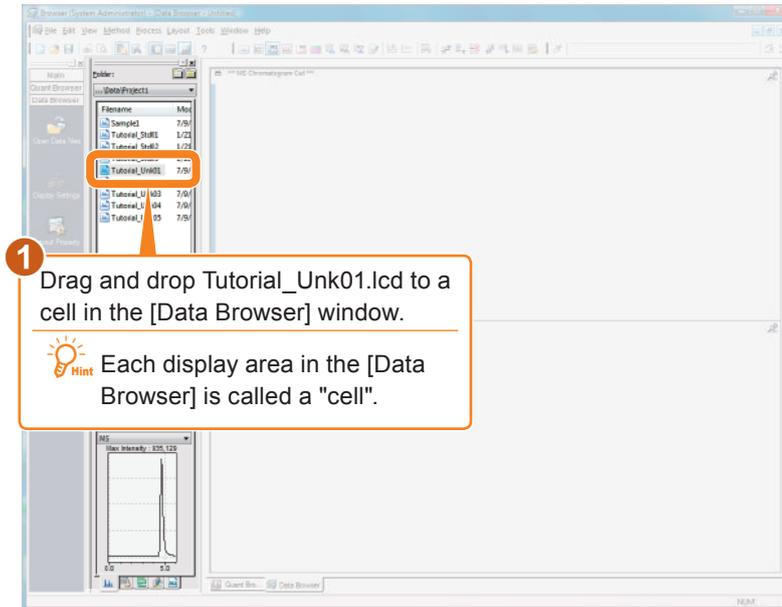
1 Start the [Browser] program.



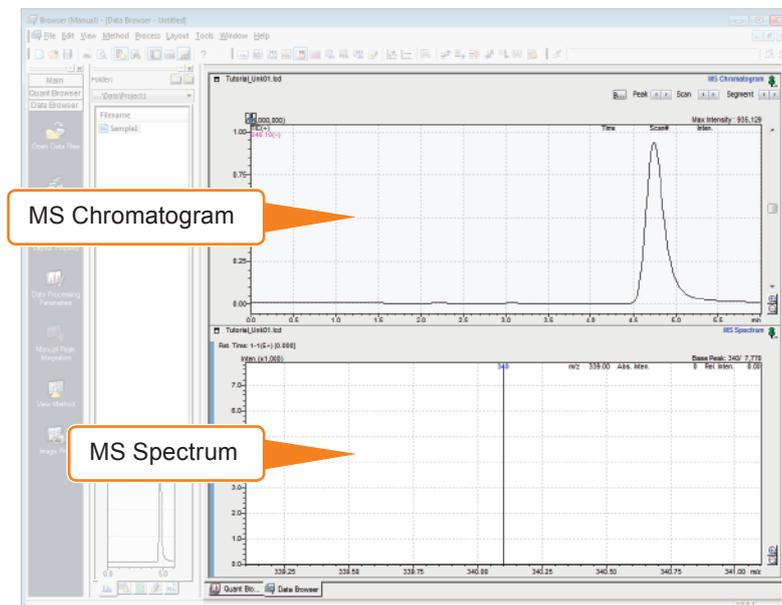
2 Open the [Data Browser] window.



3 Select a data file.



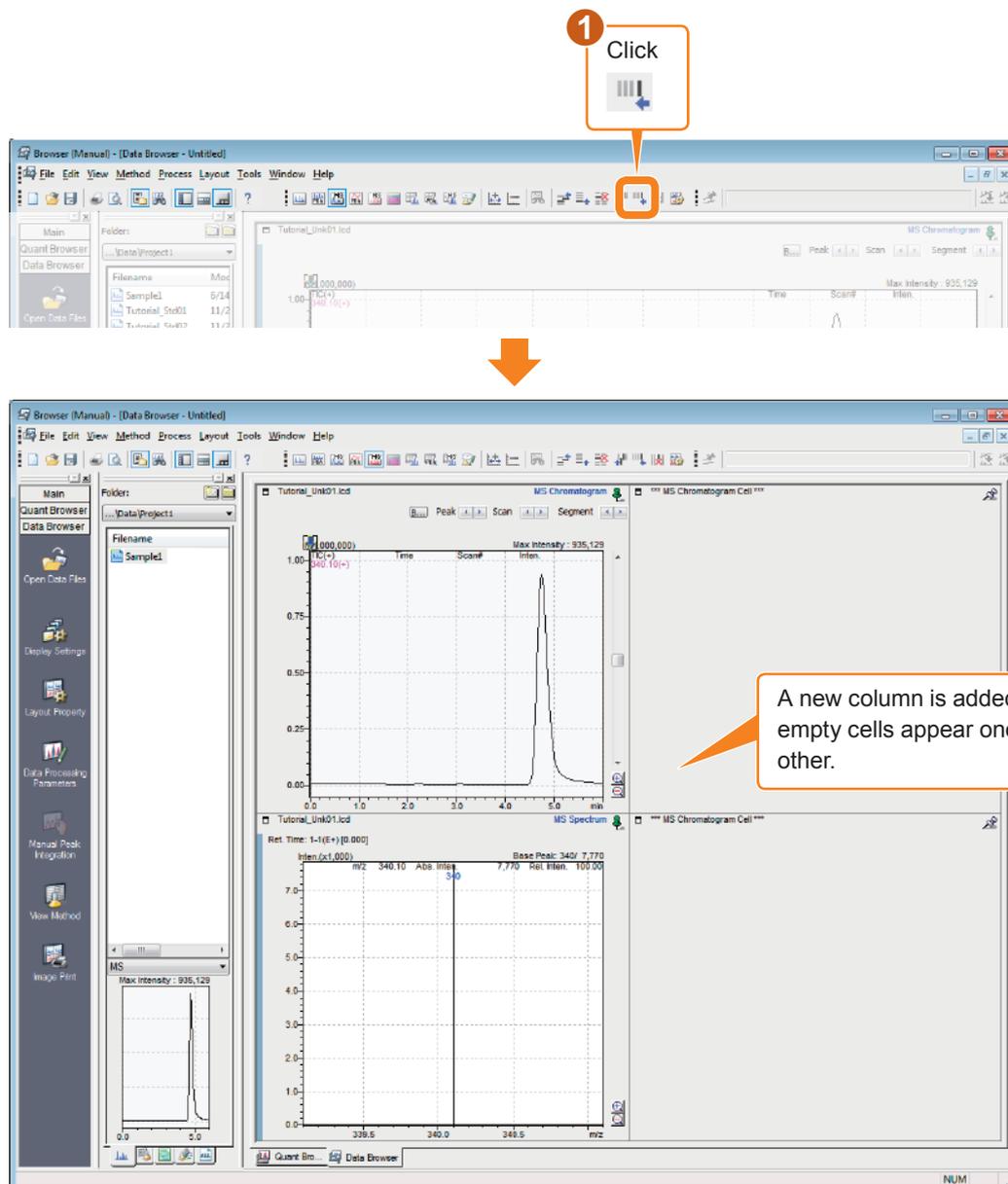
The MS chromatogram and MS spectrum are displayed.
Double click a point on the MS chromatogram to display the MS spectrum at that point.



6.2 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.

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.

3 Change the data type.

2 Click 

1 Click on the cell whose data type is to be changed to move the focus to this cell.

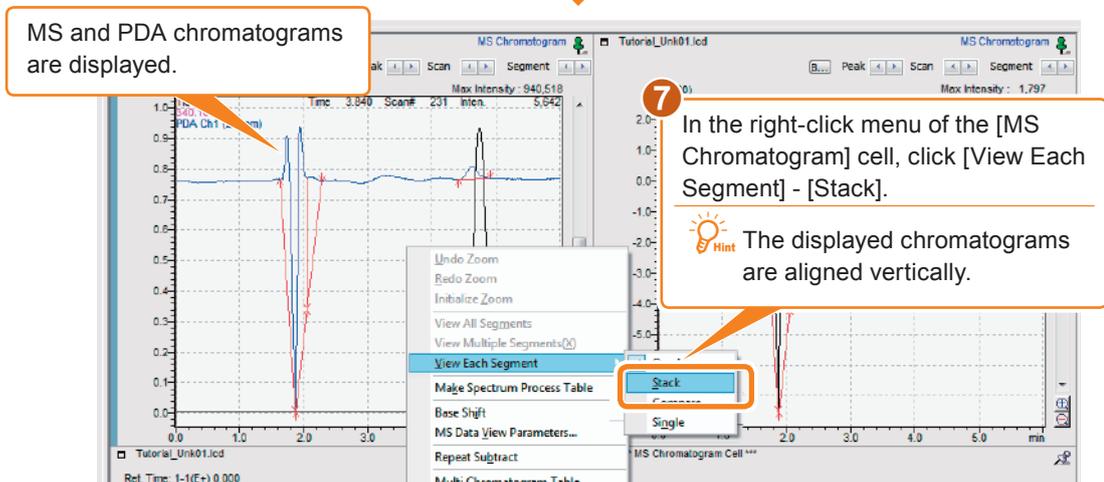
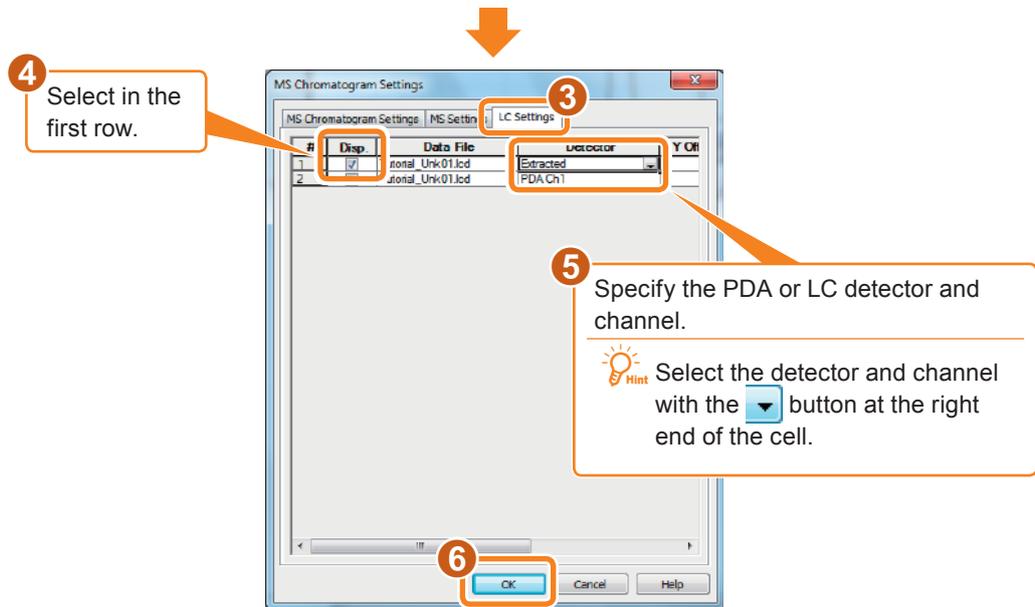
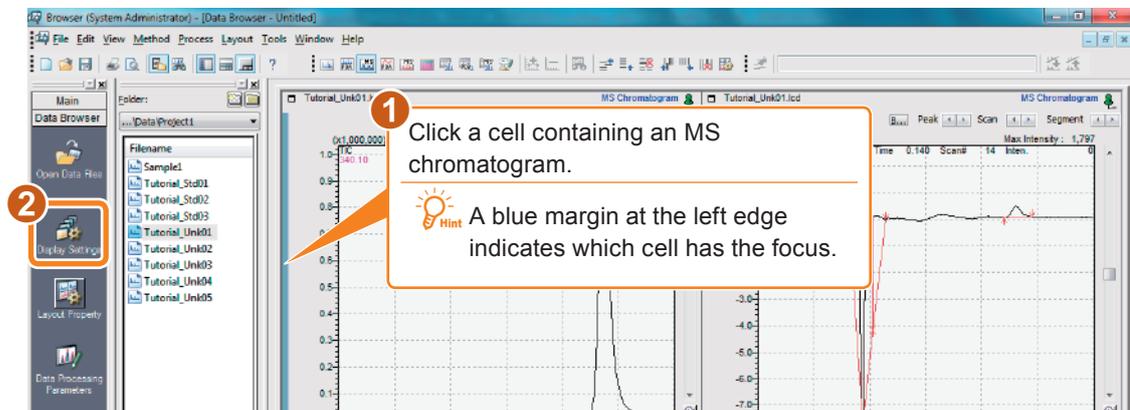
Hint A blue margin at the left edge indicates which cell has the focus.

The display changes to the PDA chromatogram.

6.3 Compare Different Types of Chromatograms

1 Compare MS and PDA chromatograms.

Chromatograms from different detectors can be overlaid and stacked in an [MS Chromatogram Cell]. Make these selections in the [MS Chromatogram Settings] sub-window.



2 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 [OK]

The names of the open files are displayed.

*** MS Chromatogram Cell ***

Tutorial_Std02.lcd
Tutorial_Std03.lcd

MS Chromatogram

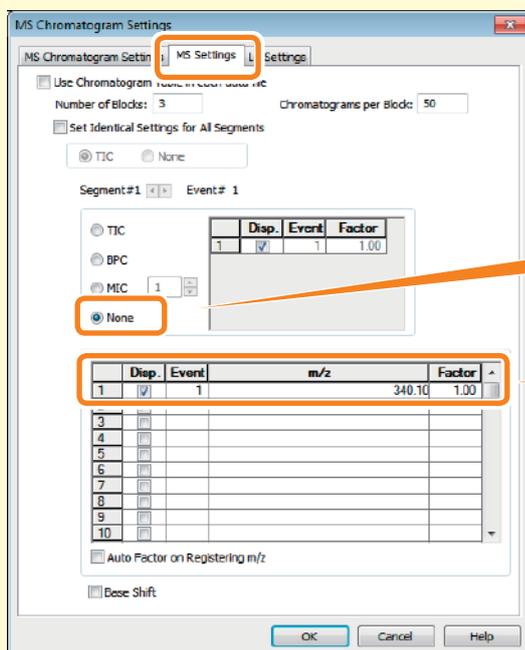
Time: 0.093 Scan: 7 Inten: 7,689
Max Intensity: 984,908

TC: Tutorial_Std02.lcd
TC: Tutorial_Std03.lcd
TC: Tutorial_Std03.lcd

▼ 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.

6.4 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 

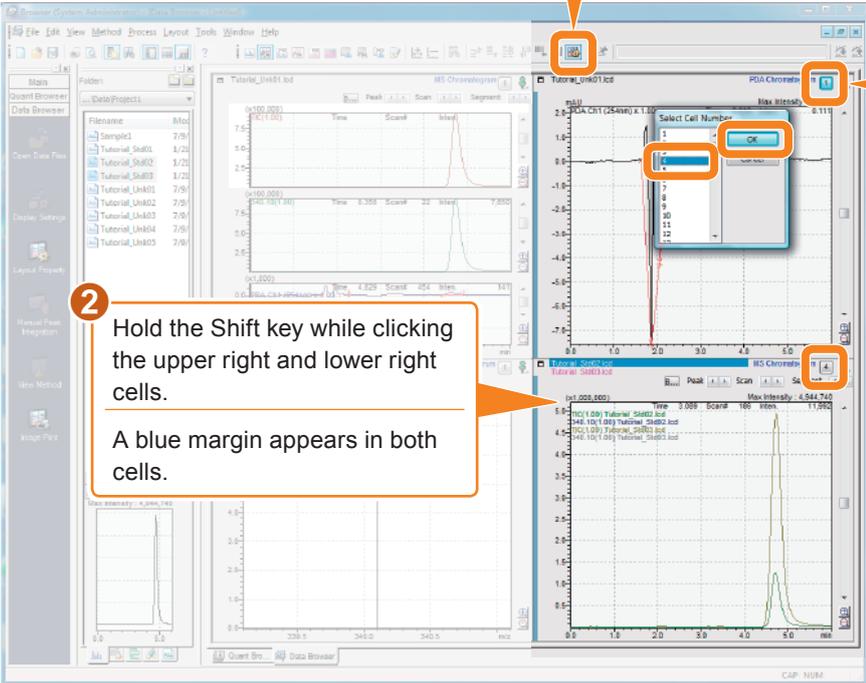
The entire [Data Browser] window enters the [Cell Fix] mode with [Cell Number] displayed at the top right of each cell.

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].

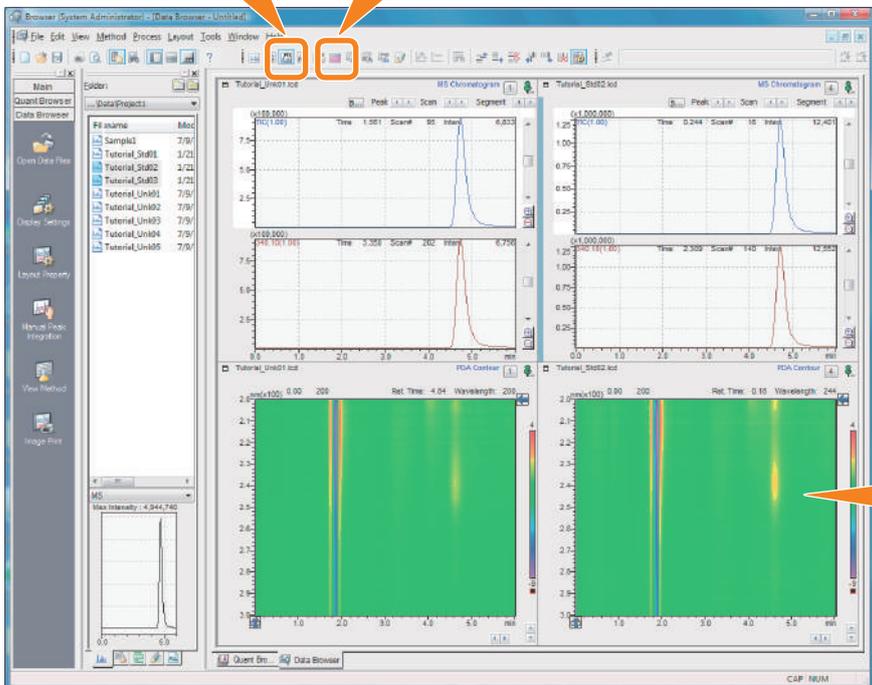
The cell numbers of two cells are both changed to 4.



2 Display an MS chromatogram and PDA contour.

1 Click (MS Chromatogram)

3 Click (PDA Contour)



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

Hint 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.

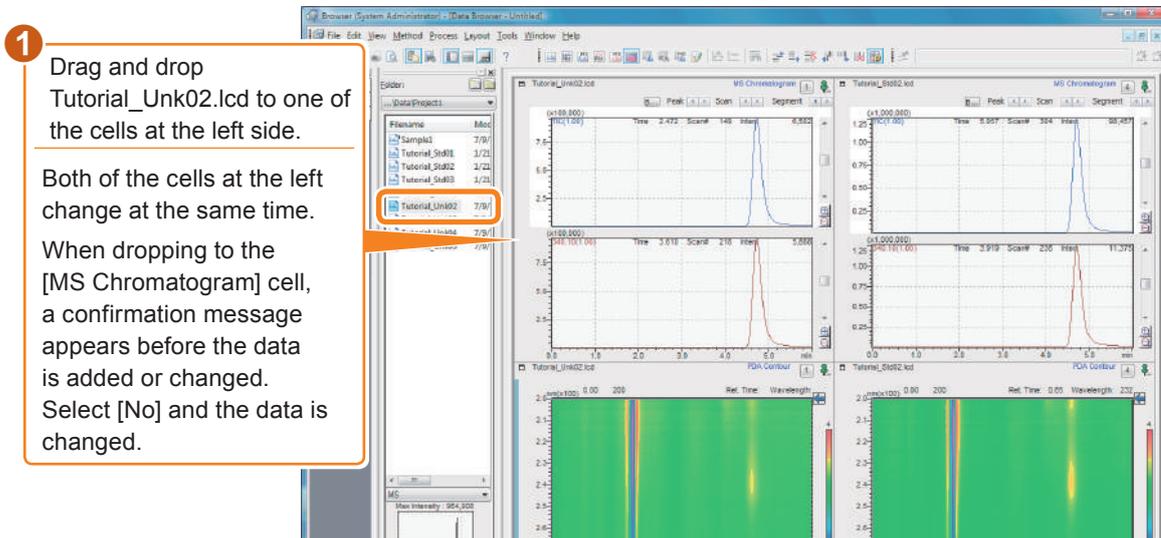
3 Confirm while comparing data.

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.



6.5 Qualitative Processing in the [Data Browser] Window

1 Load the data file.

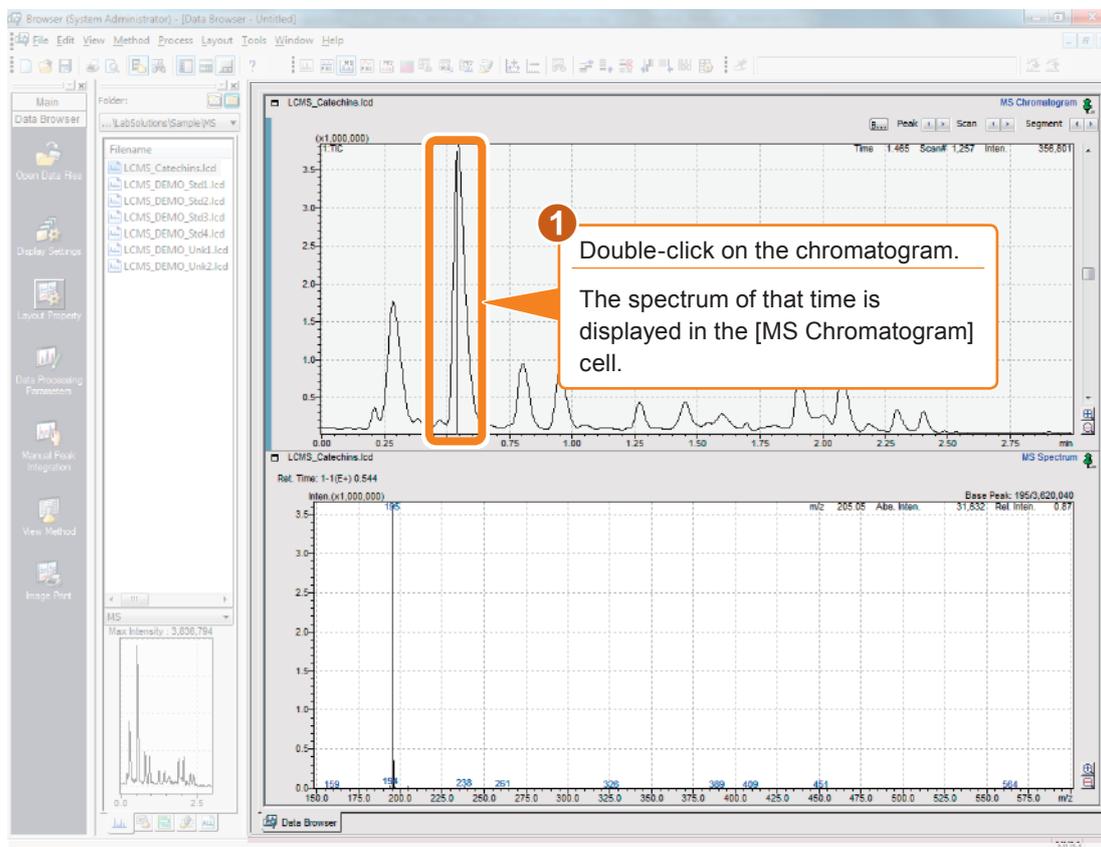
The screenshot shows the Data Browser window with the following elements:

- Data Browser Panel:** A list of files is shown, with 'LCMS_Catechins.lcd' selected. A callout box labeled '1' points to this file with the text: "Drag-and-drop LCMS_Catechins.lcd onto the cell in the [Data Browser] window."
- MS Chromatogram:** A plot showing intensity versus time (min). A callout box labeled '2' points to a green pin icon in the top right corner of the plot area with the text: "Turn pin (📌) on."
- MS Spectrum:** A plot showing intensity versus m/z. A callout box labeled 'MS spectrum' points to the plot area.



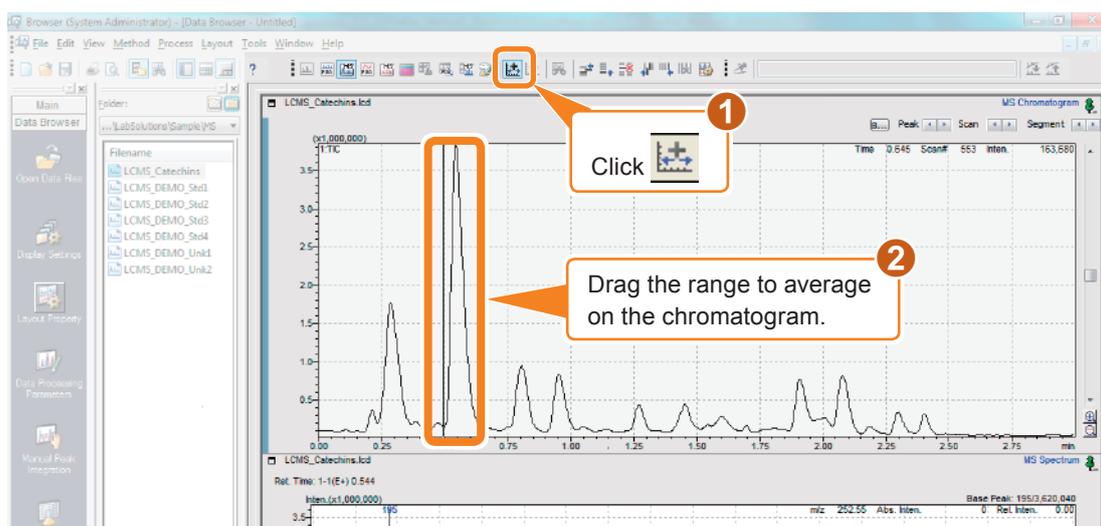
Clicking the pin switches toggles it on and off. Cells are interlocked when the pin is on. Browser functions applied to one pinned cell are executed in all of the pinned cells.

2 Display the MS spectrum.



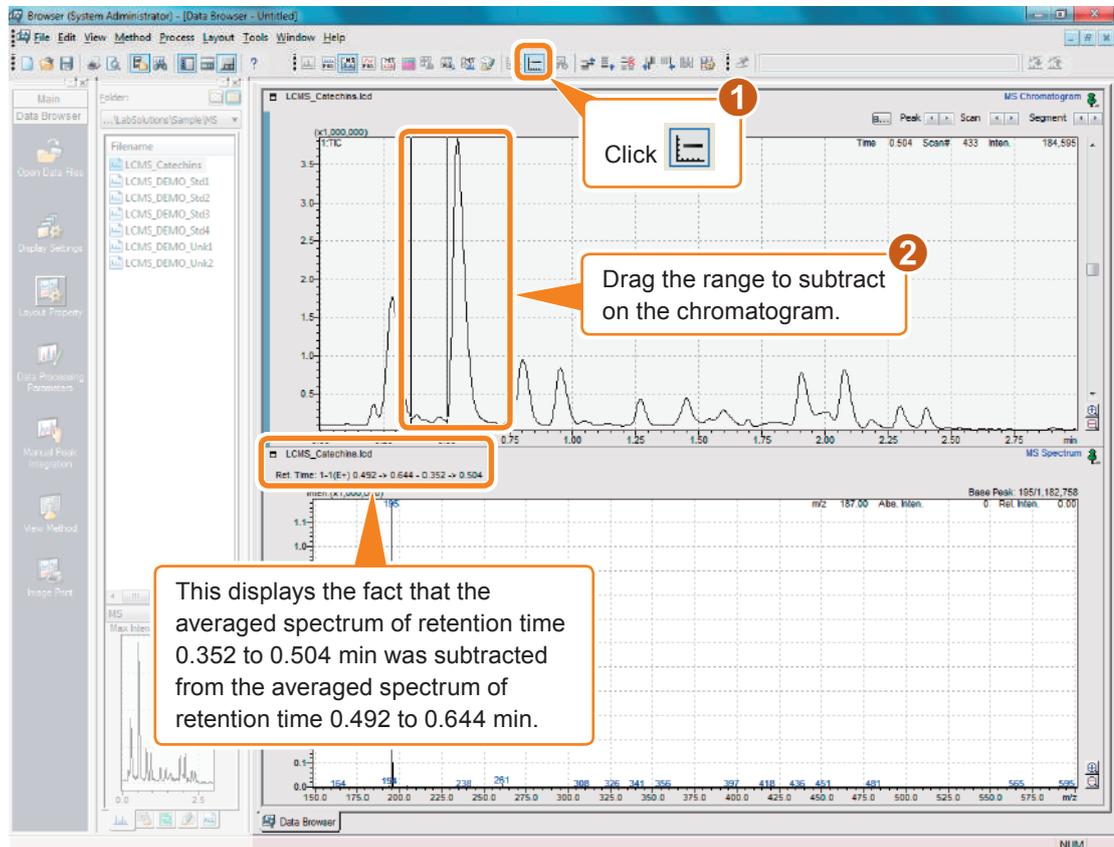
3 Average the MS spectrum.

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



4 Perform subtraction on the MS spectra.

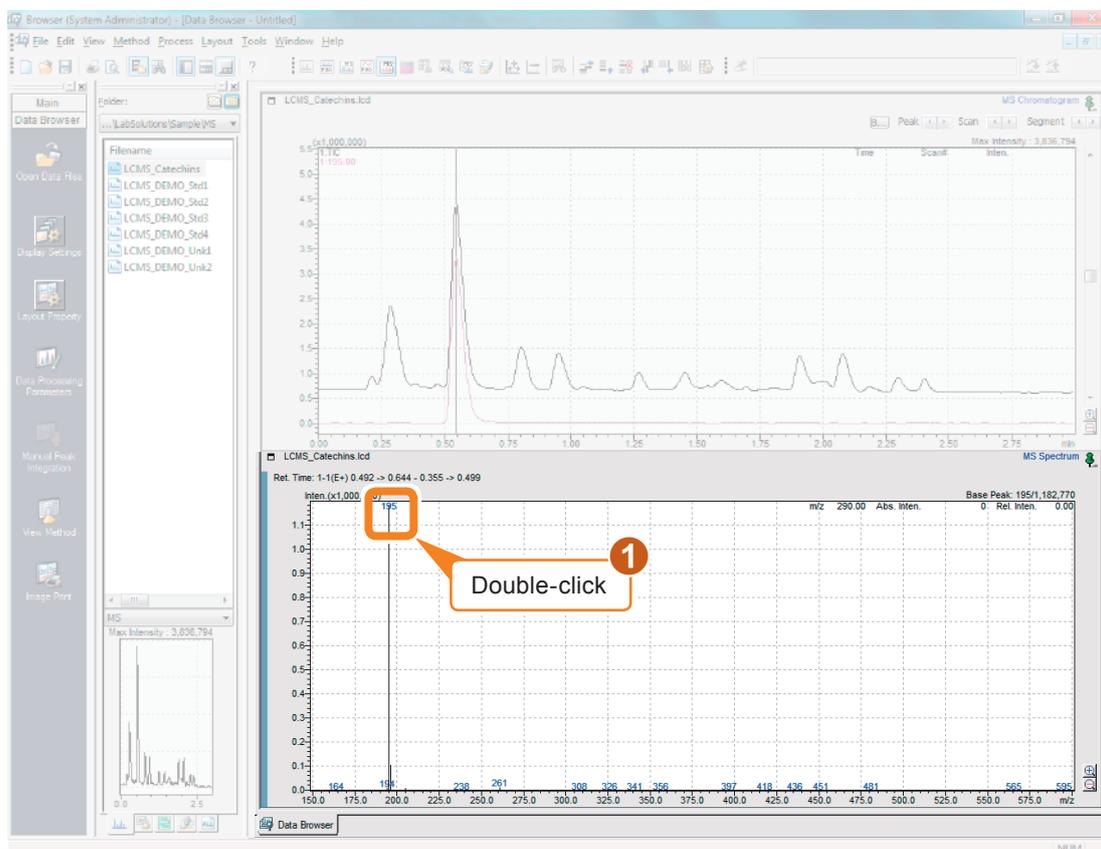
A cleaner-looking spectrum can be displayed by subtracting the background MS spectrum from the averaged spectrum.



 **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.

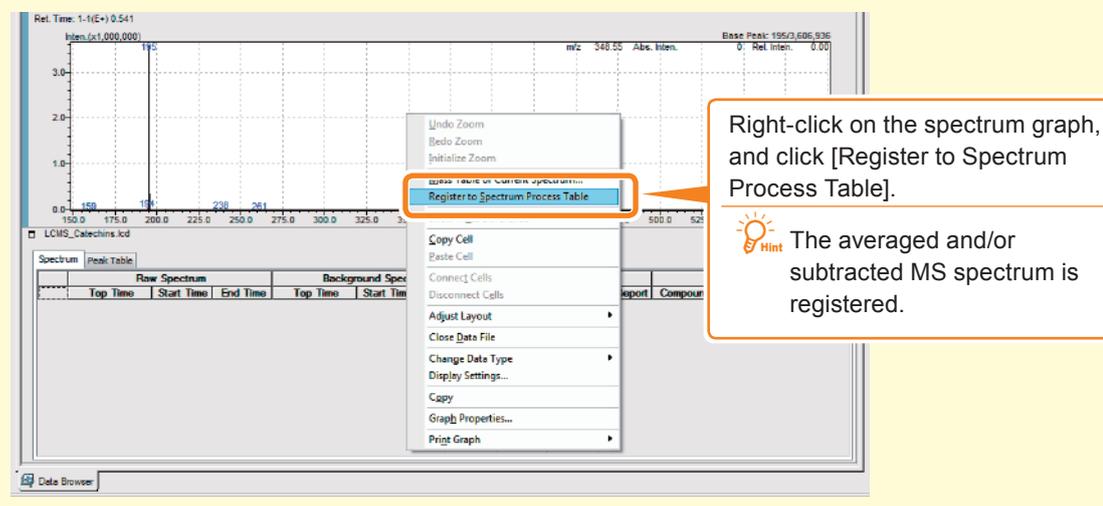


▼ Tips

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.

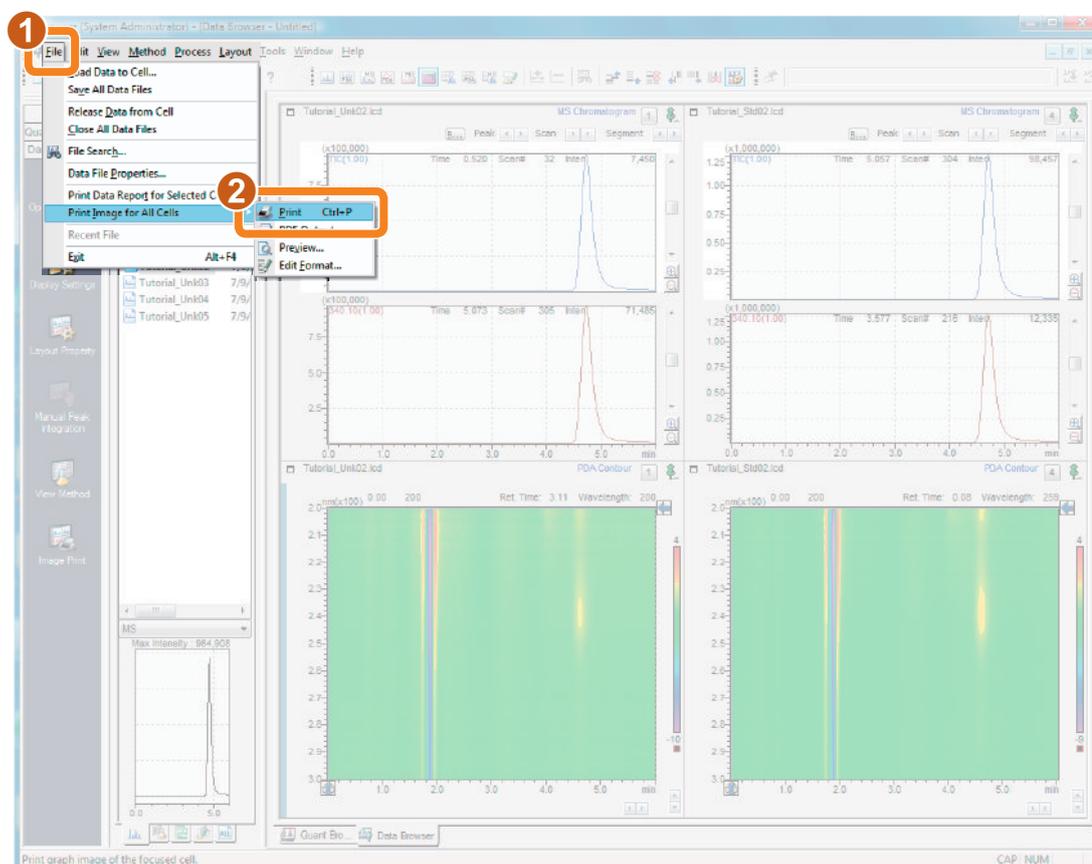
The spectrum can also be printed in the [Report] window.



6.6 Print from the [Data Browser] Window

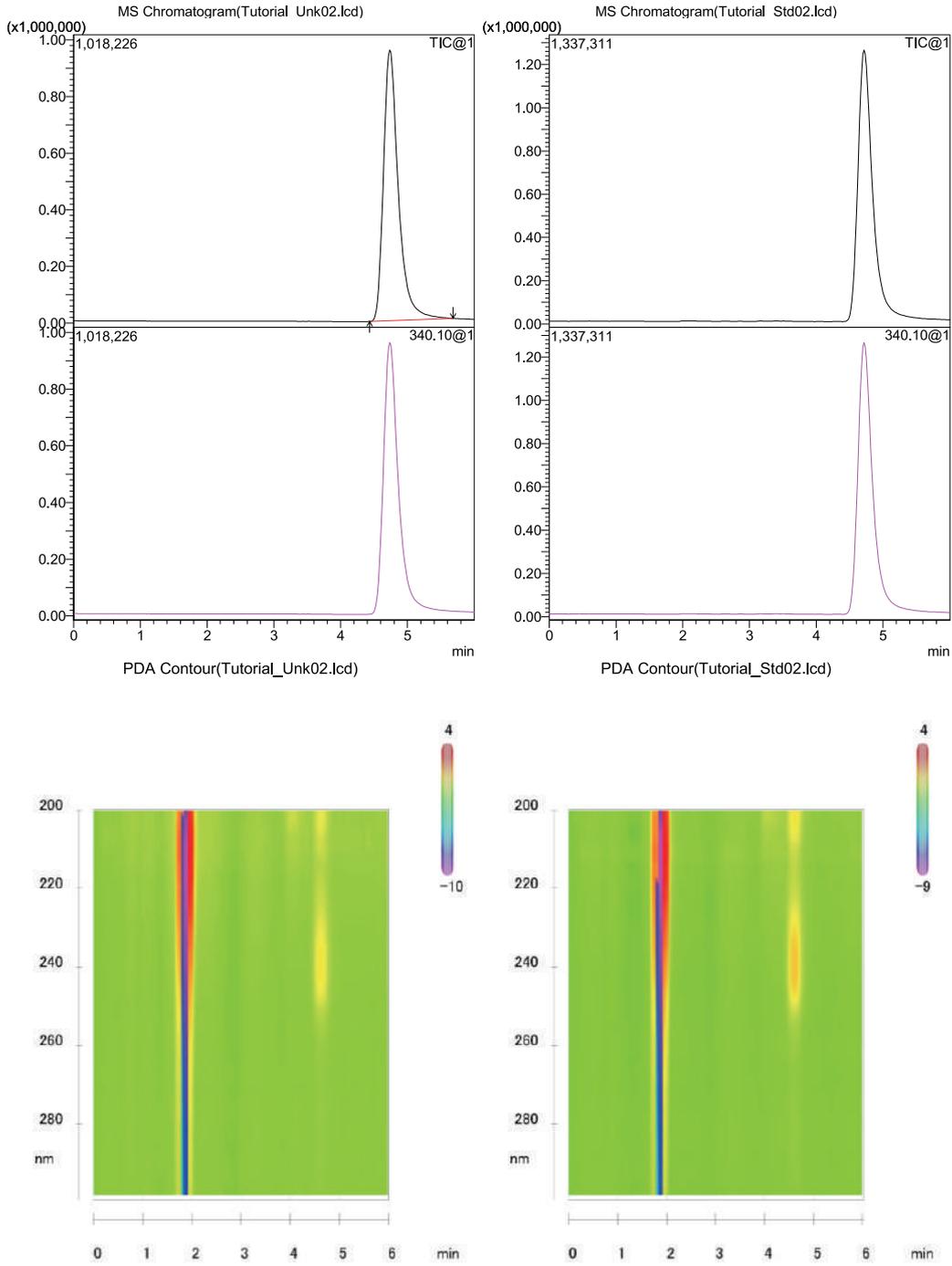
1 Print an image of the display.

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



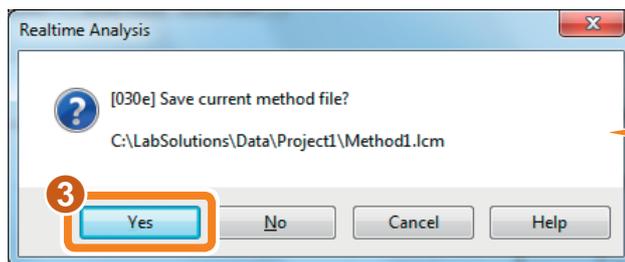
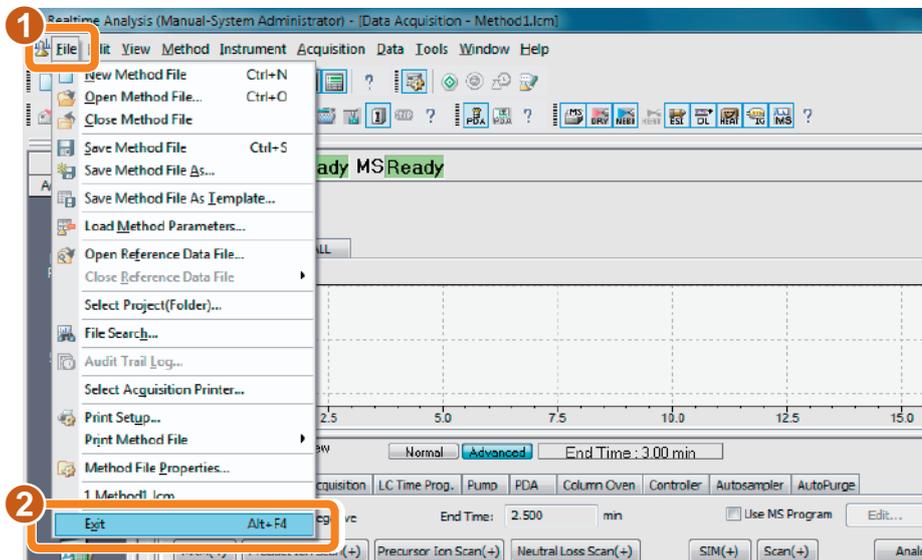
Hint Select [Print Data Report for Selected Cell] from the [File] menu to print using the report format saved in the data file.

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



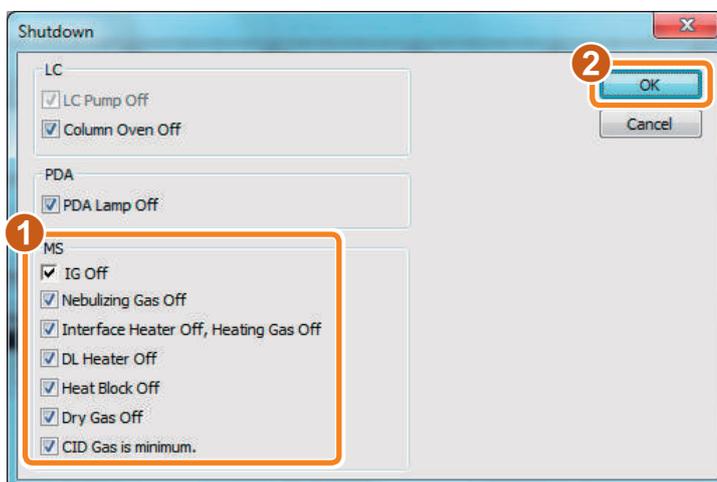
Chapter 7. Shutdown

1 Close any open windows.

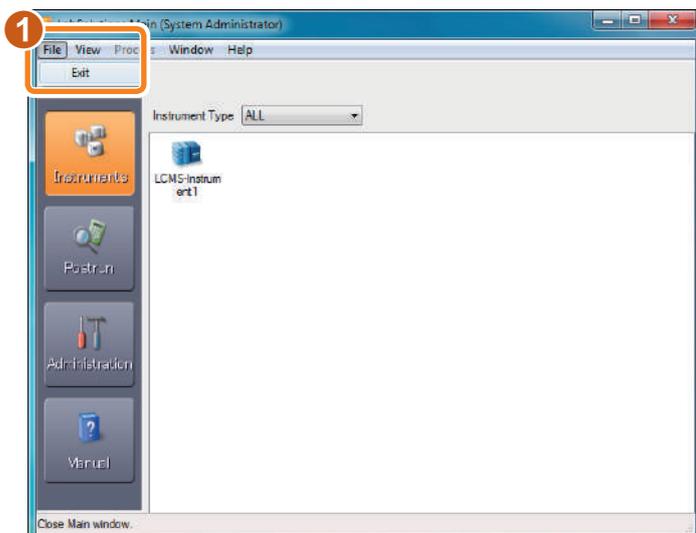


 **Hint** This sub-window appears if there are any unsaved files.

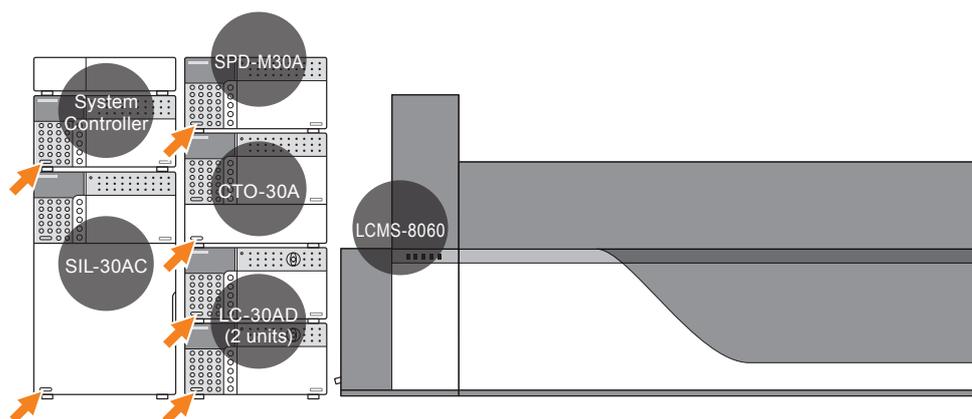
2 Stop the LC pumps, gas flows and heaters from the [Shutdown] sub-window.



3 Exit LabSolutions.



4 Turn off the power to the LC modules.



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

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