SHIMADZU

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LabSolutions LCMS

Getting Started Guide

NOTICES

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

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.

Hint	Useful advice for convenient instrument operation
Reference	Shows where to refer to.
Tips	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:

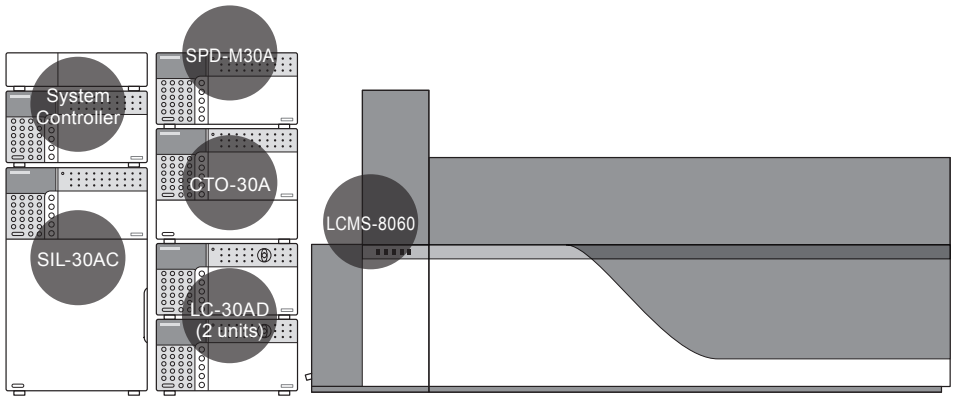
- Data acquisition and control of analytical instruments
- Data analysis and viewing of data
- Creation and printing of various customizable reports

System Structure

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

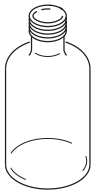
High-pressure gradient LCMS + PDA system

- 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.

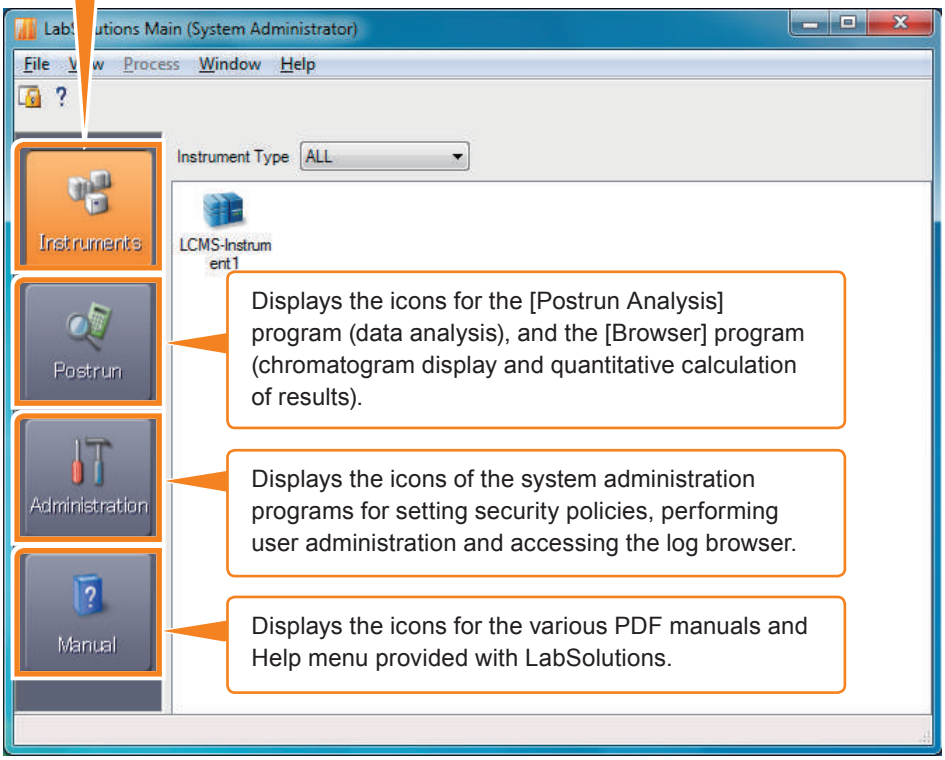
Report format file (.lsr)

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.



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

Displays the icons of the system administration programs for setting security policies, performing user administration and accessing the log browser.

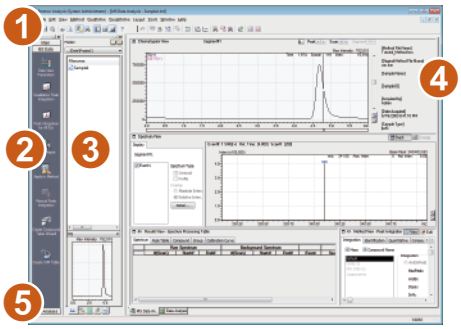
Displays the icons for the various PDF manuals and Help menu provided with LabSolutions.

LabSolutions Main Programs and Main Windows

- [Realtime Analysis] program
  - **[Data Acquisition] window** for acquiring data
  - **[Realtime Batch] window** for continuous data acquisition
- [Postrun Analysis] program
  - **[MS Data Analysis] window** for analyzing data
- [Browser] program
  - **[Quant Browser] window** for analyzing data from multiple samples
  - **[Data Browser] window** for comparing data

LabSolutions Windows

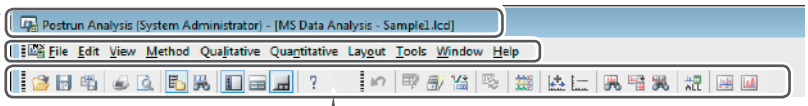
The following example describes the [Postrun Analysis] program window.



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.

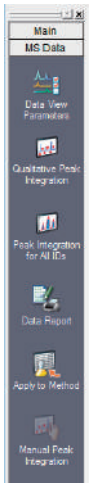
Toolbar

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.

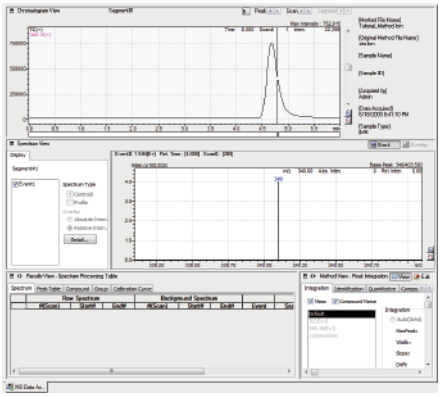
4

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.

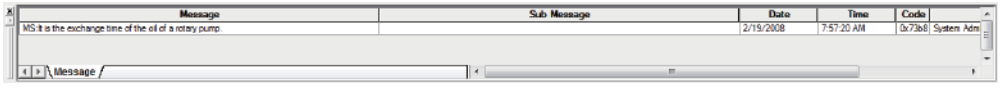
Switch the windows by clicking the icons on the assistant bar.



5

Output Window

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



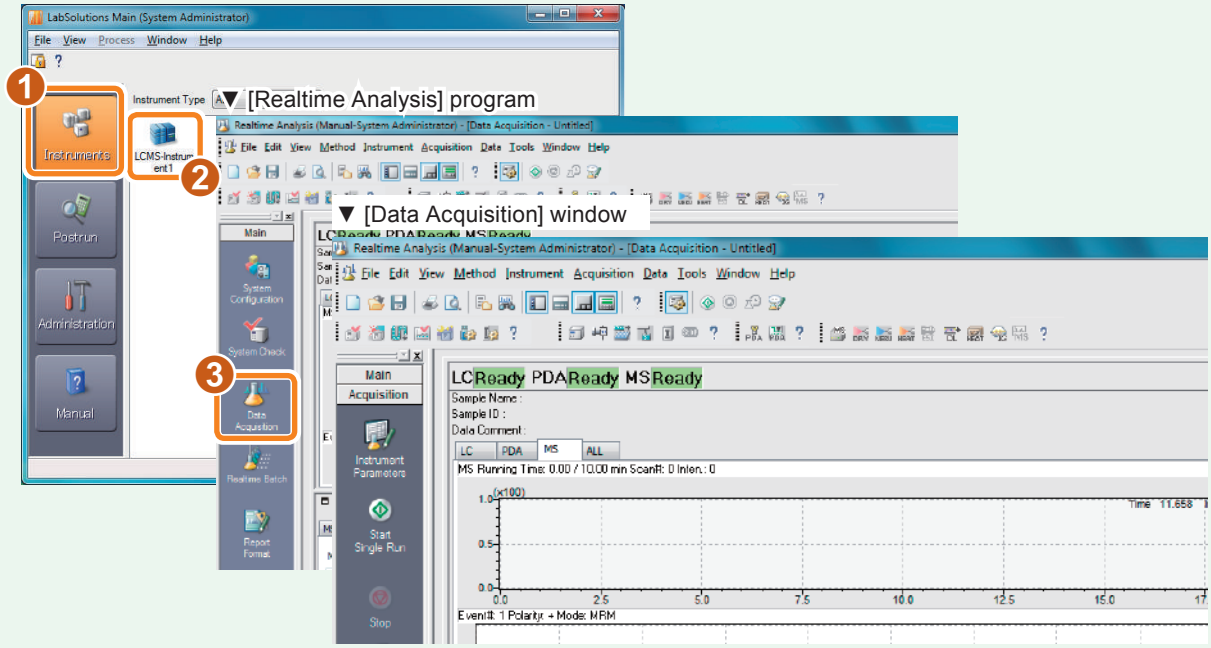
How to Open Windows

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

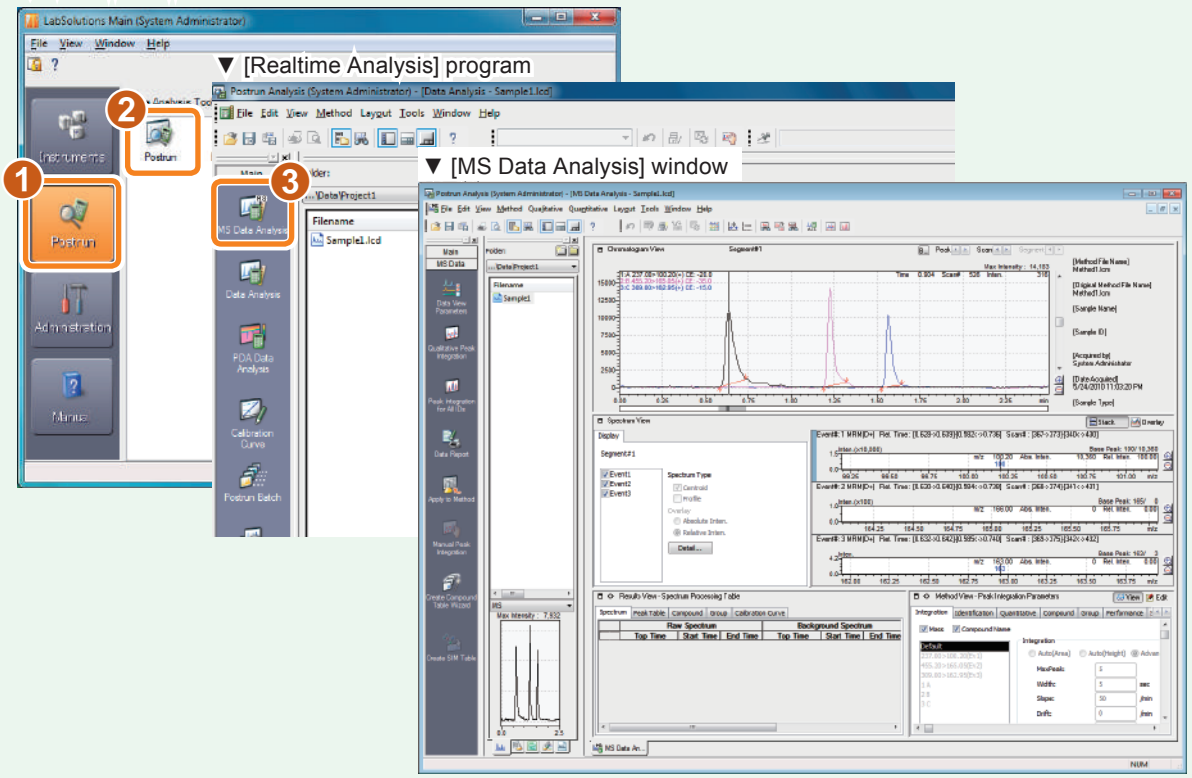


Data Analysis and Qualitative Calculations

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

Reference 3. Confirm Single Run Results

▼ Main window

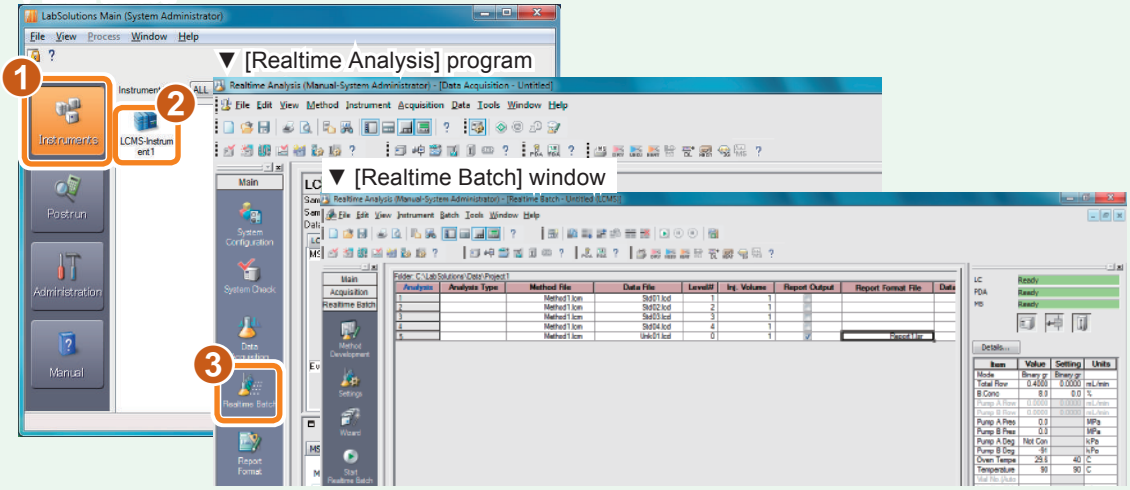


Continuous Data Acquisition of Sequential Samples

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

Reference 4. Realtime Batch

▼ Main window

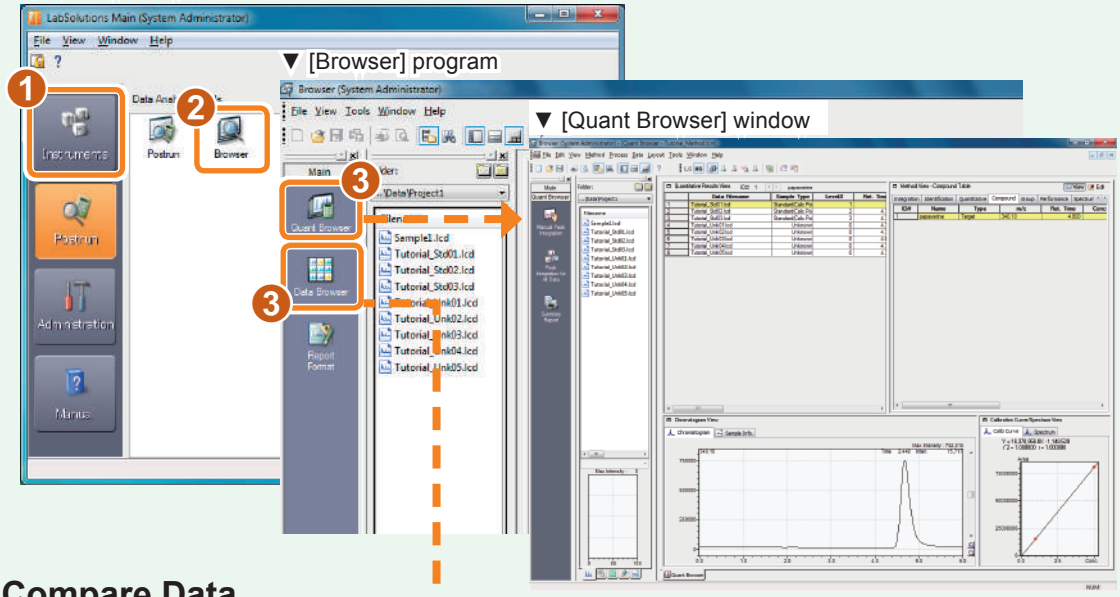


Confirm Quantitative Results

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

Reference 5. Quantitative Data Analysis

▼ Main window

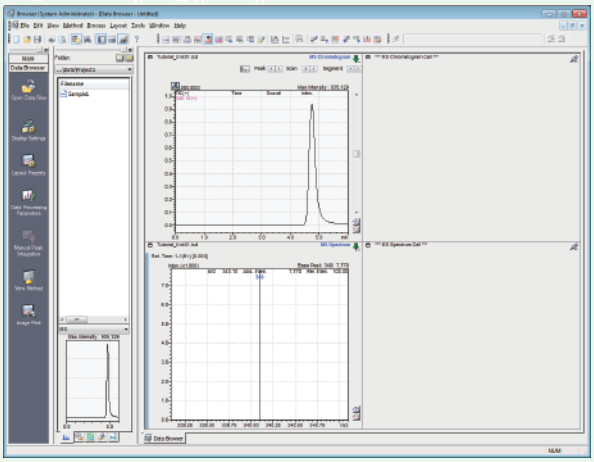


Compare Data

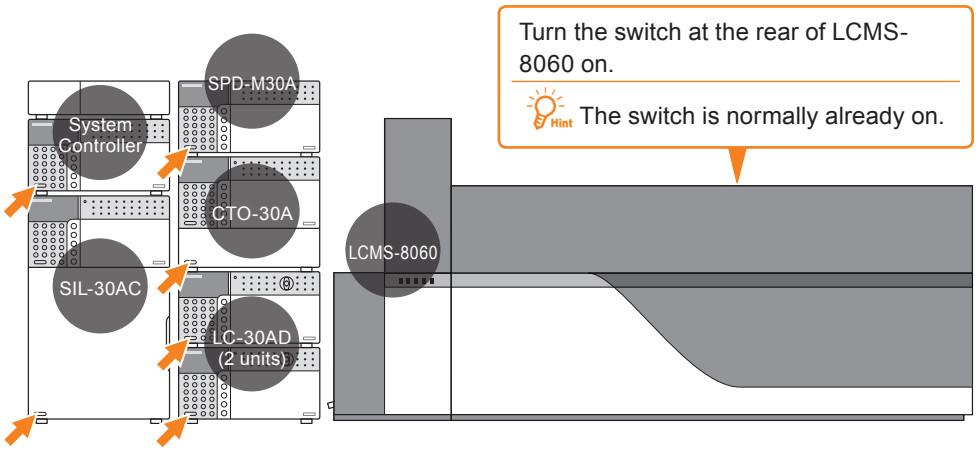
Open the [Data Browser] window from the main window.

Reference 6. Qualitative Data Analysis

▼ [Data Browser] window



1 Turn ON all of the instruments.



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

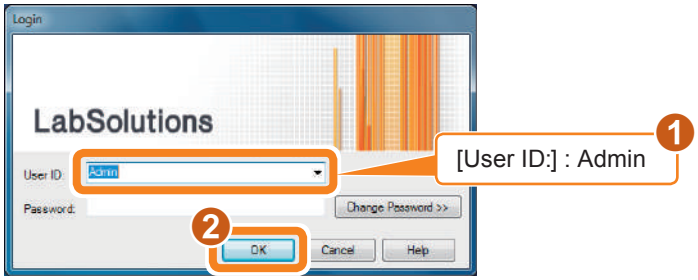
3 Start the PC.

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

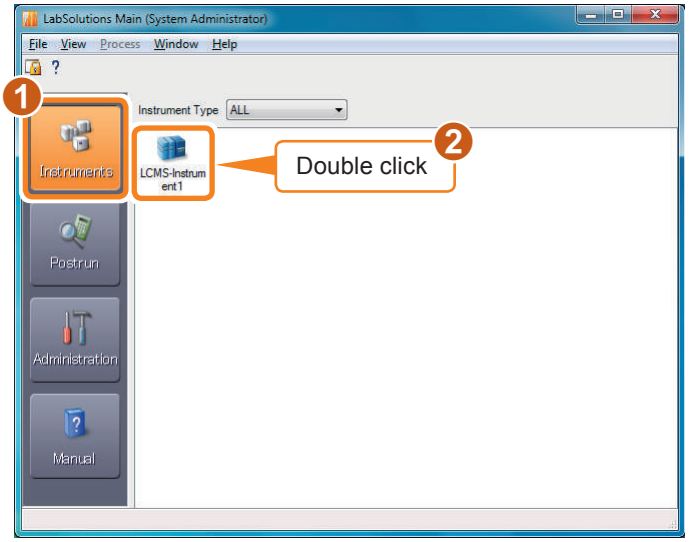
Icon Color	LabSolutions Status	Operation
Green	Normal	
Yellow	Starting up	Please wait
Red	Error	Please restart the PC.

5 Double-click  on the desktop.

6 Log in.



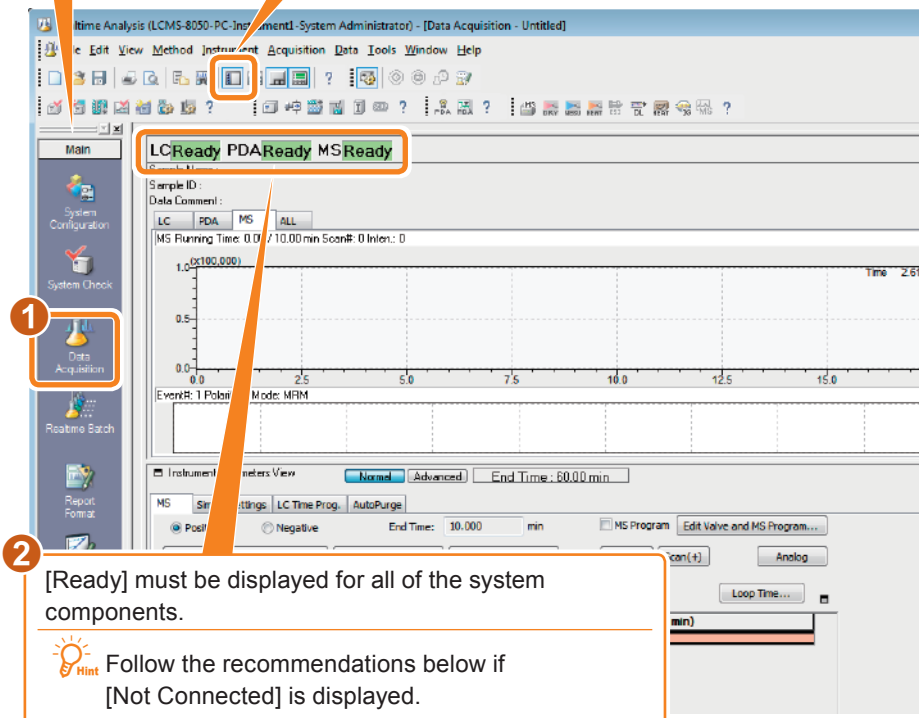
7 Start the [Realtime Analysis] program.



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.



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

Hint 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. Single Run

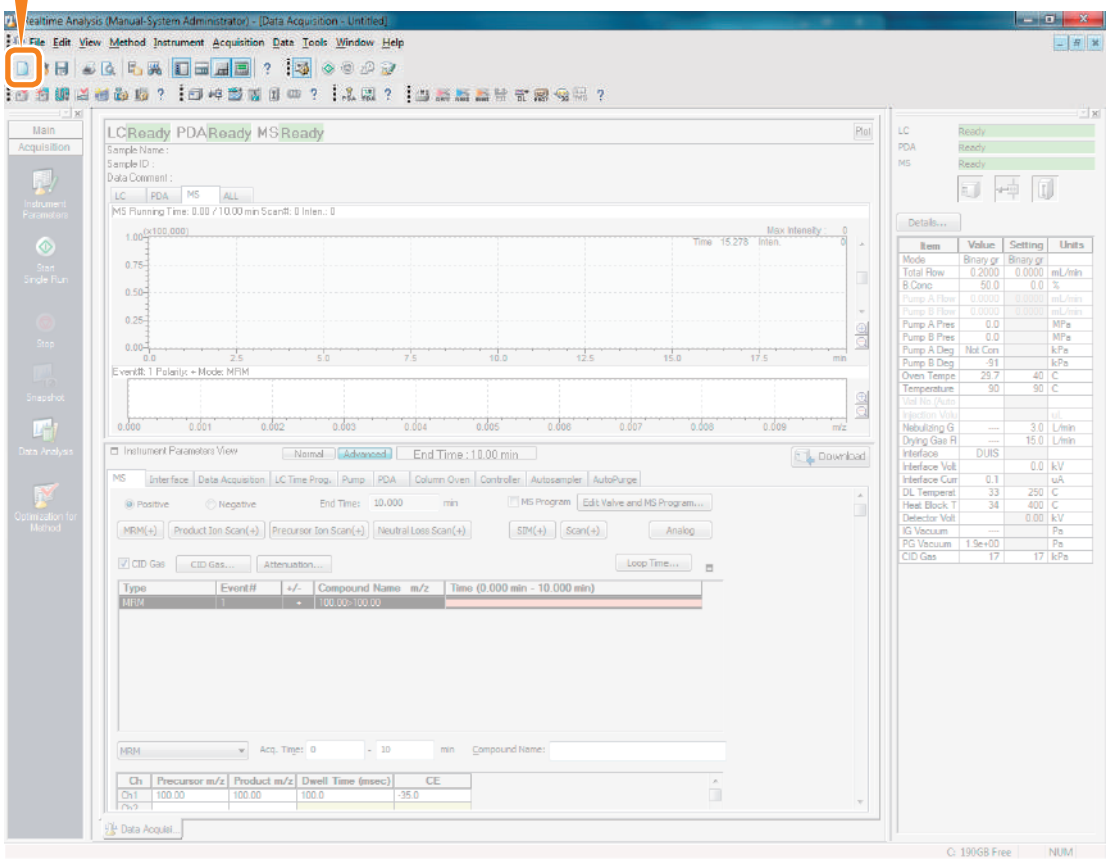
Set the LC instrument parameters and MS instrument parameters (acquisition conditions) in the [Data Acquisition] window, and perform method optimization and single run.

2.1 Create a Method File

1 Click [New] on the toolbar.

Click 

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



2.2 Prepare for Method Optimization

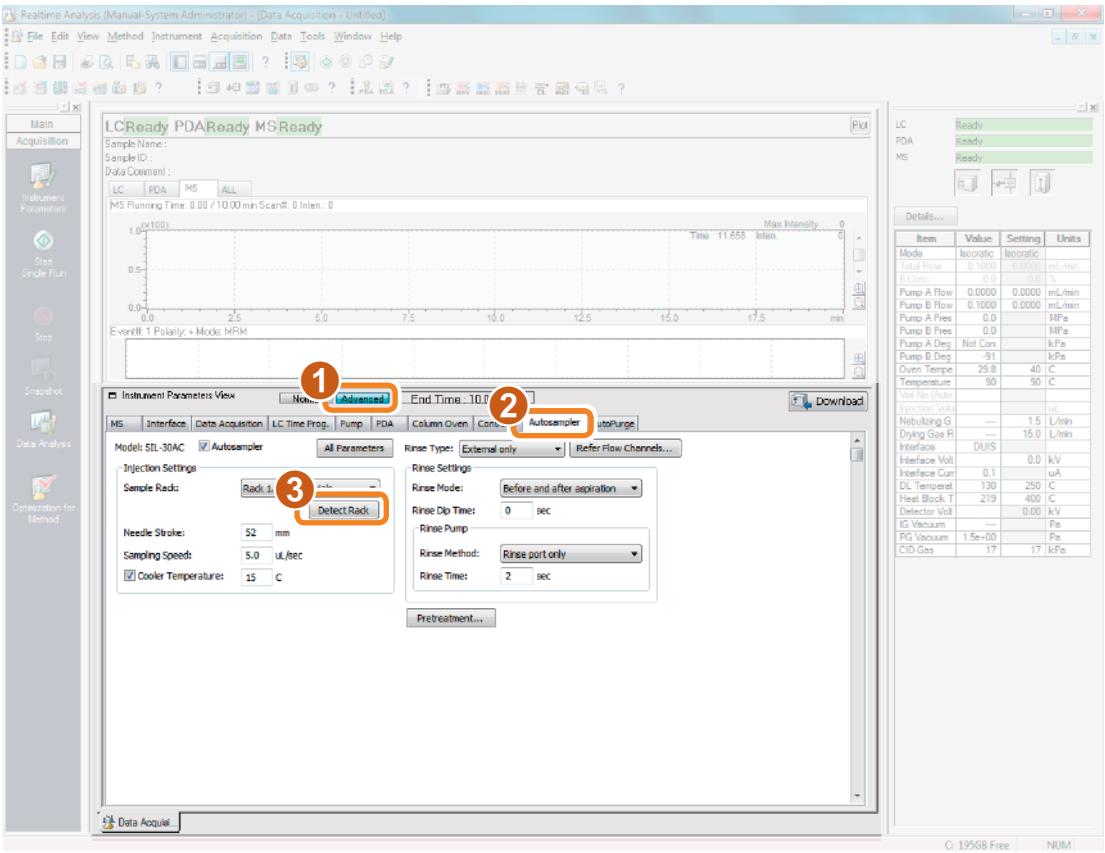
MRM (Multiple Reaction Monitoring) measurement on the LCMS-8030/8040/8045/8050/8060 enables high-sensitivity quantitative data acquisition.
The optimum conditions for MRM data acquisition can automatically be determined by executing method optimization.
In this example, we enter the 3-component precursor *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*.

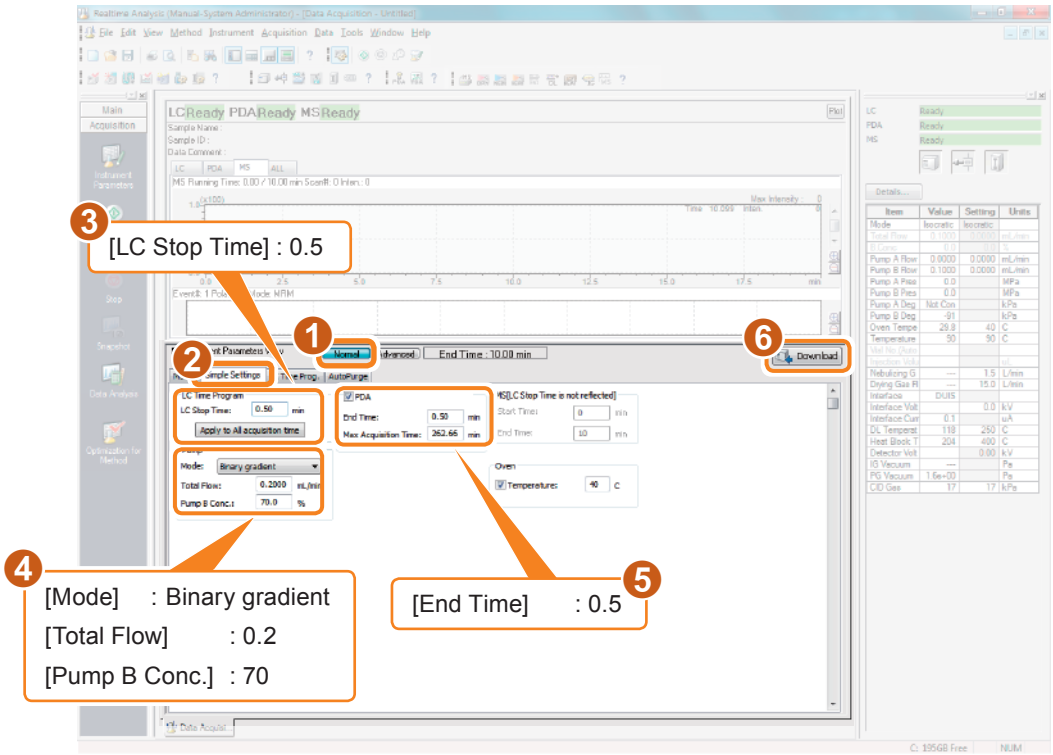
1 Remove the column.

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

2 Detect the type of autosampler rack.

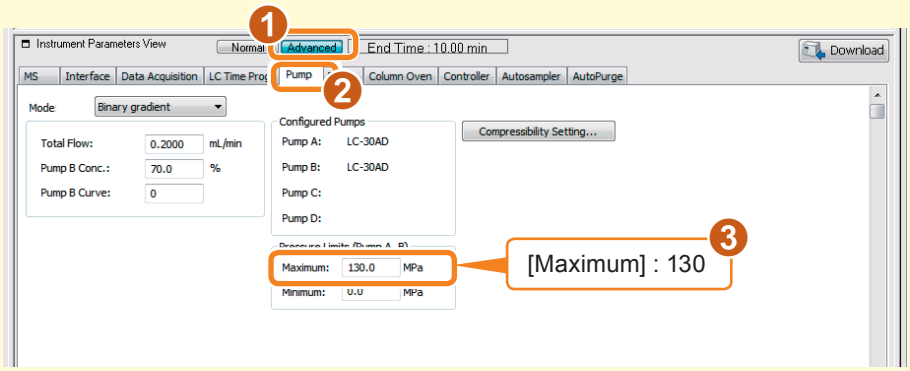


3 Set the LC instrument parameters.



▼Tips Pump Pressure Limits

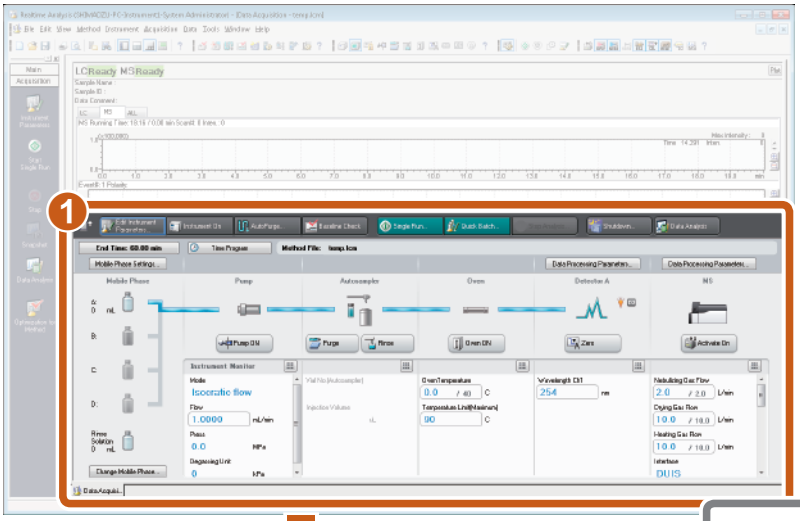
The maximum column pressure (pressure resistance) value is specified in the column's instruction manual. Use the following procedure to set the pressure threshold (typically, the column's pressure resistance) at which the pump automatically stops to protect the column. This procedure changes the upper pressure value to 130 MPa, as an example.



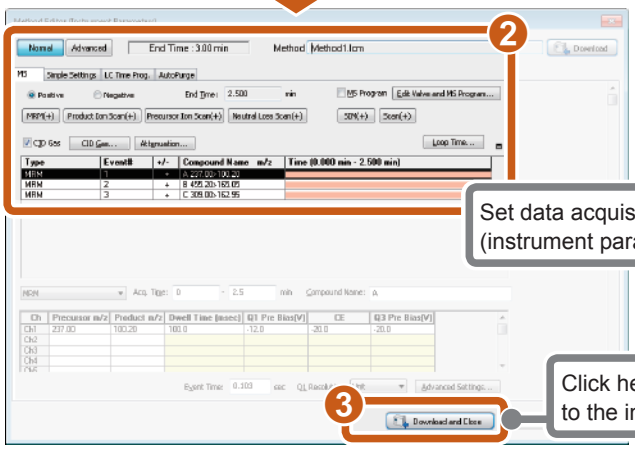
LabSolutions SUPPLEMENT

Control Panel

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



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



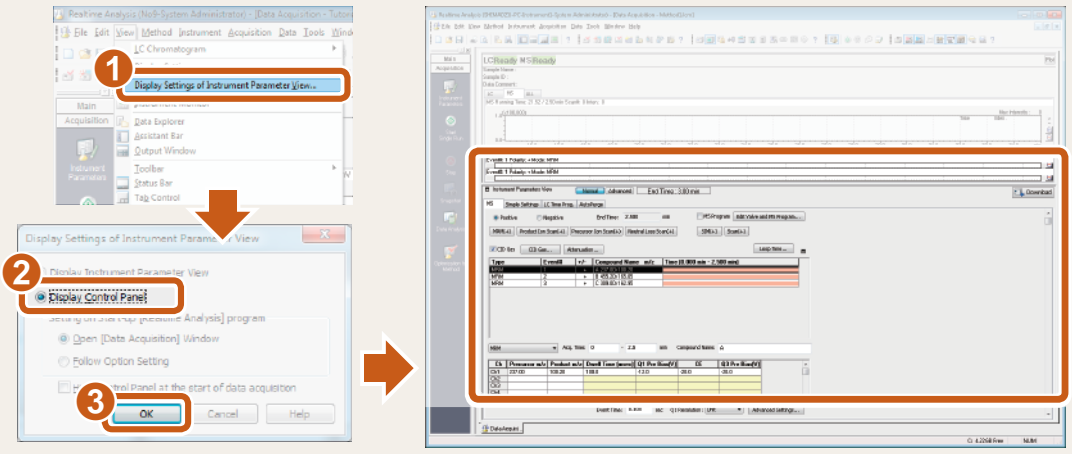
Set data acquisition conditions (instrument parameters).

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

Hint

Switching Display Settings

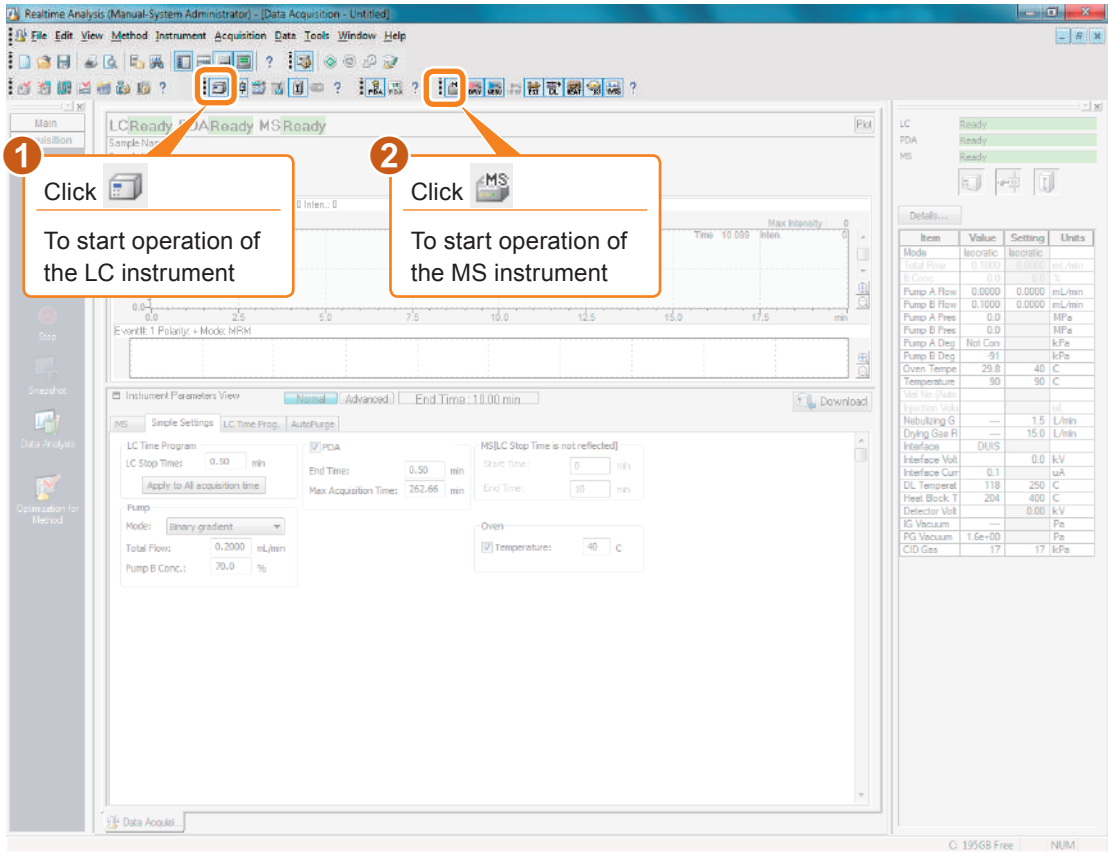
In the [Display Settings of Instrument Parameter View] sub-window, you can select displaying either the control panel or the instrument parameter view.



2.3 Instrument Control

1 Take control of the instrument.

The DL plug must be removed before starting analysis.

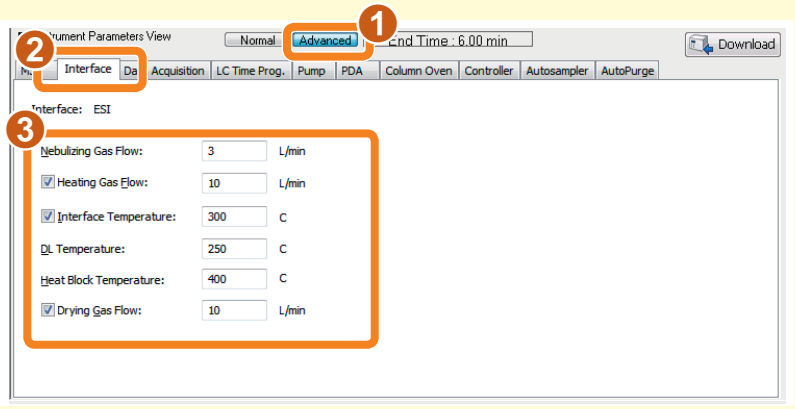


2 Purge the LC pump and the autosampler.

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.



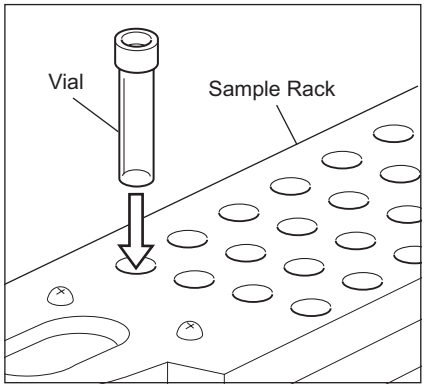
2.4 Execute Method Optimization

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

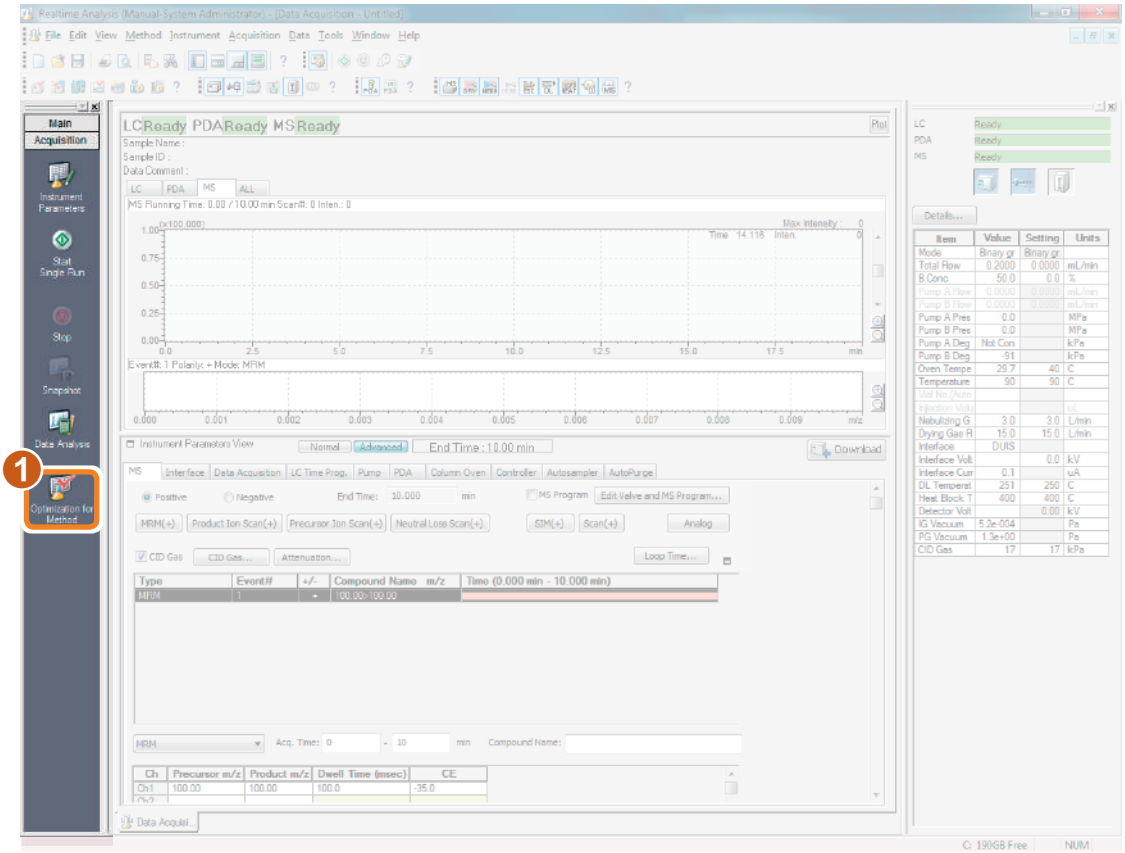
Reference "11 Method Optimization" in *Operators Guide*.

1 Place the samples in the autosampler.

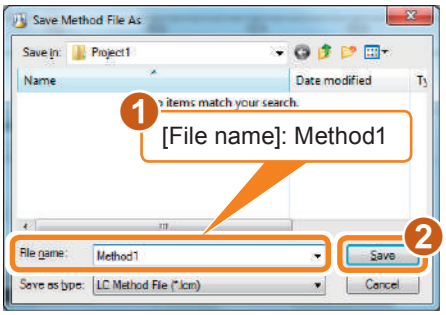
Vial 1, sample A 0.5 ng/µL solution
Vial 2, sample B 0.5 ng/µL solution
Vial 3, sample C 0.5 ng/µL solution



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

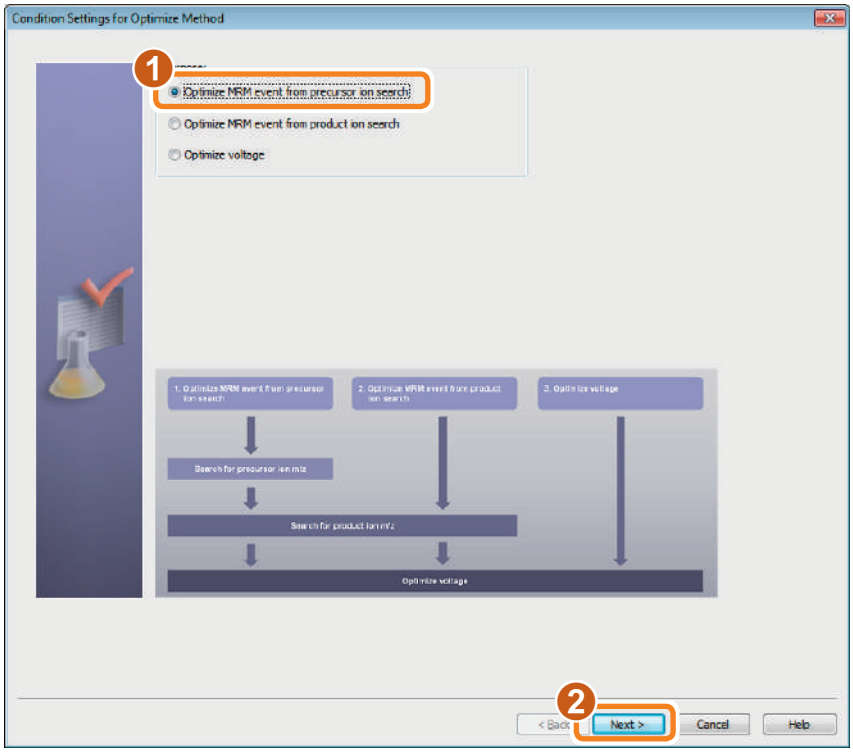


3 Save the method file.

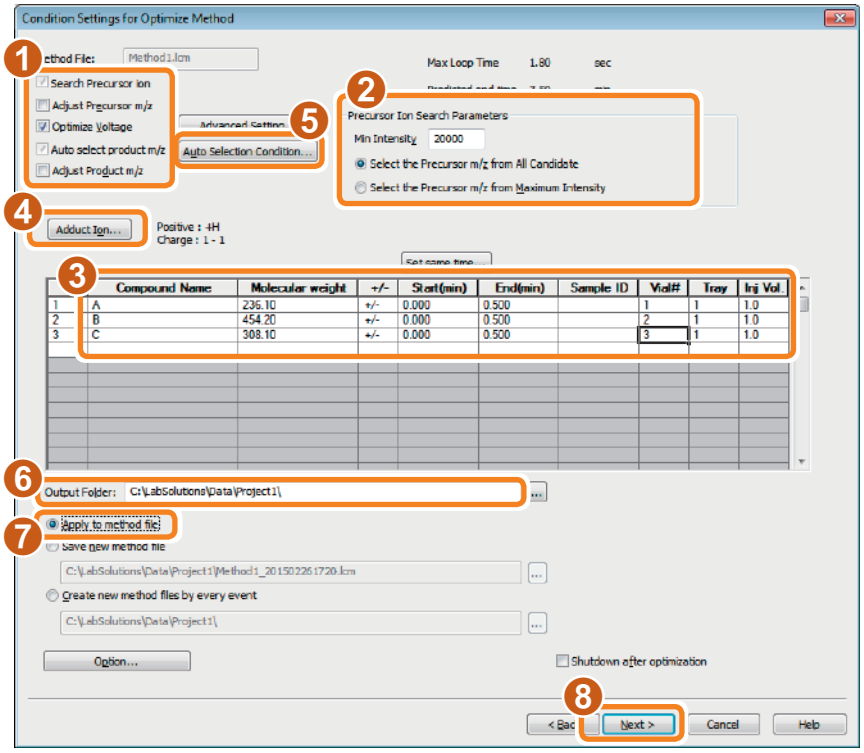


Hint This sub-window is not displayed when a method file is already saved.

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



5 Set the parameters.



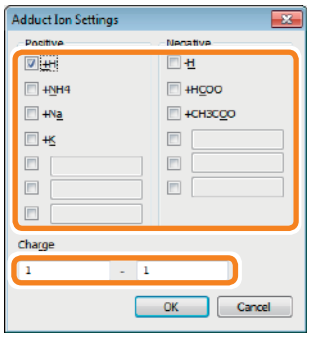
1 Check [Optimize Voltage].

2 Set the parameters for selecting precursor ions.

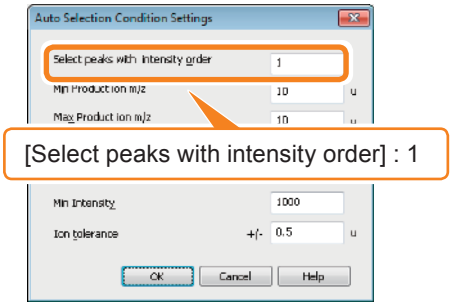
3 Set the information of compounds to be searched for.

	#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.



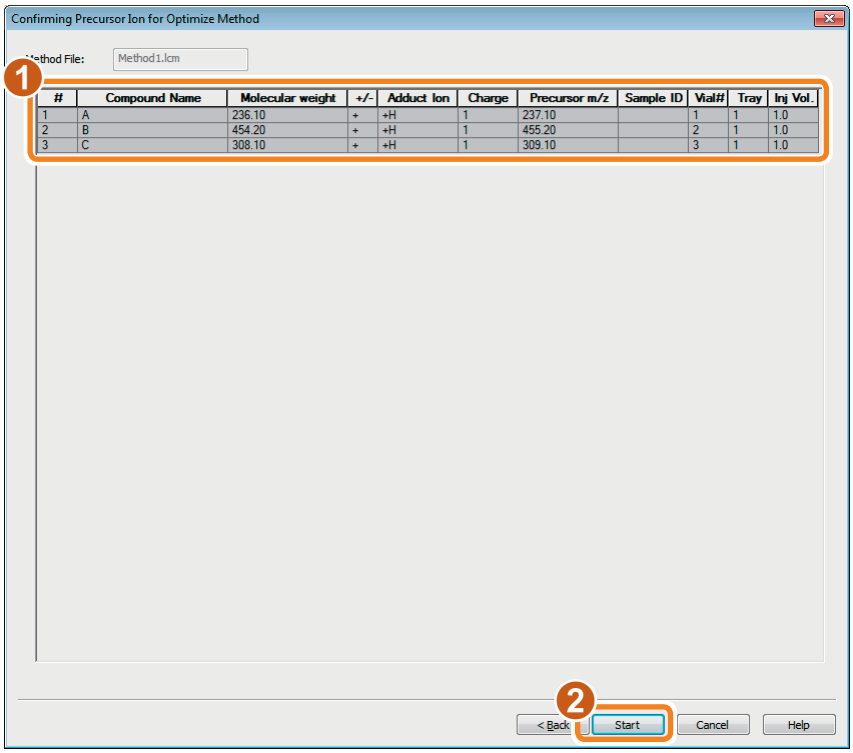
6 A subfolder is created under the folder specified here. The name of the subfolder is determined by the date and time. The files automatically created during the optimization are output in this folder.

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

7 Select [Apply to method file].

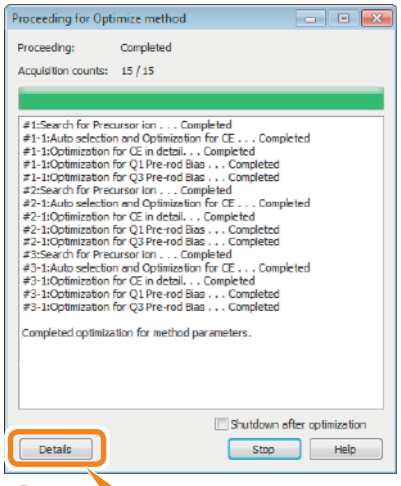
8 Open the [Confirming Precursor Ion for Optimize Method] sub-window.

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



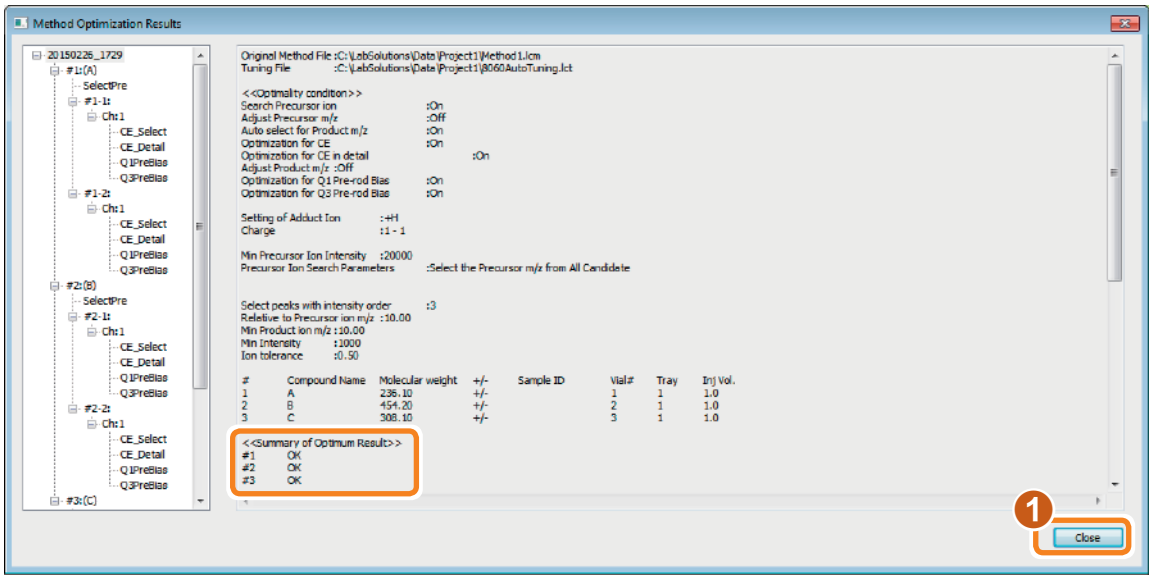
Measurement having a data acquisition time of 0.5 minutes is repeated 15 times.

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

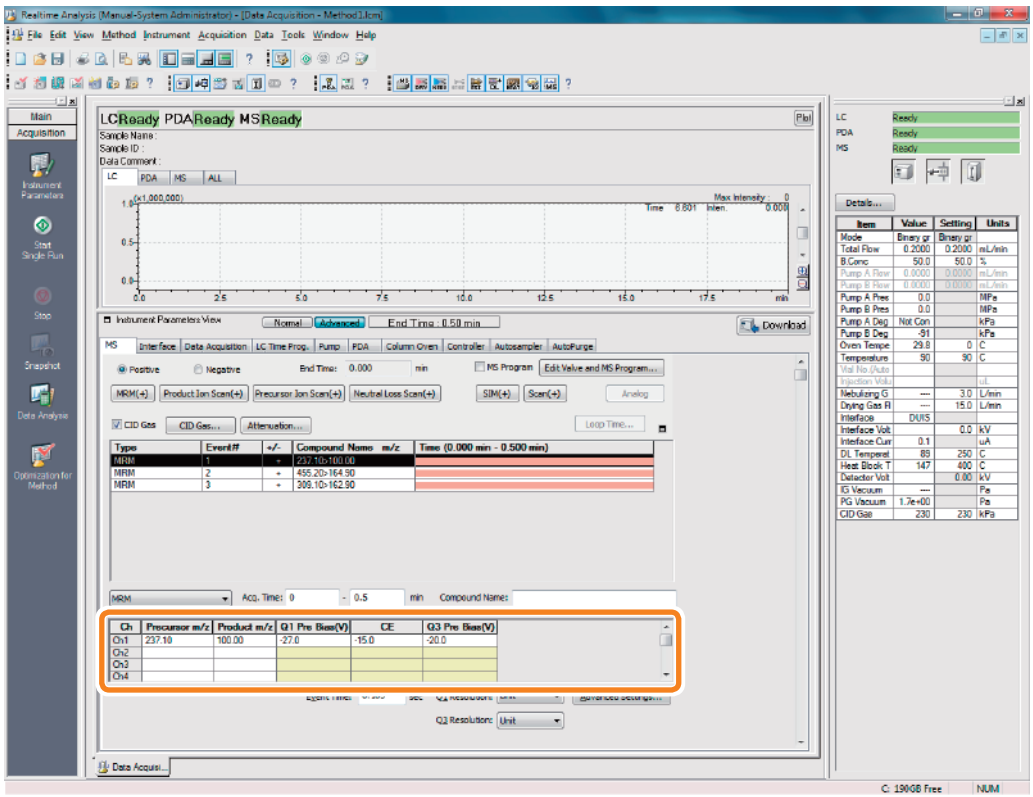


3 To check optimization results, click [Details].

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

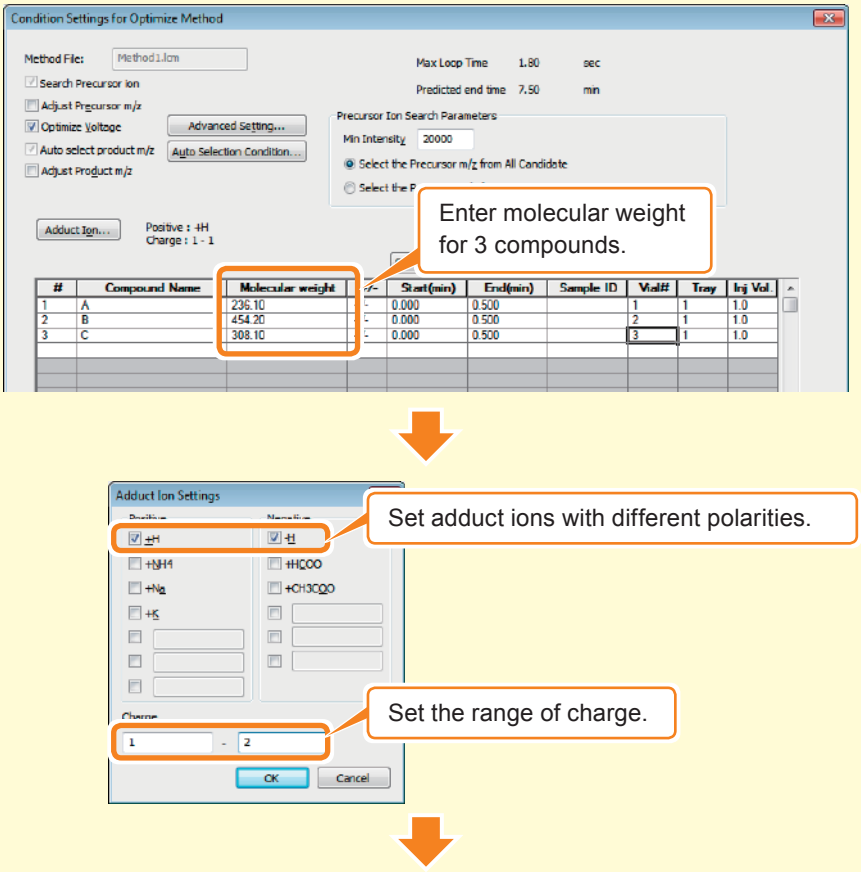


The results reflected in the method parameters.

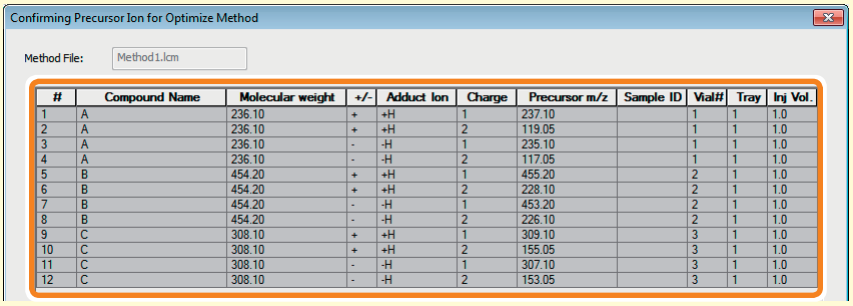


▼Tips

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.



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



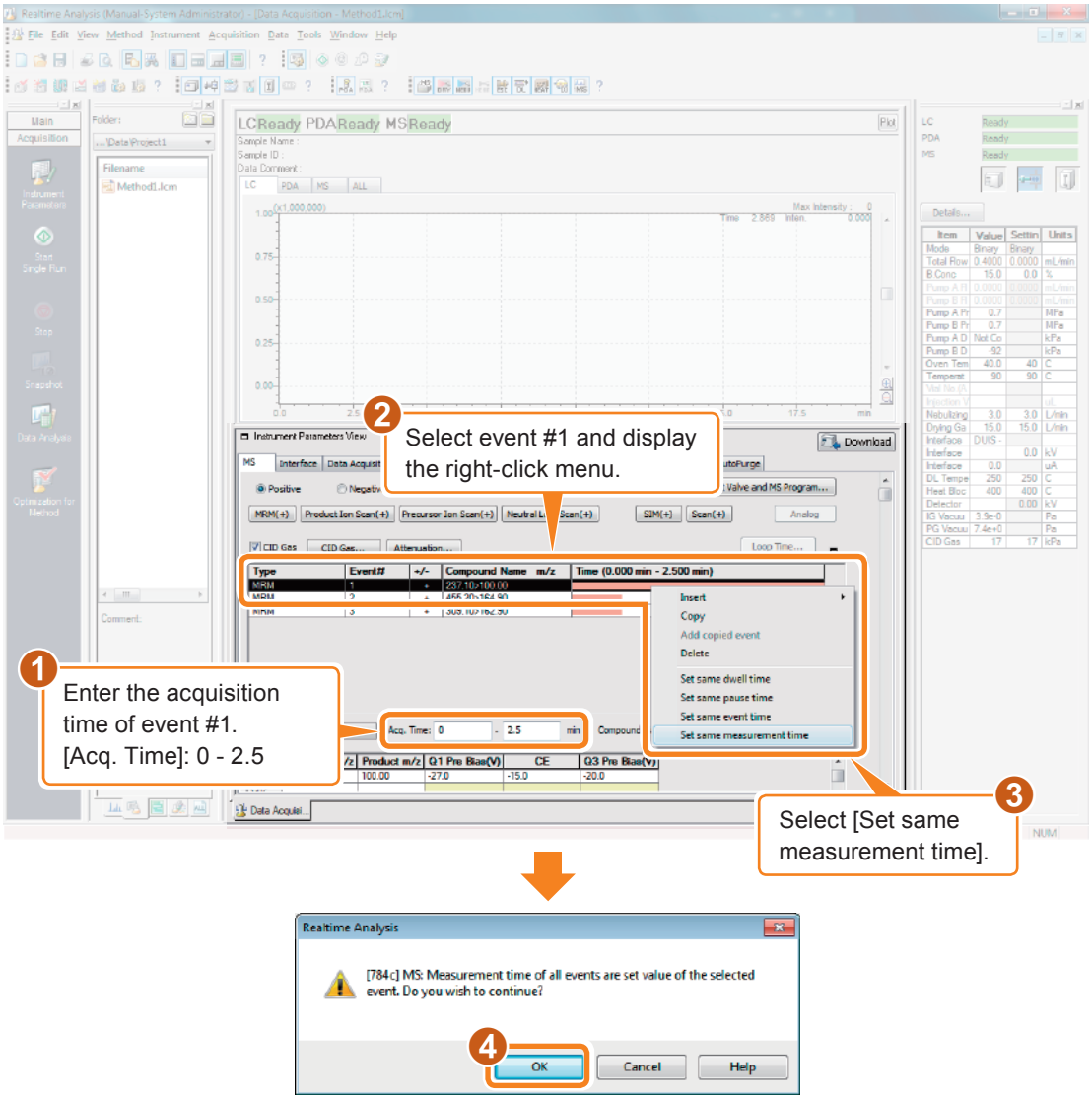
2.5 Set the Parameters for Single Run

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

1 Install the column.

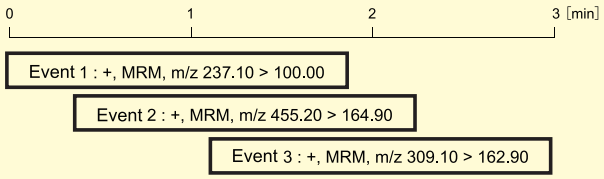
Open the CTO-30A door, and install the column.

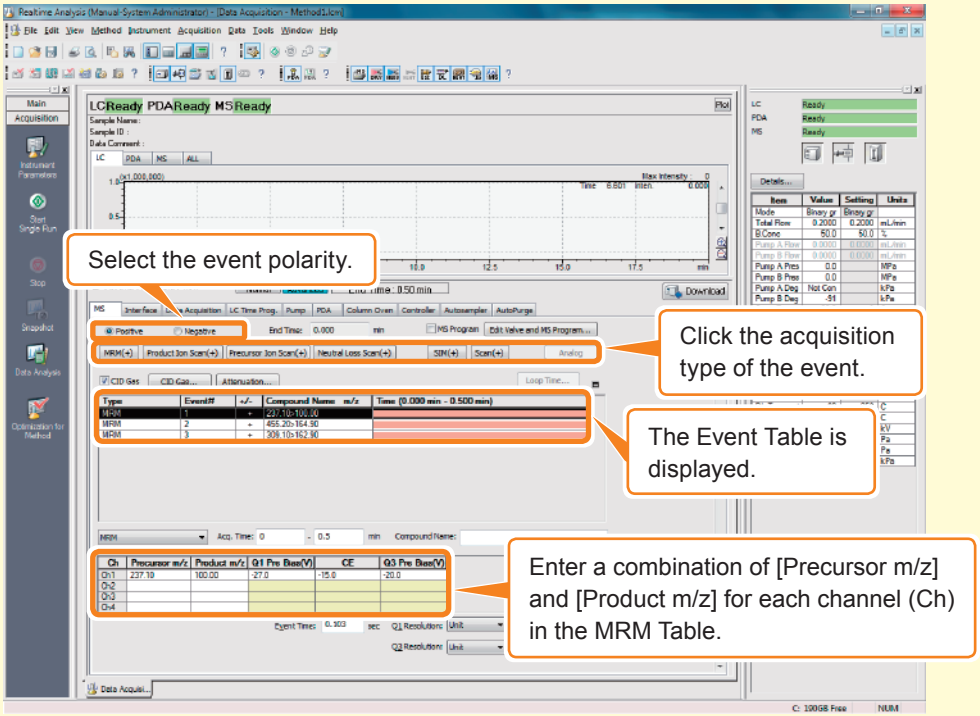
2 Set the MS instrument parameters.



▼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."





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].

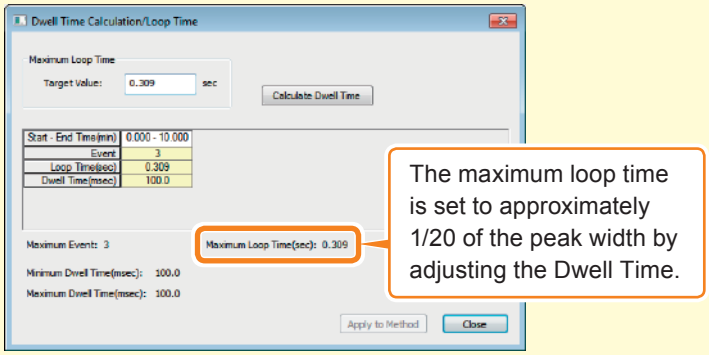
Hint When compounds are different, please change and set the event number.

Hint Ch1 is used for the quantitative calculation.

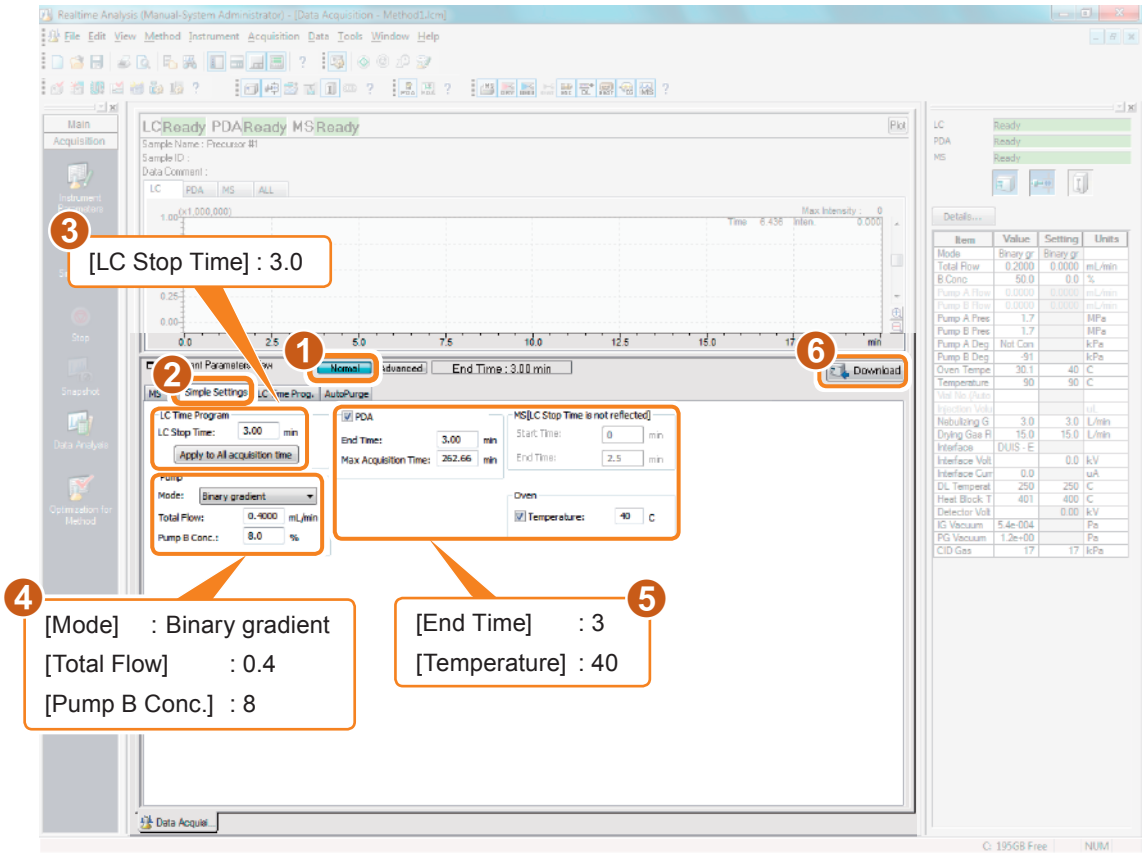
Reference "2 Data Acquisition" in *Operators Guide*.

▼Tips Check the loop time

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

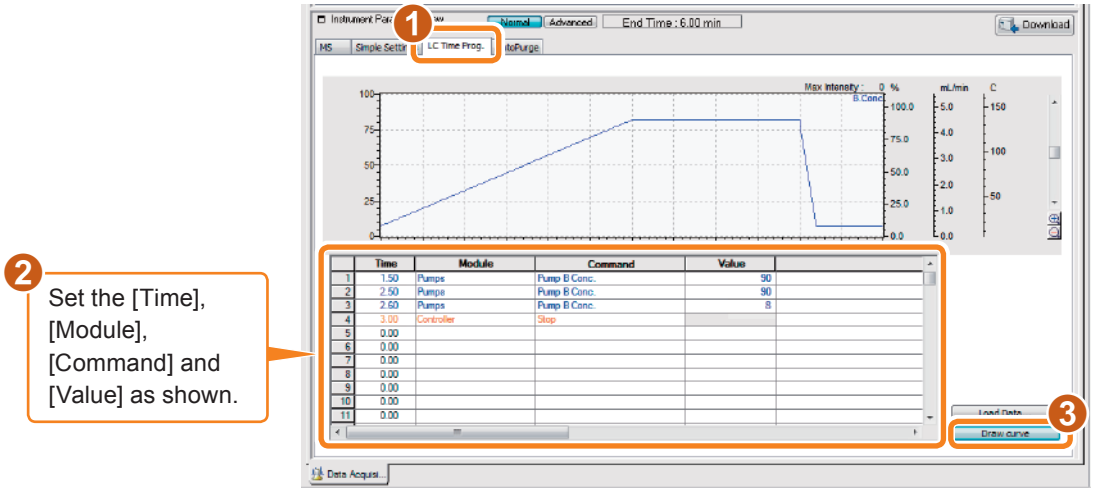


3 Set the LC instrument parameters.



4 Set the Gradient conditions.

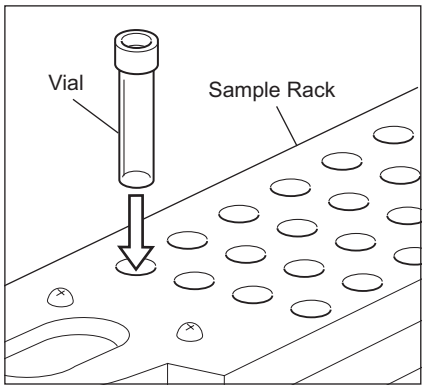
Change the mobile phase mixture ratio.



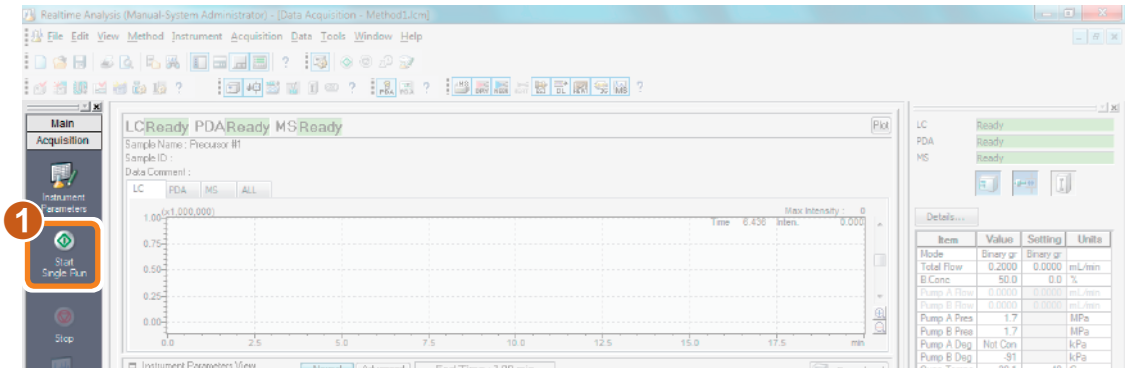
2.6 Execute Single Run to Determine Retention Time

1 Place the samples in the autosampler.

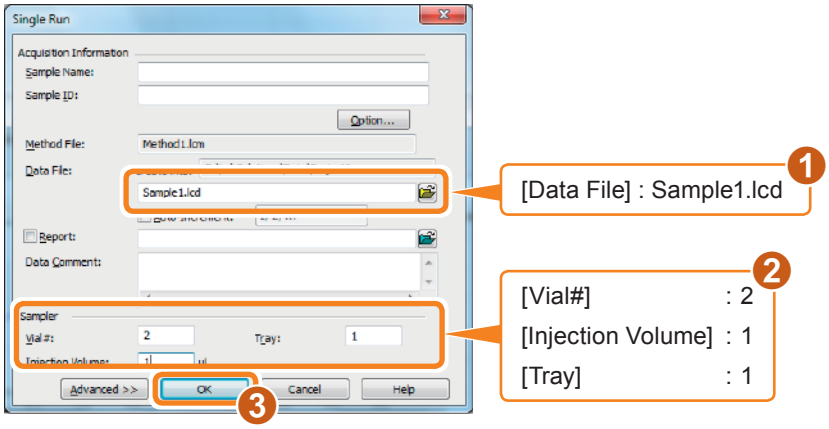
Vial 2, analytes A, B, C 0.05 ng/µL mixture



2 Open the [Single Run] sub-window.



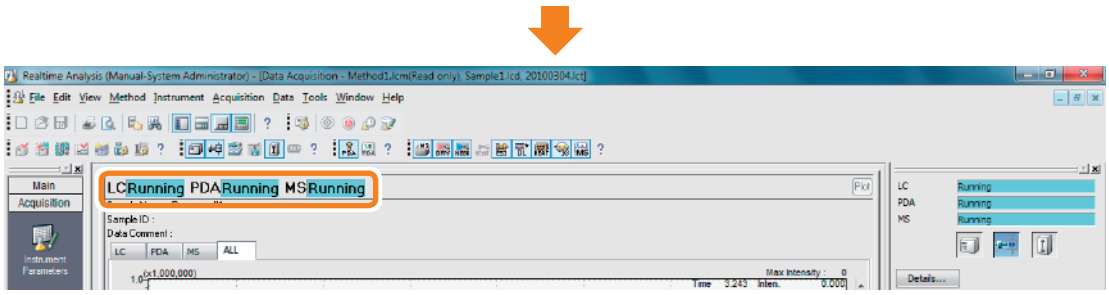
3 Set the conditions for a single run.



❶ [Data File] : Sample1.lcd

❷ [Vial#] : 2
[Injection Volume] : 1
[Tray] : 1

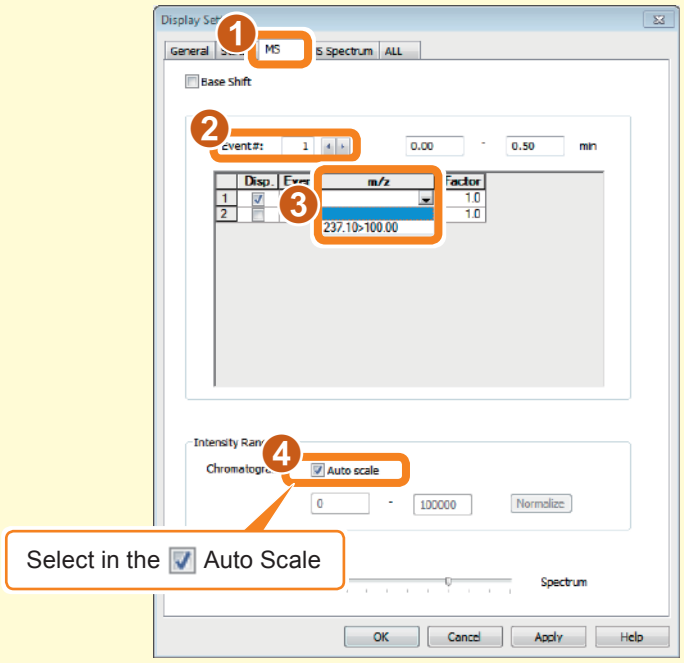
❸ Click [OK] to start the acquisition.



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

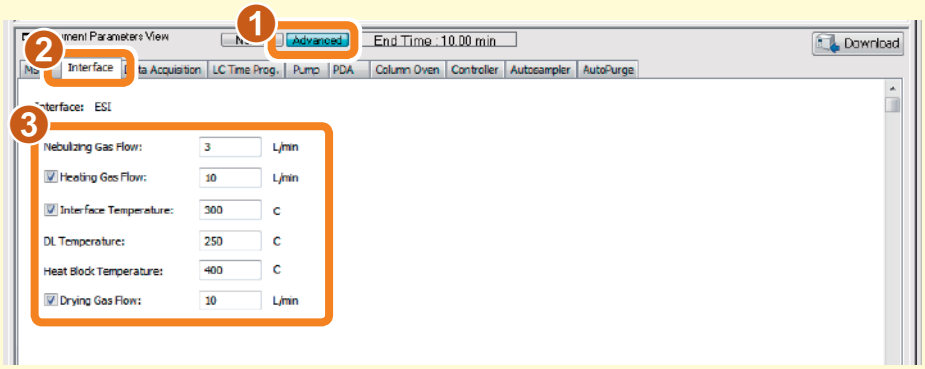
▼Tips Change the Displayed Chromatograph

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



▼Tips Set the interface temperature and the gas flow

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

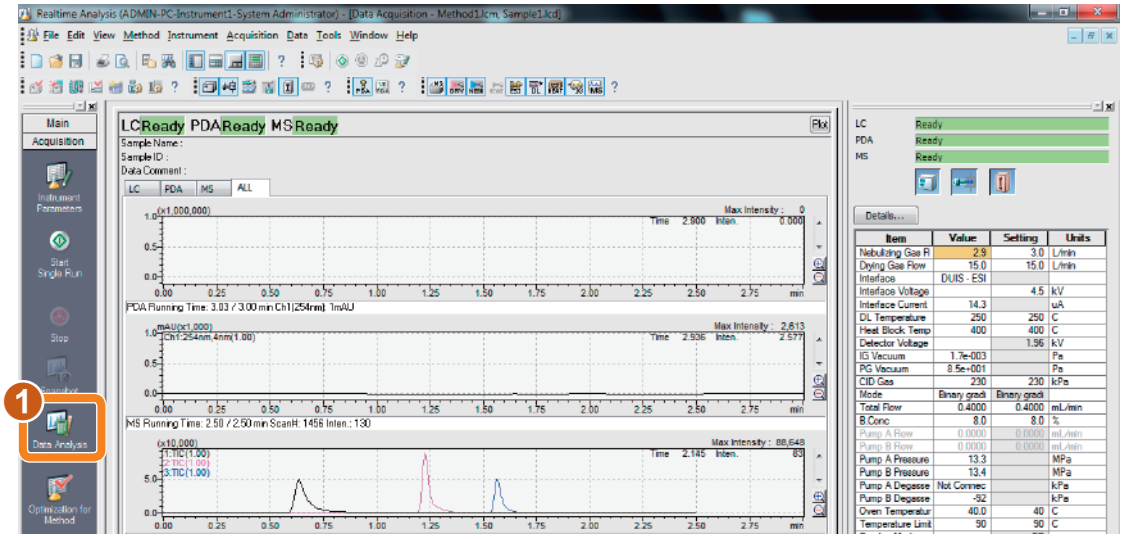


Chapter 3. Confirm Single Run Results

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

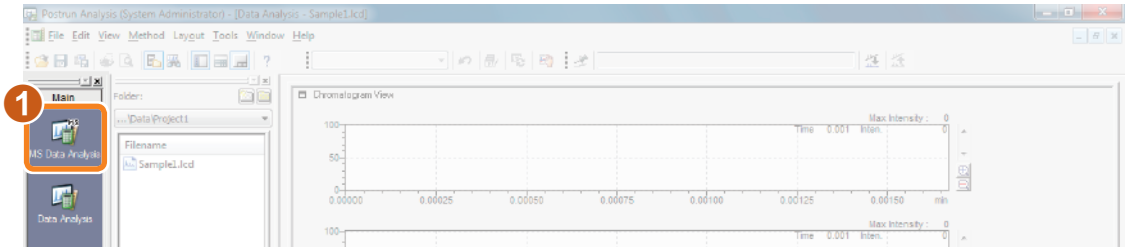
Display the results of single run in the [MS Data Analysis] window, and set the parameters for quantitative data acquisition.

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

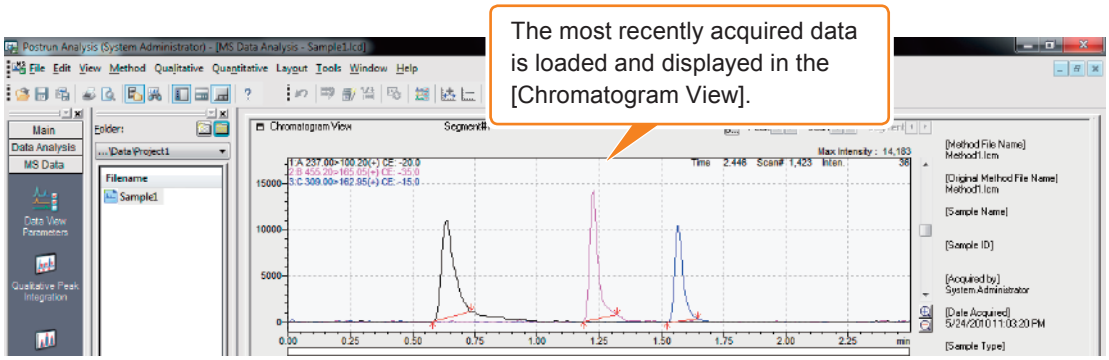


The [Postrun Analysis] program starts.

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



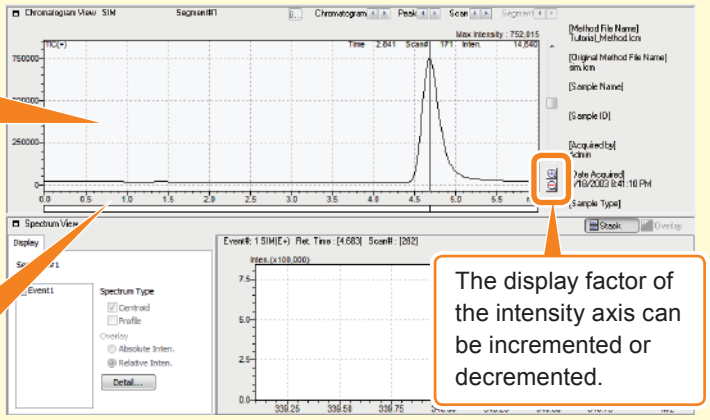
The [MS Data Analysis] window opens.



▼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.

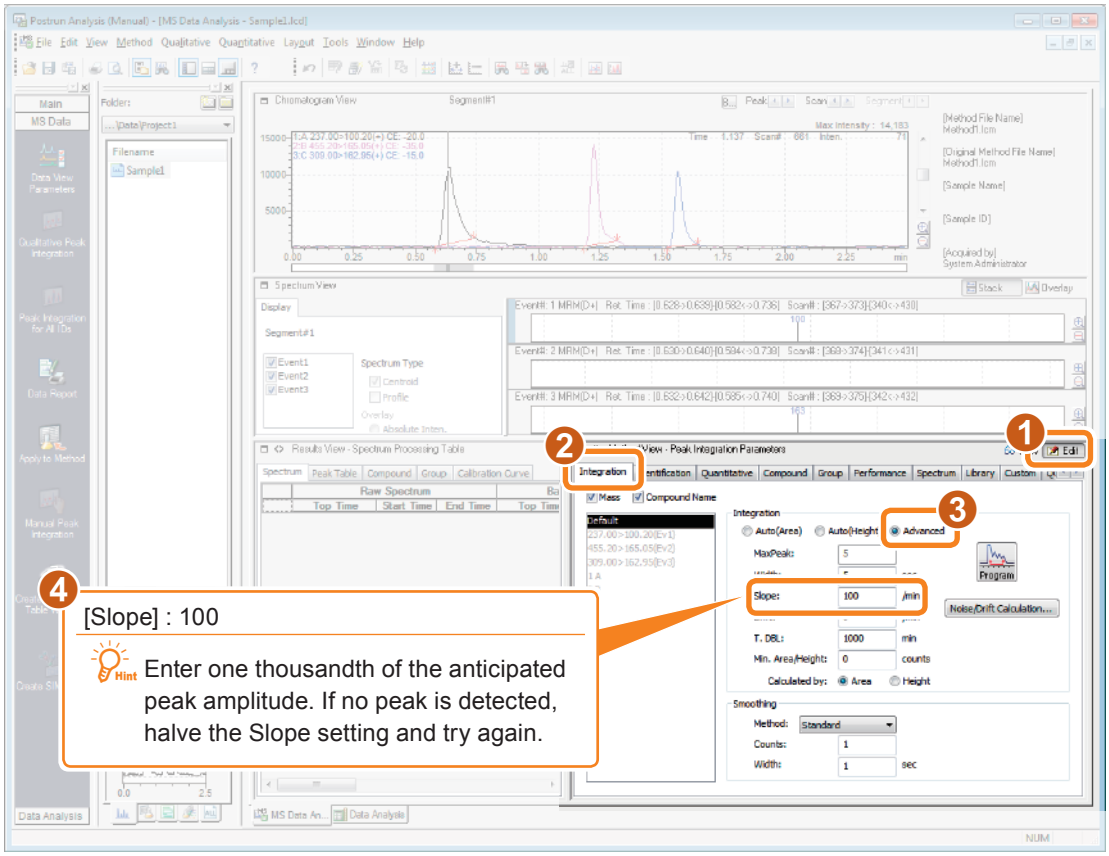


The display factor of the intensity axis can be incremented or decremented.

3.2 Compound Table Setup

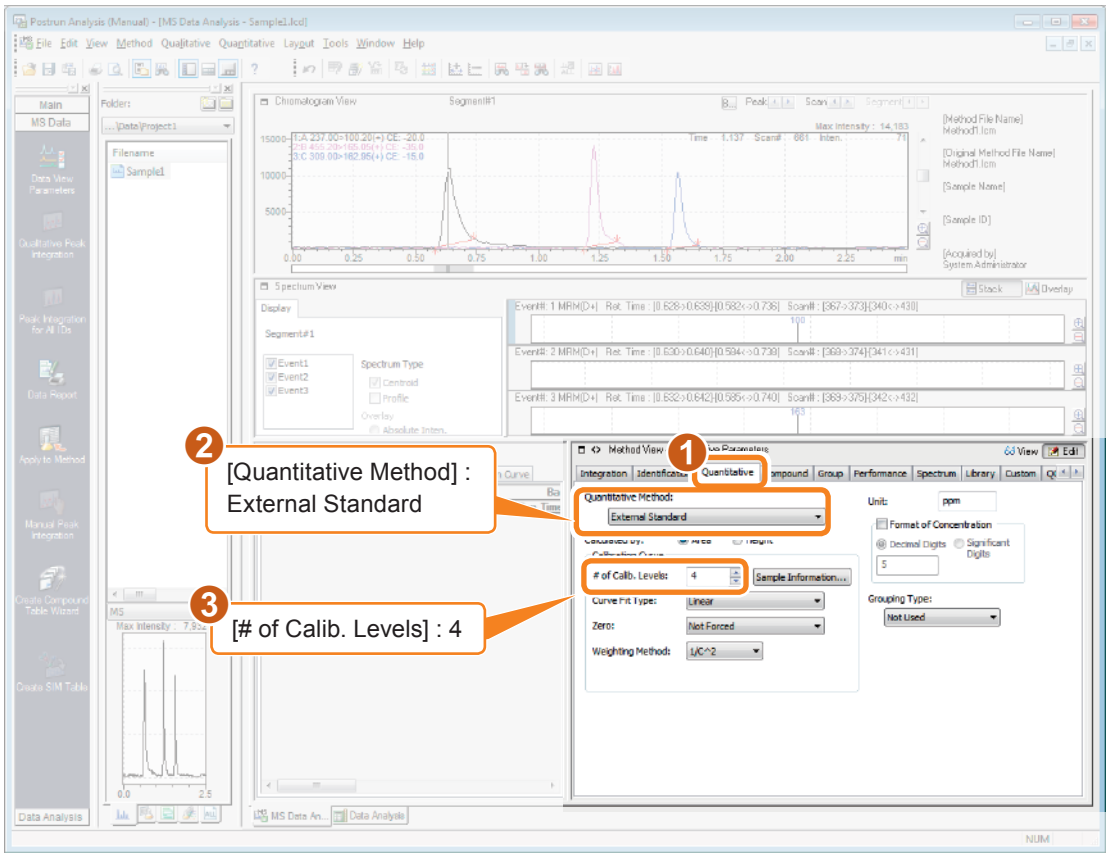
For quantitative processing, use a "standard sample" with a known concentration to create a "calibration curve".
Use this calibration curve to calculate the concentration of the components in the unknown data source.
In this example, we create a calibration curve by injecting 1 µL of 0.01, 0.05, 0.1 and 0.5 ng/µL standard sample containing analytes A, B and C.

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

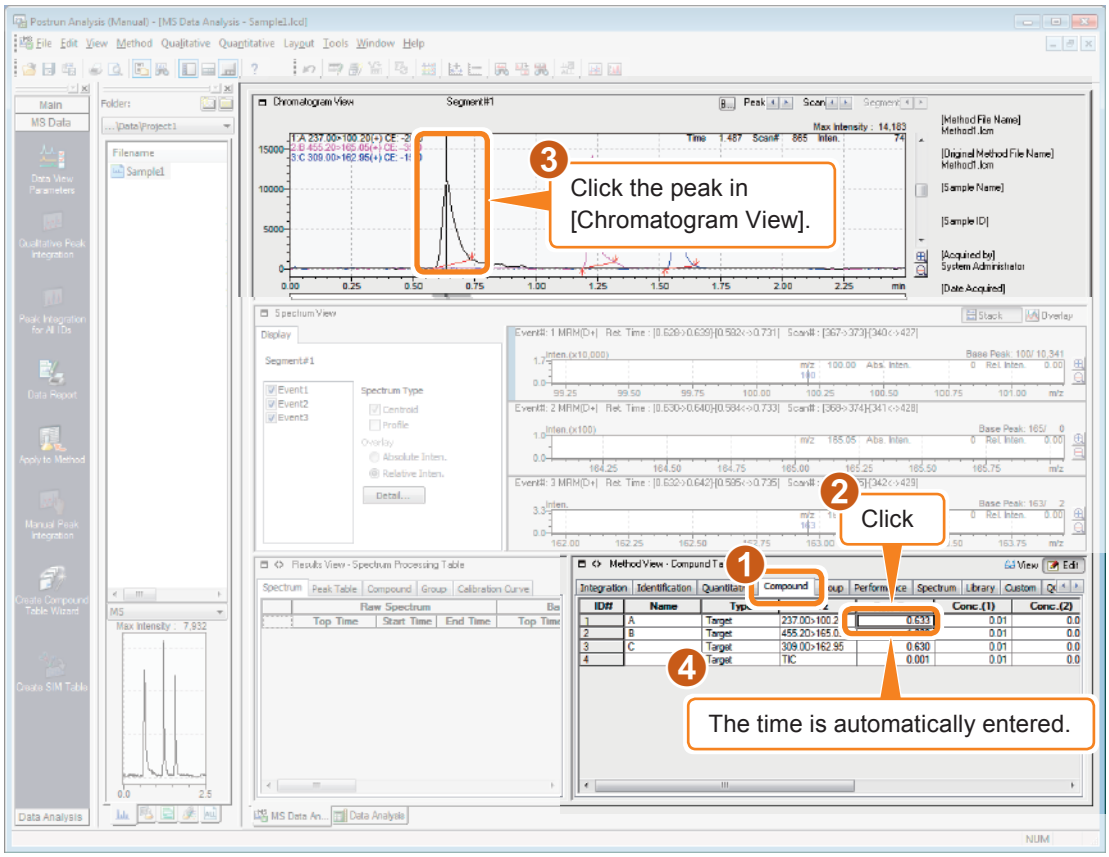


Hint The Edit and View switch between the [Edit Mode] and the [View Mode]. Parameters cannot be altered in the [View Mode]. Switching from [Edit Mode] to [View Mode] applies the changes and executes the related operations.

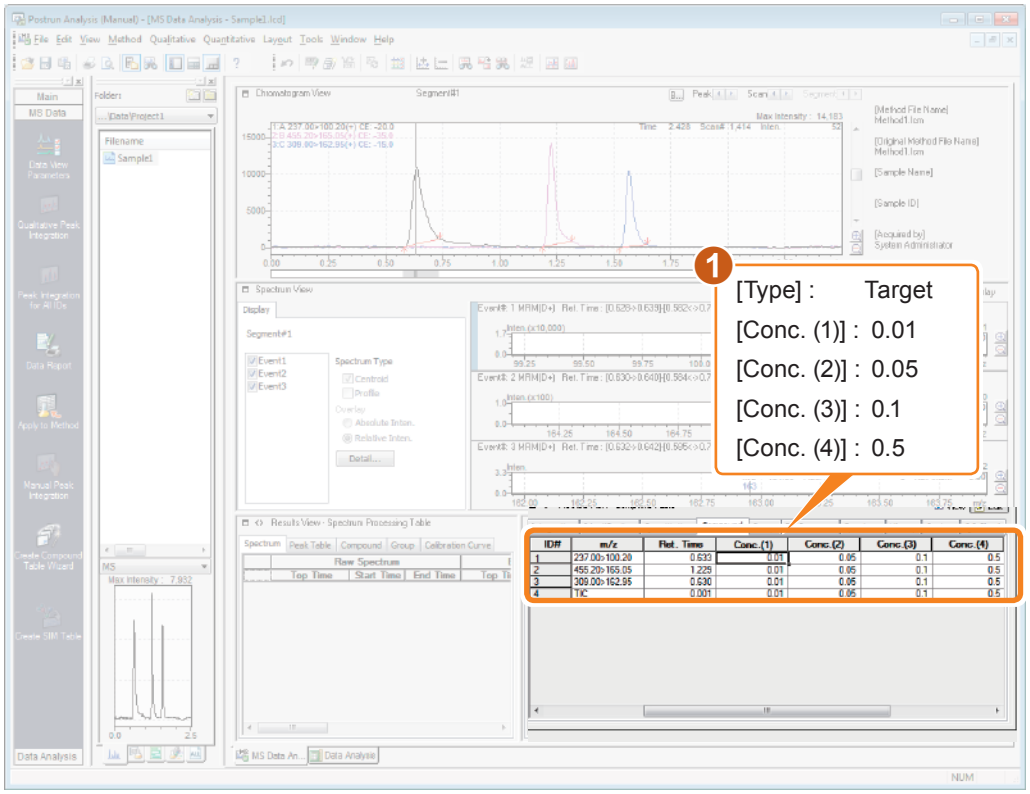
2 Enter the quantitative parameters.



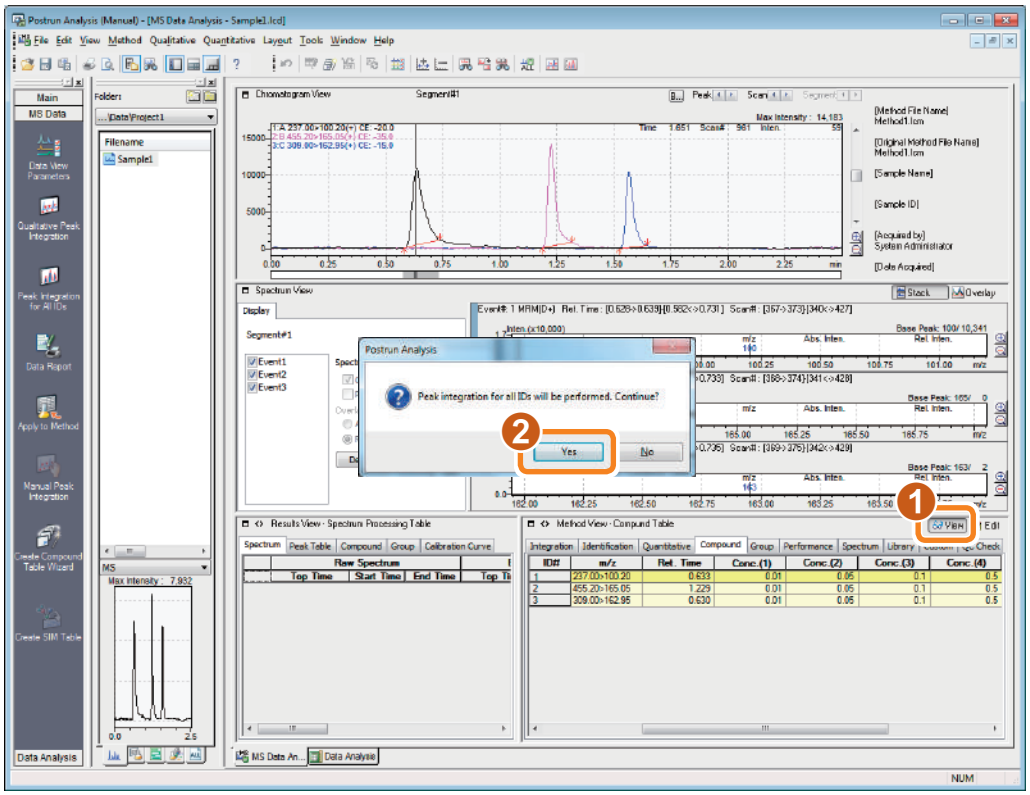
3 Enter the retention time of the sample in the Compound Table.



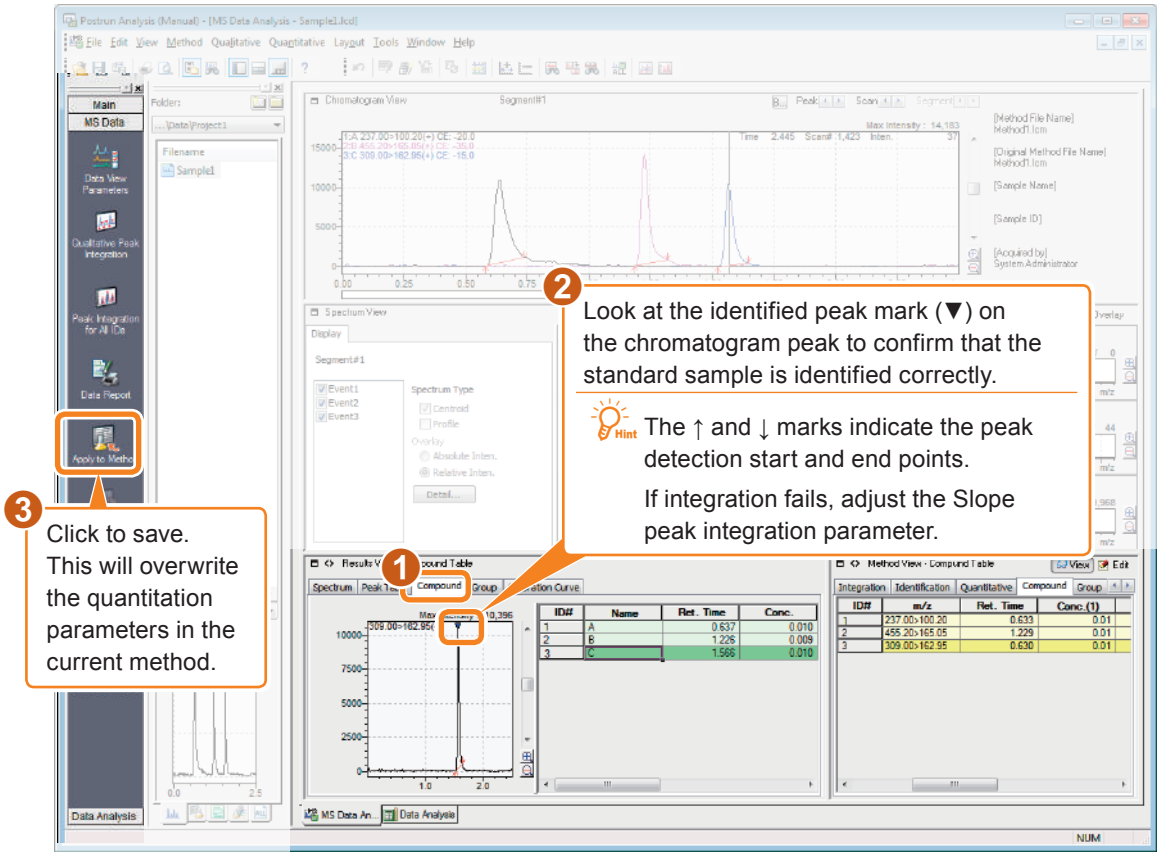
4 Enter the concentration of the standard sample in the Compound Table.

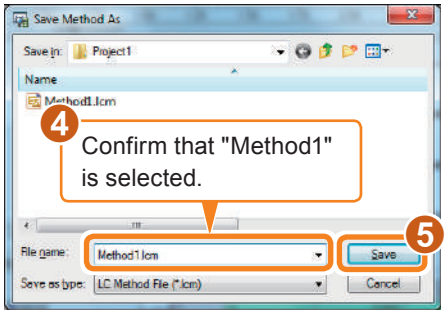


5 Click the View to exit [Edit Mode]and execute quantitative peak integration.



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

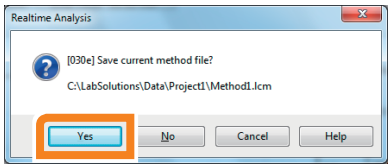




Hint
If a peak is detected but not identified, check the retention time in the compound table and window width in the identification parameters.

The method file is overwritten and saved.

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

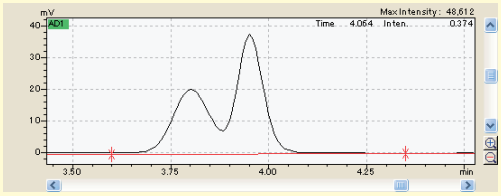


Click [Yes] to continue processing.

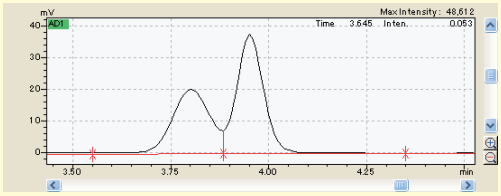
▼Tips Simple Peak Integration Parameters

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

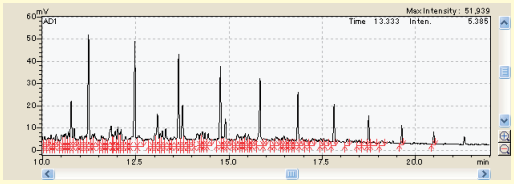


With the [Width] set to 30, the data is processed as one peak.

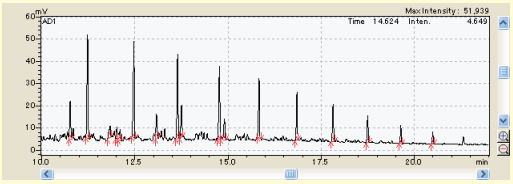


With the [Width] set to 10, the data is processed as two peaks.

Slope Setting Example



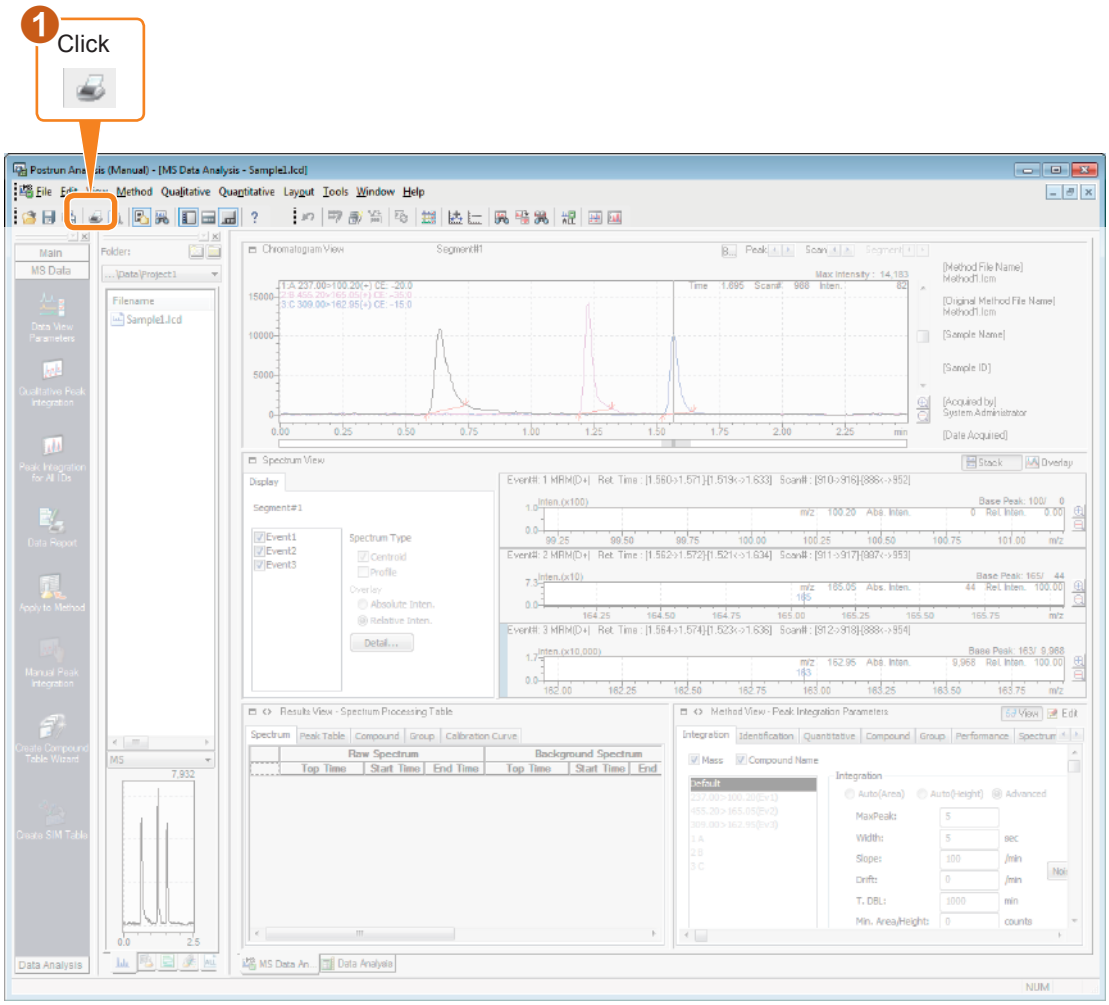
When the [Slope] is set to 1000, even small noise peaks are detected.



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

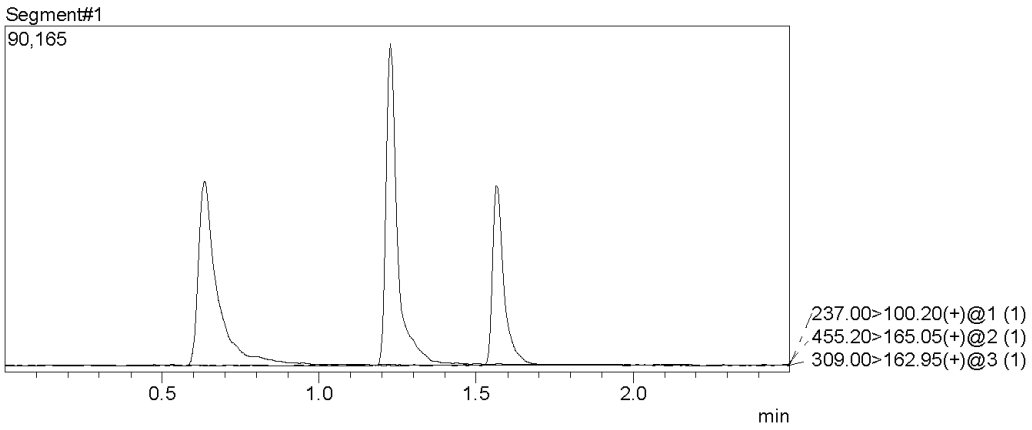


Graphic Image Printout Example

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

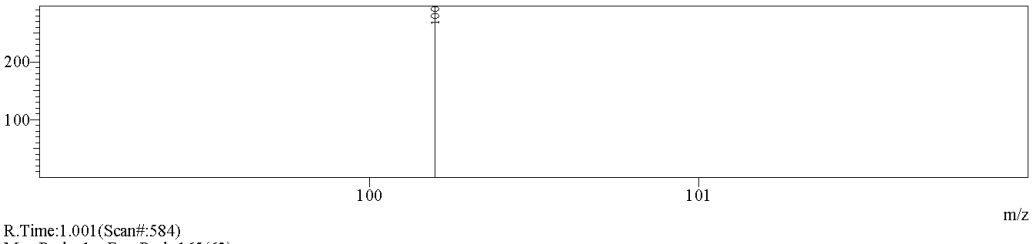
Sample ID :
Data Filename : Sample1.lcd
Date Acquired :5/25/2010 2:38:05 PM

<Chromatogram>

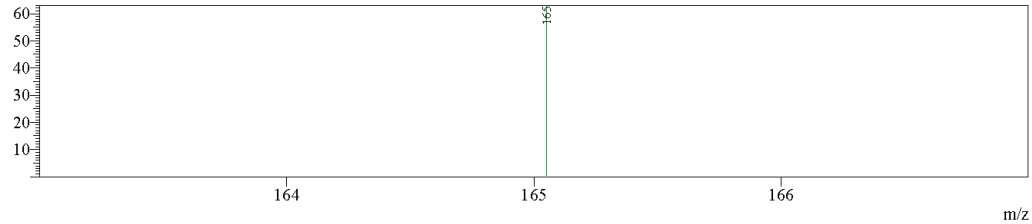


<Spectrum>

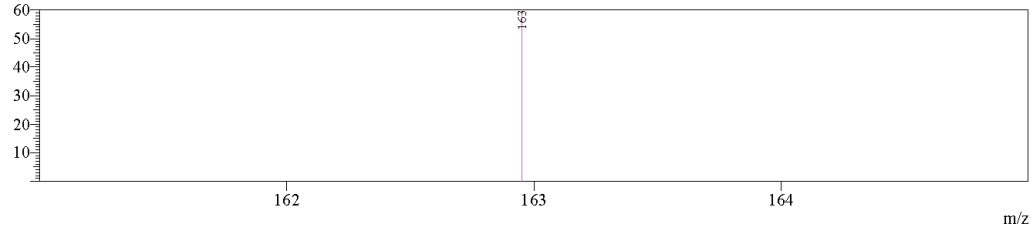
R.Time:0.999(Scan#:583)
MassPeaks:1 BasePeak:100(297)
Polarity:Positive Segment 1 - Event 1



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



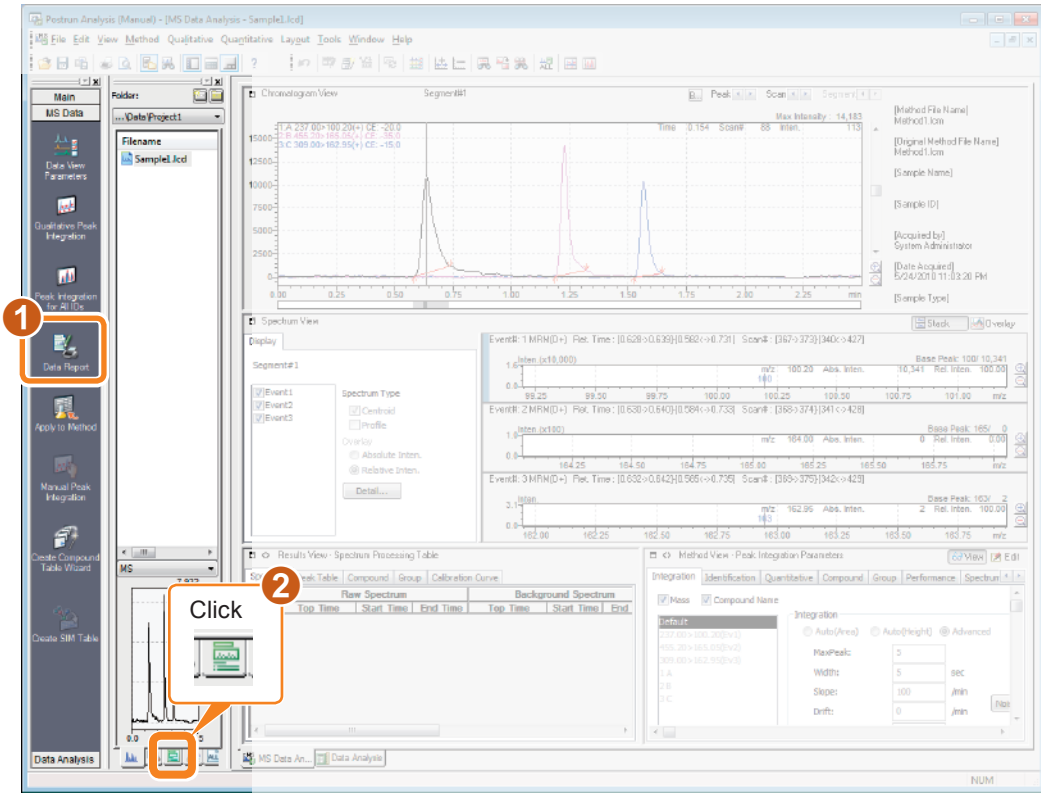
R.Time:1.003(Scan#:585)
MassPeaks:1 BasePeak:163(60)
Polarity:Positive Segment 1 - Event 3

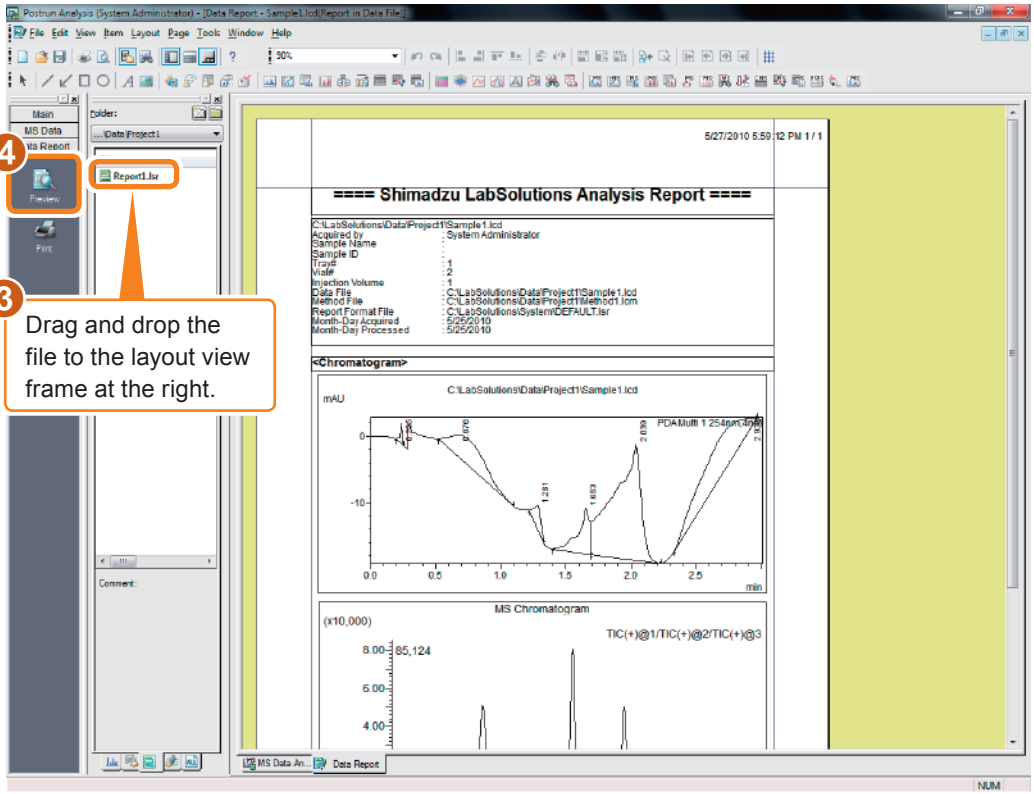


Layout the report format

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.



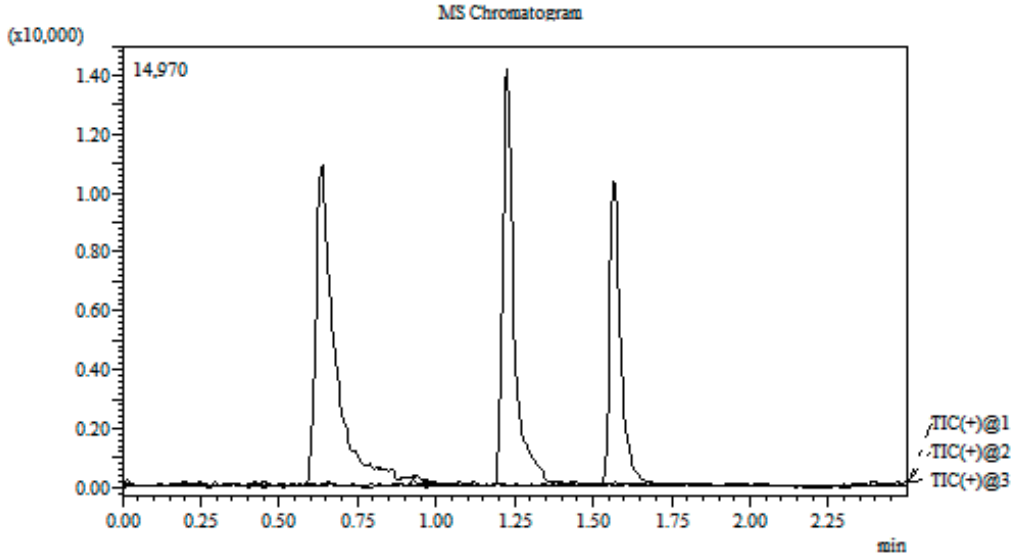


Report Format Printout Example

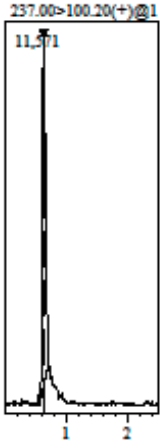
Sample Information

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.lcd
Method File	: Method1.lcm
Original Method File	: Method1.lcm
Report Format File	: DEFAULT.lsr
Tuning File	: Tuning.lct
Processed by	: Manual
Date Processed	: 6/14/2013 3:09:25 PM

MS Chromatogram



Mass Quant Graph



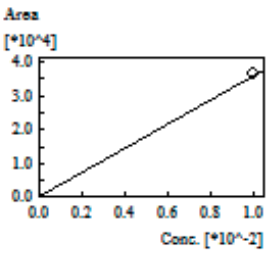
ID#: 1
Type:
Name:

Ret.Time: 0.637
Area: 35904
Conc.: 0.010ppm
Event:1

m/z: 237.
Target
A

Calibration Curve

ID# : 1 m/z : 237.00>
Name : A
Function : f(x)=3.61950e+006*x+0
Rr1=1.000000 Rr2=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



#	Conc.(Ratio)
1	0.01

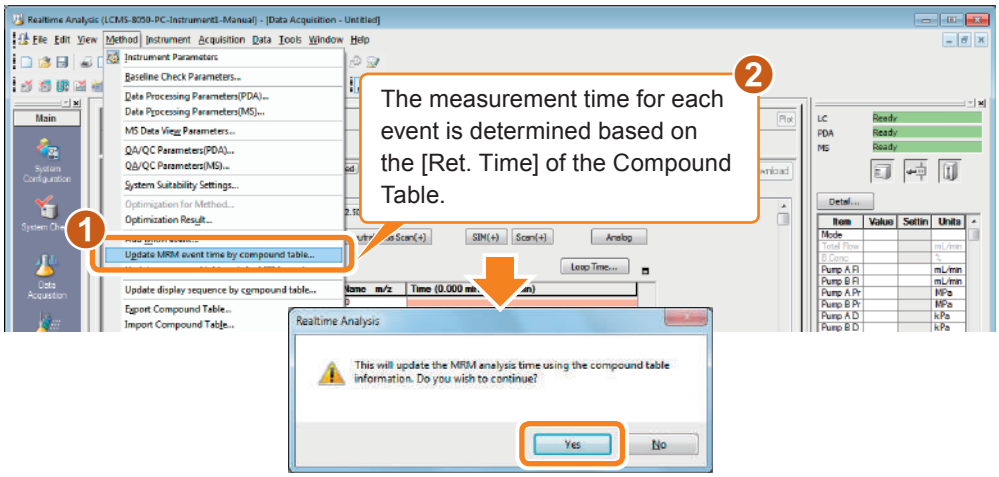
MeanArea	Area
36195	36195

Chapter 4. Realtime Batch

4.1 Create a Batch Table

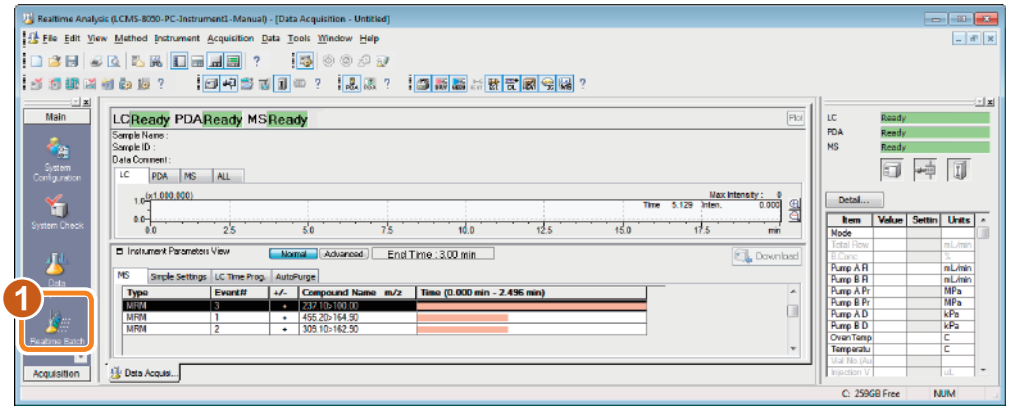
Select a batch table using the method file created for realtime sequential batch analysis.
Here we perform quantitative calculation for a sample containing A, B and C at 0.075 ng/µL each.

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



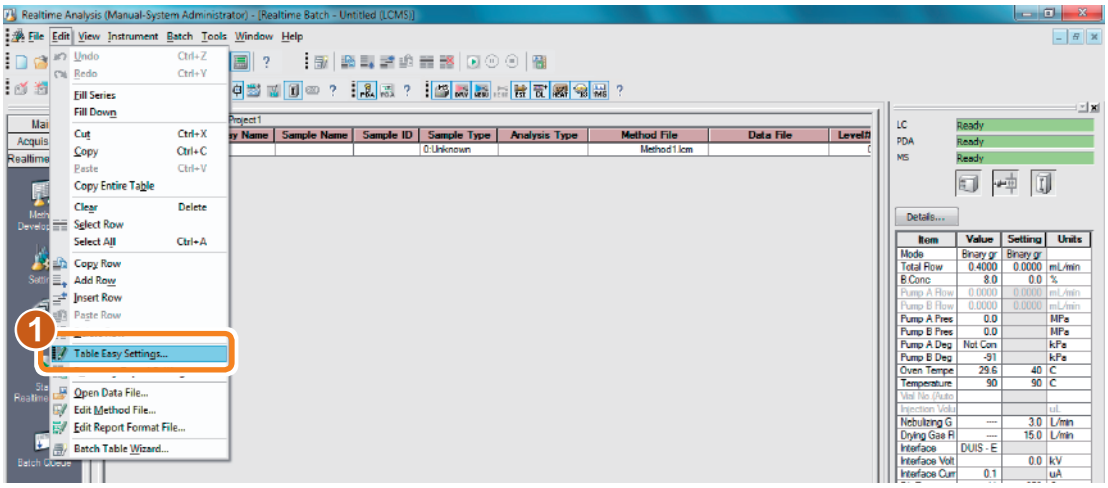
The measurement time for each event is determined based on the [Ret. Time] of the Compound Table.
The start time of measurement = [Ret. Time]
- [process time in the identification parameters]
The end time of measurement = [Ret. Time]
+ [process time in the identification parameters]

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

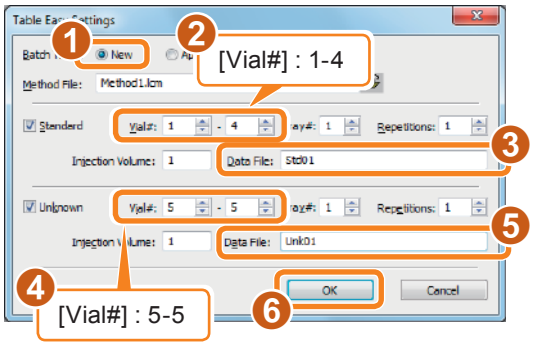


The [Batch Table] window is displayed.
Create the Batch Table using the following procedure.
Use the first four rows for the standard sample and the fifth row for the unknown sample.

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

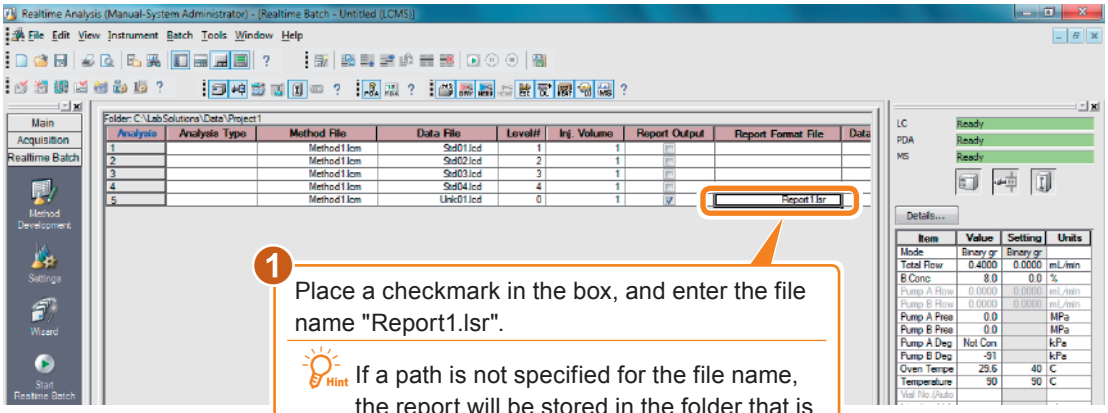


4 Make the following settings on the [Table Easy Settings] sub-window.

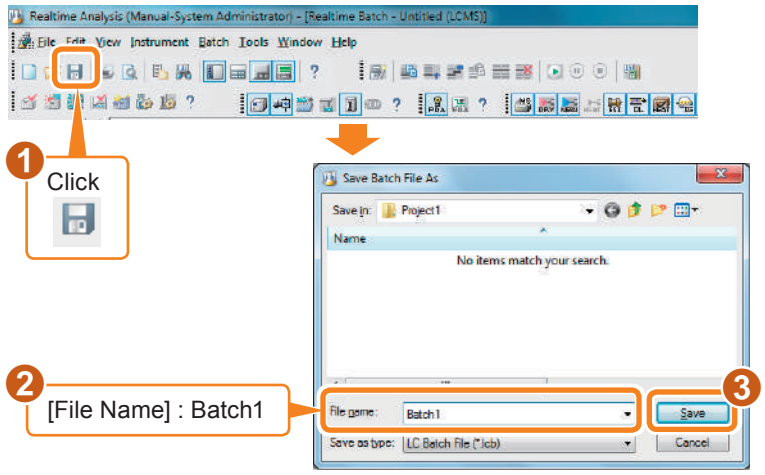


A five-row Batch Table is created.

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



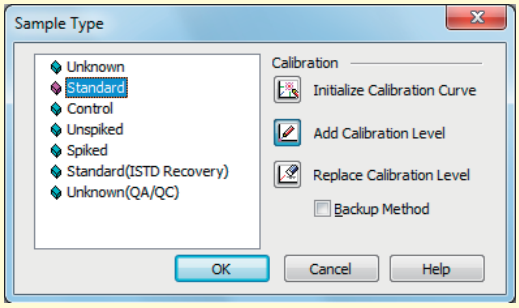
6 Save the Batch Table settings.



▼Tips Batch Table Settings

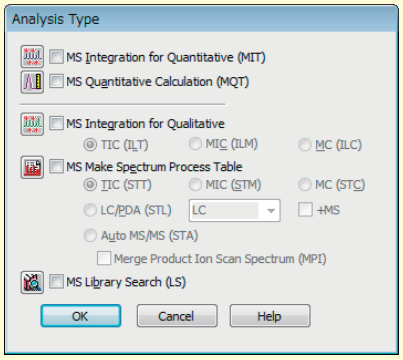
Sample Type

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

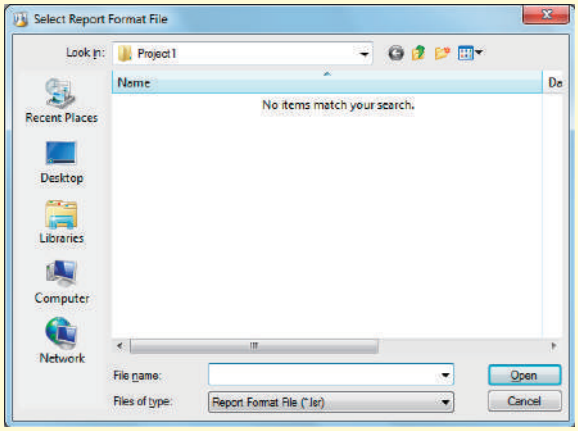
Enter a level number for all of the standard samples.

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.

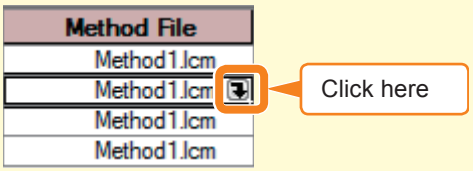


Reference *Help*

Tips — Table Entries

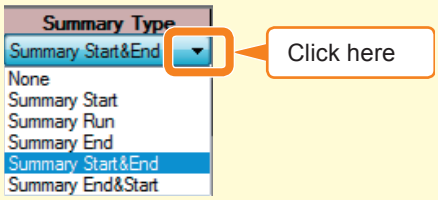
Popup Windows (for complex settings)

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.



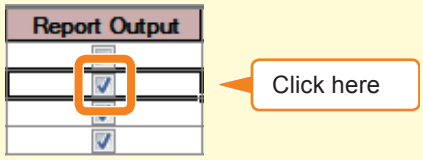
Drop-Down List (to select from a list of choices)

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)

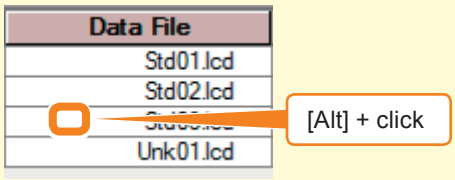
Click the displayed check box to select or clear a checkmark.



[Alt] + click (to open a file)

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

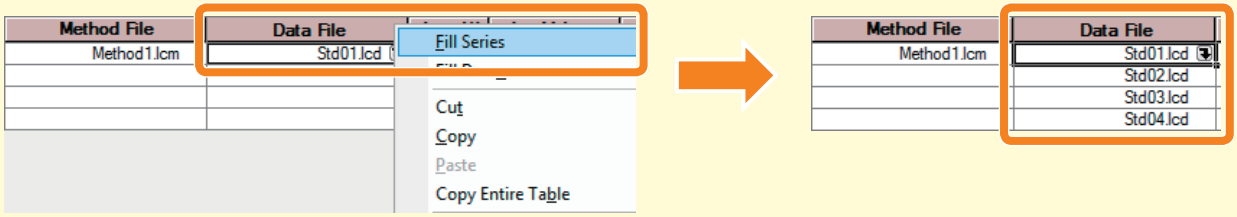
The data or method file for the selected row in a Batch Table can also be opened from the [Edit] menu.



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.

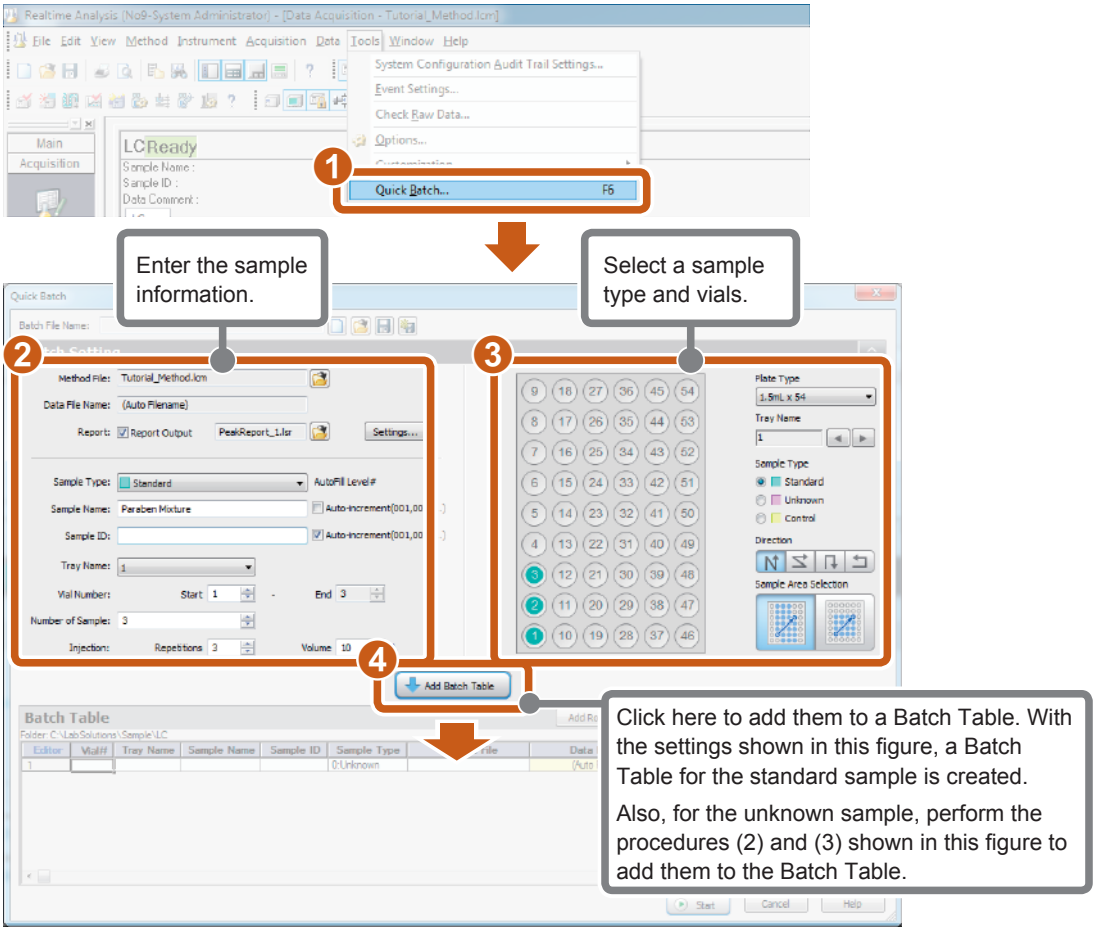
Hint To add rows, select [Add Row] from the right-click menu of the batch table.

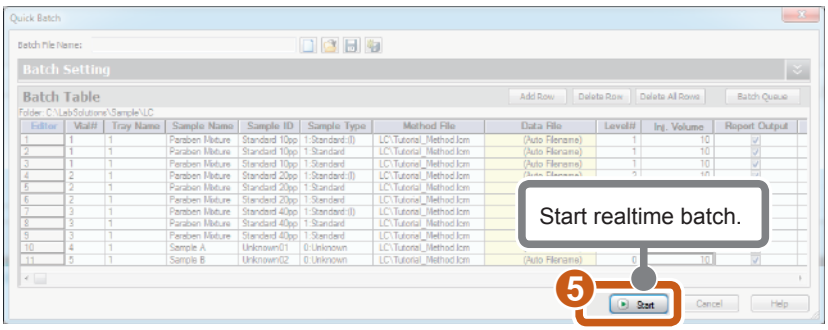
LabSolutions

SUPPLEMENT

Create a Batch Table Using Quick Batch

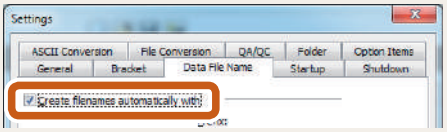
You can also create a Batch Table using quick batch.





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

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

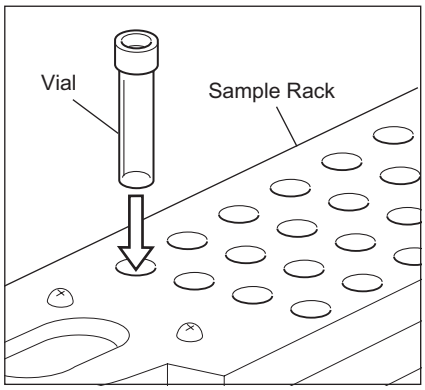


4.2 Realtime Batch Processing

Execute batch processing.

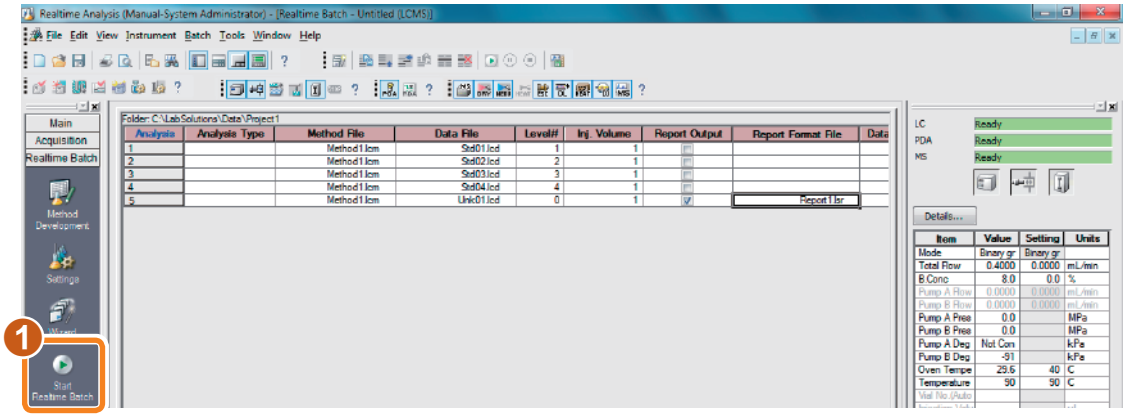
1 Place the samples in the autosampler.

Vial 1, sample solution containing A, B, C at 0.01 ng/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.



Hint Click Stop to stop batch processing.

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

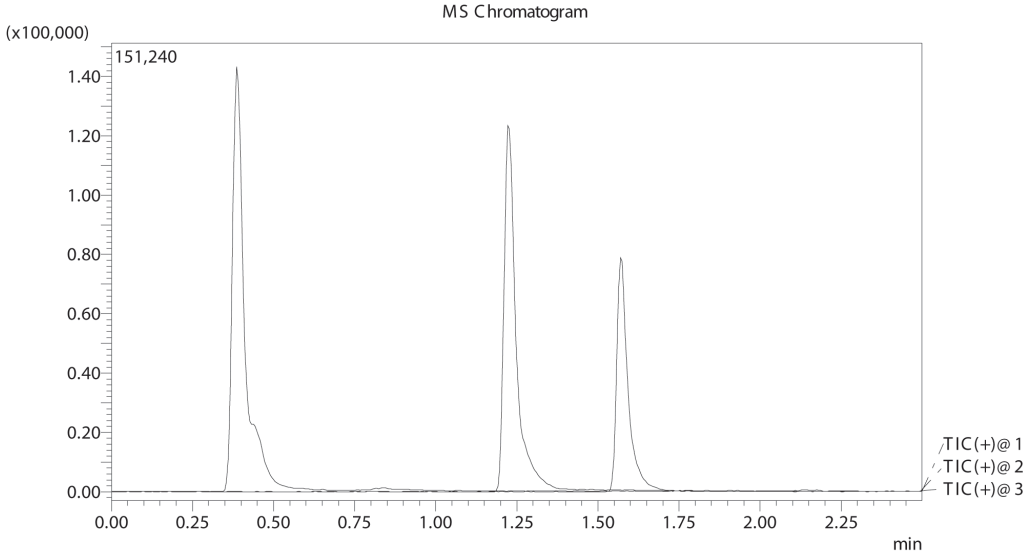
Hint You can take a snapshot to view the data during acquisition. To take a snapshot, click Snapshot in the [Data Acquisition] assistant bar during acquisition.

Realtime Batch Report Printout Example

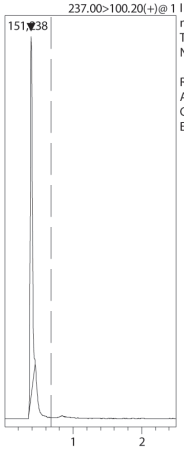
Sample Information

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

MS Chromatogram



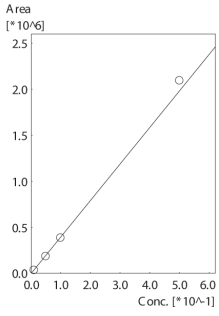
Mass Quant Graph



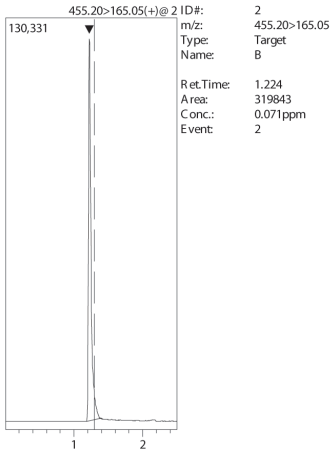
ID#:	1
m/z:	237.00>100.20
Type:	Target
Name:	A
Ret.Time:	0.387
Area:	279676
Conc.:	0.071ppm
Event:	1

Calibration Curve

ID# : 1 m/z : 237.00
Name : A
Function : f(x)=3.98377e+006*x-4014.10
Rr1=0.9988958 Rr2=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

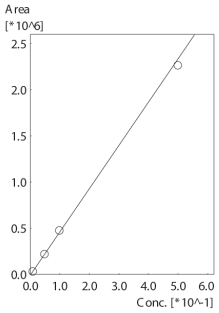


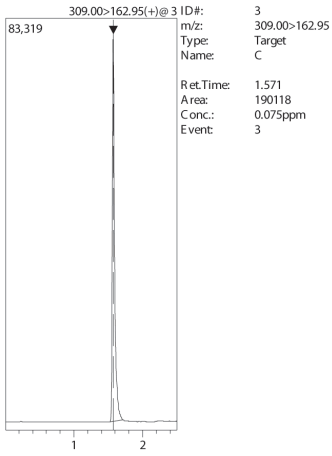
ID#: 2
m/z: 455.20>165.05
Type: Target
Name: B

Ret.Time: 1.224
Area: 319843
Conc.: 0.071ppm
Event: 2

ID# : 2 m/z : 455.20
Name : B
Function : f(x)=4.71632e+006*x-15222.7
Rr1=0.9994071 Rr2=0.9988146
MeanRF: 4.213971e+006 RF SD: 7.039121e+005 RF %RSD: 16.704248
FitType : Linear
ZeroThrough : Not Through
Weighted Regression : 1/C^2
Quantitation Method : External Standard

#	Conc.(Ratio)	MeanArea	Area
1	0.01	31817	31817
2	0.05	219764	219764
3	0.1	475316	475316
4	0.5	2262891	2262891



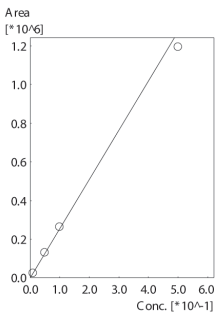


ID#: 3
m/z: 309.00>162.95
Type: Target
Name: C

Ret.Time: 1.571
Area: 190118
Conc.: 0.075ppm
Event: 3

ID# : 3 m/z : 309.00
Name : C
Function : f(x)=2.54851e+006*x-984.917
Rr1=0.9985671 Rr2=0.9971363
MeanRF: 2.516006e+006 RF SD: 1.286267e+005 RF %RSD: 5.112336
FitType : Linear
ZeroThrough : Not Through
Weighted Regression : 1/C^2
Quantitation Method : External Standard

#	Conc.(Ratio)	MeanArea	Area
1	0.01	24275	24275
2	0.05	130160	130160
3	0.1	264742	264742
4	0.5	1192961	1192961



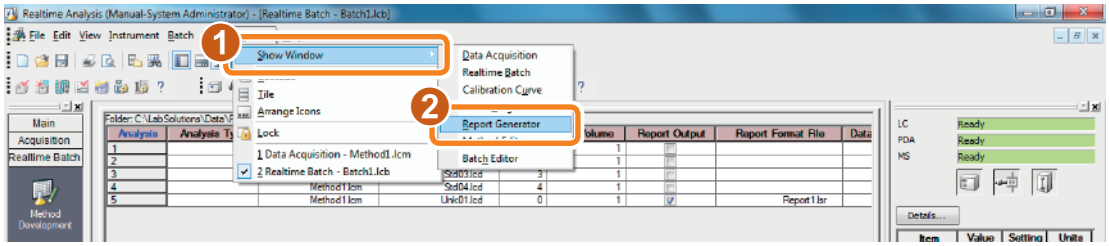
This example report for unknown sample (vial 5) shows the quantitated values for A, B and C. Also shown are the method calibration curves for A, B and C.

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

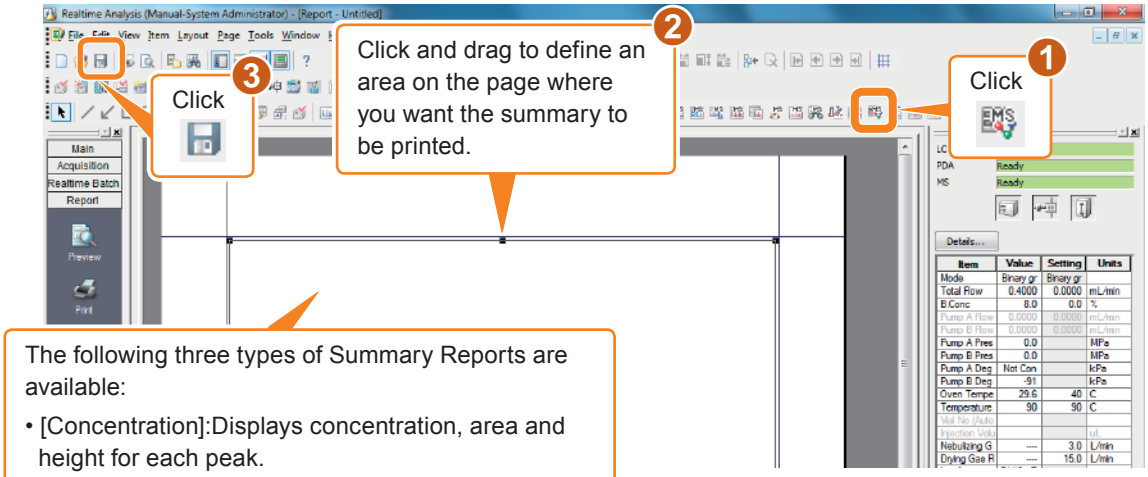
Prints a batch processing summary report (a simple combined report of two or more sets of analysis results).

1 Open the [Report] window.



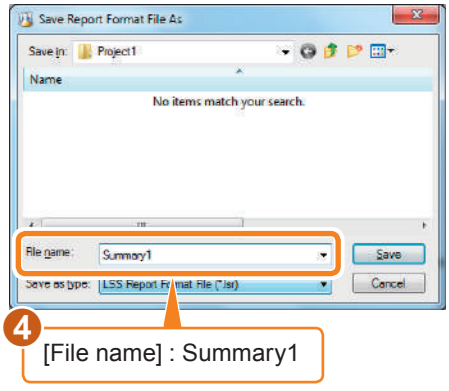
2 Create a summary report format with the [MS Summary (Compound)] report item.

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



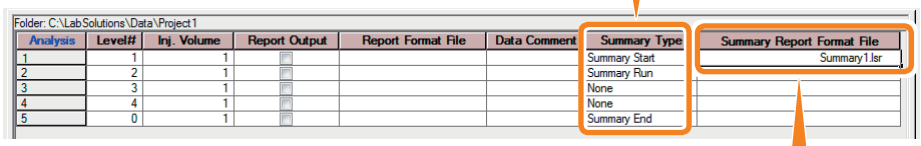
The following three types of Summary Reports are available:

- [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.

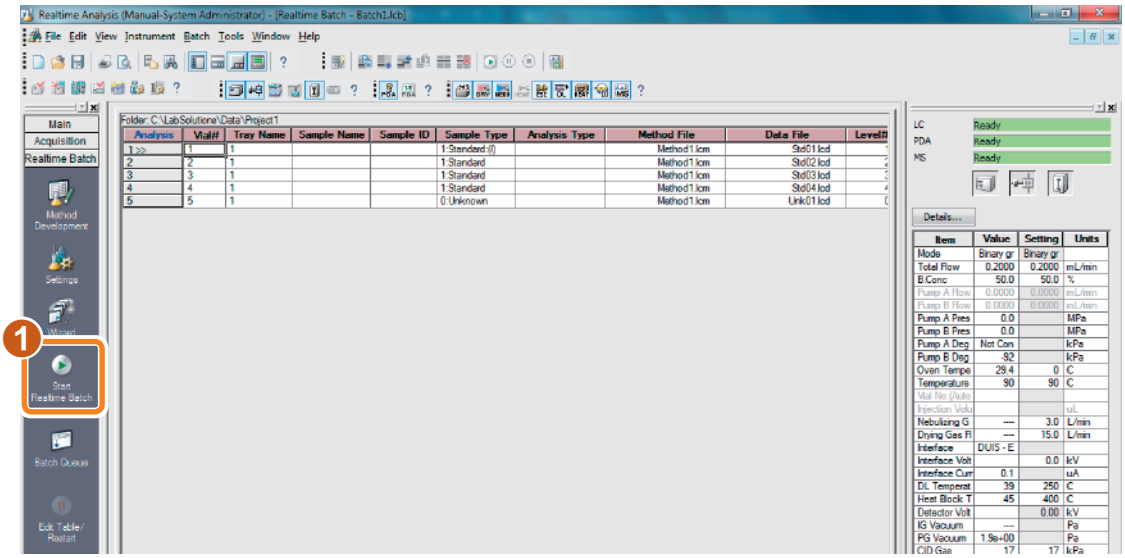
1. Enter [Summary Start] in the first data line to be included in the summary report.
   Enter [Summary Run] in all of the subsequent data lines to be included in the summary report.
   Enter [Summary End] in the last data line to be included in the summary report.



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

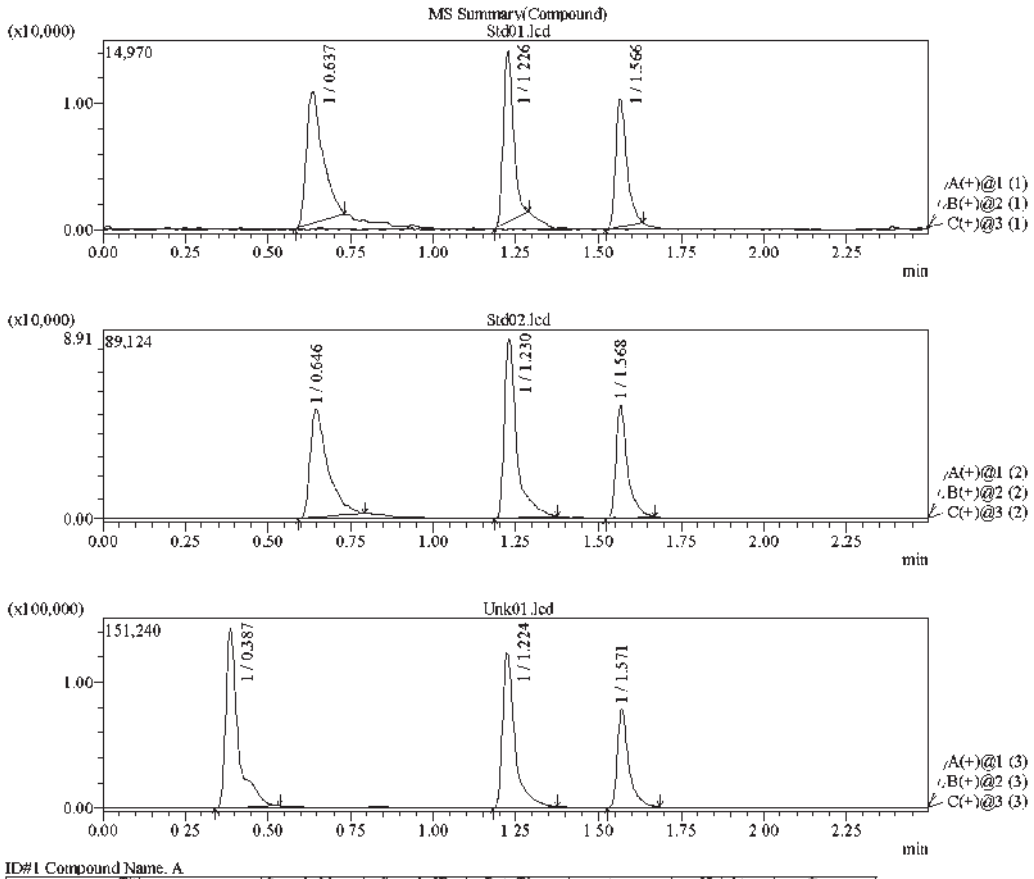
> Hint If [Summary Type] and [Summary Report Format File] are not displayed in the Batch Table, use the right-click menu to select [Table Style] and enable display of these items.

4 Start realtime batch processing.



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

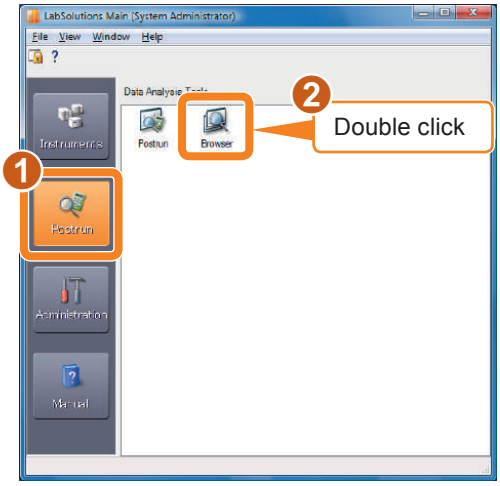
Title	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Std01.lcd			1.566	23534	10163	0.009
Std02.lcd			1.568	127900	53366	0.049
Unk01.lcd			1.571	186467	78613	0.073
Average			1.568	112634	47381	0.044
%RSD			0.164	73.275	73.058	73.335
Maximum			1.571	186467	78613	0.073
Minimum			1.566	23534	10163	0.009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

Chapter 5. Quantitative Data Analysis

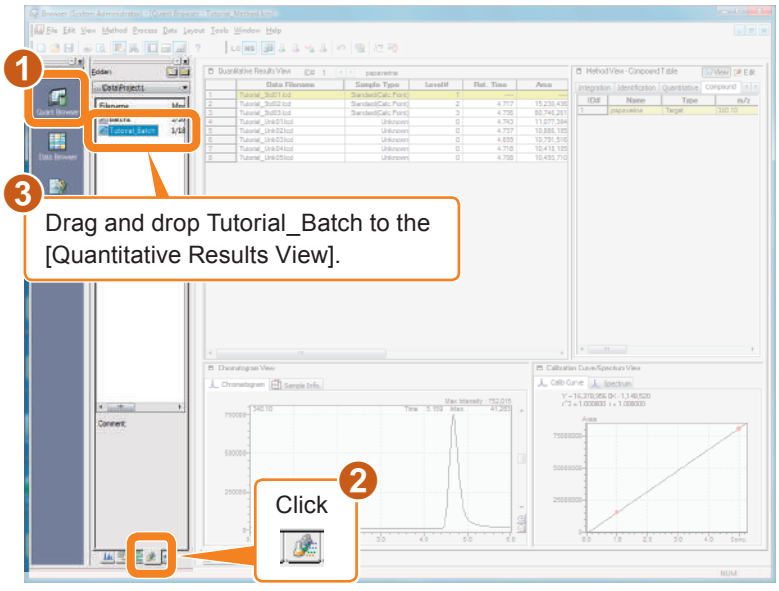
5.1 Confirm Quantitative Results in the [Quant Browser] Window

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

1 Start the [Browser] program.

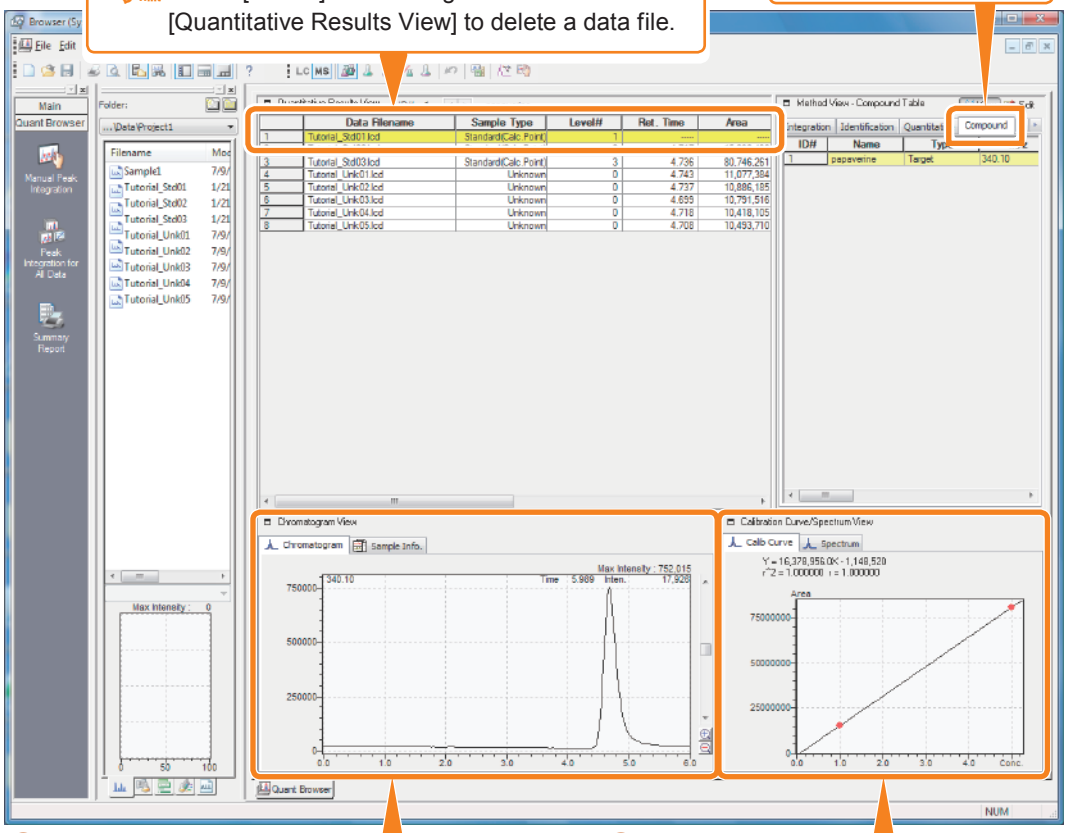


2 Load the sample data.



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.

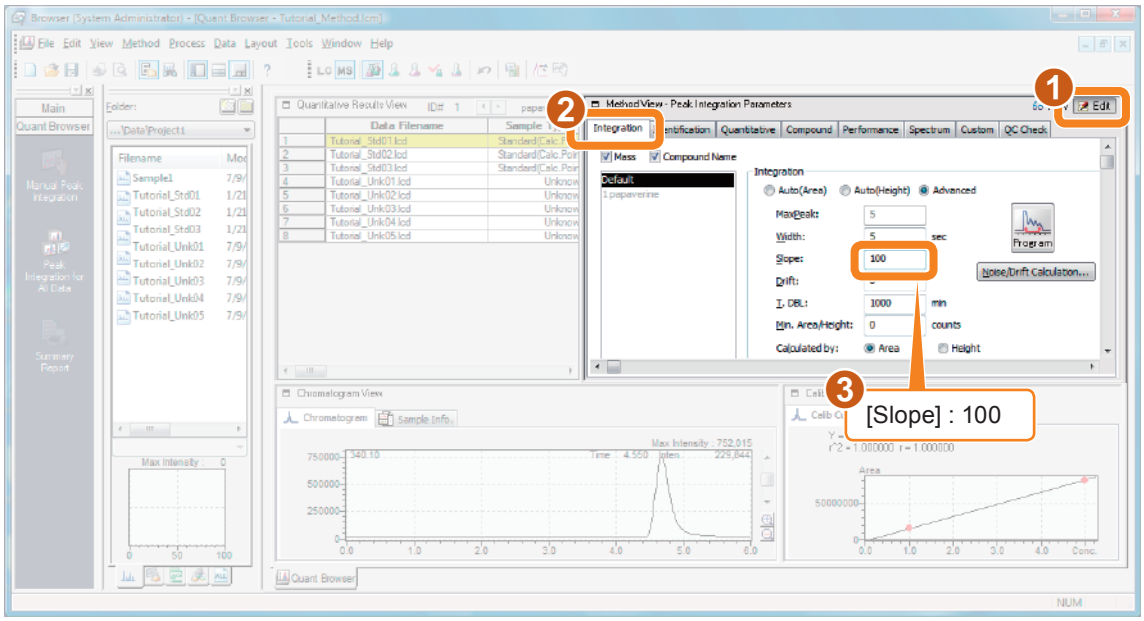
The calibration curve of the selected compound in the [Method View] is displayed.

5.2 Edit Integration Parameters and Re-Integrate

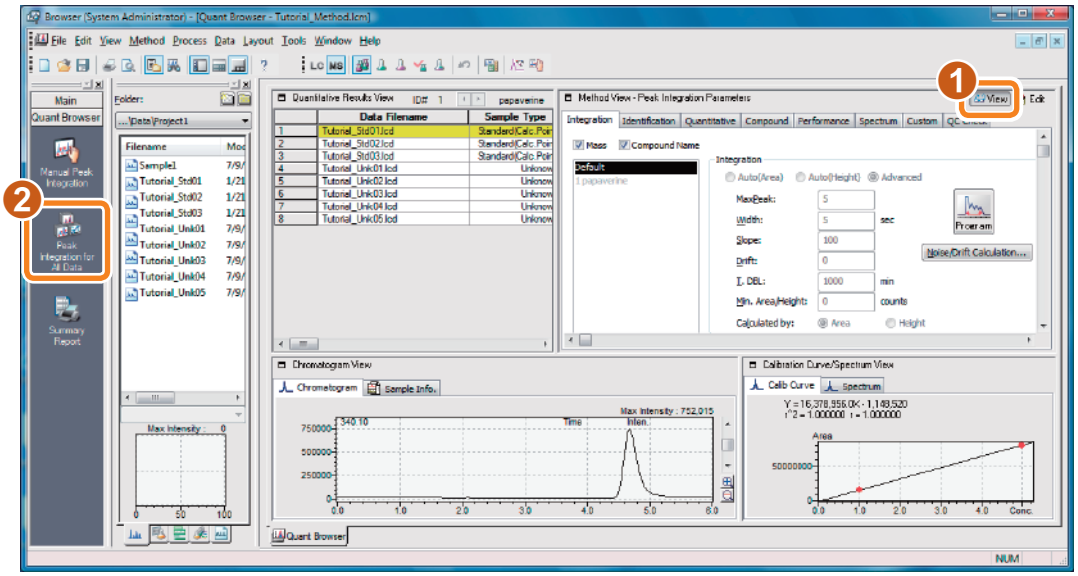
The sample data on the previous page is quantitative data for a three-point absolute calibration curve. However, if the area value for the first line of data (Tutorial_Std01.lcd) in the [Quantitative Results View] is found to be "----", or if confirming the [Chromatogram View] reveals that peak integration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

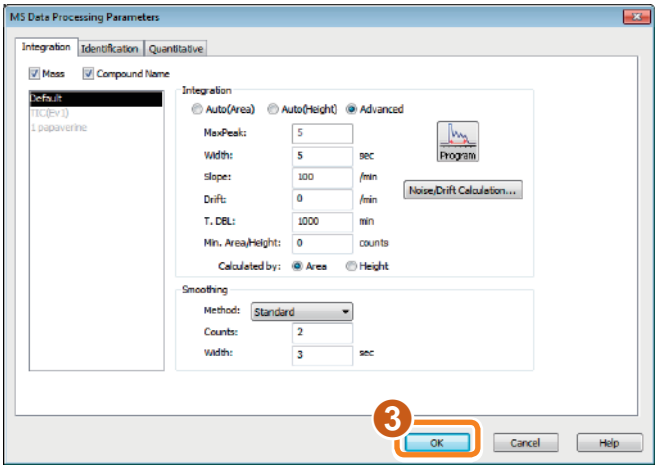
1 Edit the quantitative parameters.

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



2 Re-integrate





Original Results

Quantitative Results View ID# 1 papaverine

	Data Filename	Sample Type	Level#	Area	Conc. (ppm)	Std. Conc.
1	Tutorial_Std01.lcd	Standard(Calc.Point)	1	-	----	0.500
2	Tutorial_Std02.lcd	Standard(Calc.Point)	2	15,230.4	1.000	1.000
3	Tutorial_Std03.lcd	Standard(Calc.Point)	3	80,746.2	5.000	5.000
4	Tutorial_Unk01.lcd	Unknown	0	11,077.3	0.746	----
5	Tutorial_Unk02.lcd	Unknown	0	10,886.1	0.735	----
6	Tutorial_Unk03.lcd	Unknown	0	10,791.5	0.729	----
7	Tutorial_Unk04.lcd	Unknown	0	10,418.1	0.706	----
8	Tutorial_Unk05.lcd	Unknown	0	10,493.7	0.711	----

Edited Results

Quantitative Results View ID# 1 papaverine

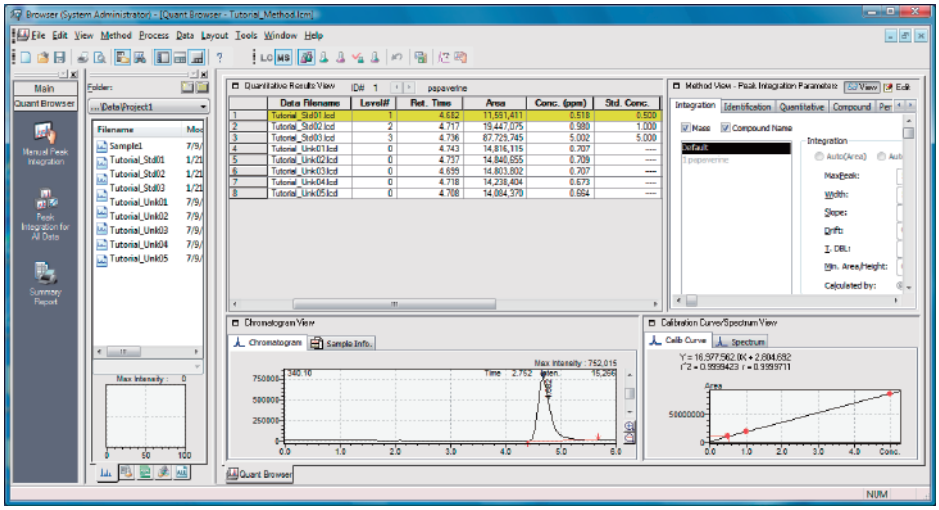
	Data Filename	Sample Type	Level#	Area	Conc. (ppm)	Std. Conc.
1	Tutorial_Std01.lcd	Standard(Calc.Point)	1	11,591.4	0.518	0.500
2	Tutorial_Std02.lcd	Standard(Calc.Point)	2	19,447.0	0.980	1.000
3	Tutorial_Std03.lcd	Standard(Calc.Point)	3	87,729.7	5.002	5.000
4	Tutorial_Unk01.lcd	Unknown	0	14,816.1	0.707	----
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	----

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

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

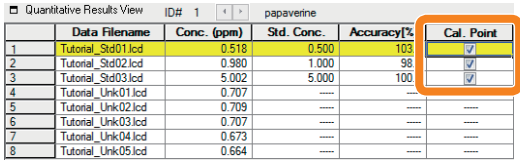
Reference "7.5.6 Manual Quantitative Peak Integration" in *Operators Guide*.

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].



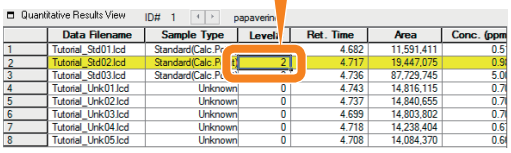
	Data Filename	Conc. (ppm)	Std. Conc.	Accuracy[%	Cal. Point
1	Tutorial_Std01.lcd	0.518	0.500	103	☑
2	Tutorial_Std02.lcd	0.980	1.000	98	☑
3	Tutorial_Std03.lcd	5.002	5.000	100	☑
4	Tutorial_Unk01.lcd	0.707	-----	-----	-----
5	Tutorial_Unk02.lcd	0.709	-----	-----	-----
6	Tutorial_Unk03.lcd	0.707	-----	-----	-----
7	Tutorial_Unk04.lcd	0.673	-----	-----	-----
8	Tutorial_Unk05.lcd	0.664	-----	-----	-----

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.

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.Pr		4.682	11,591,411	0.5
2	Tutorial_Std02.lcd	Standard(Calc.P	2	4.717	19,447,075	0.9
3	Tutorial_Std03.lcd	Standard(Calc.P		4.736	87,729,745	5.0
4	Tutorial_Unk01.lcd	Unknown	0	4.743	14,816,115	0.7
5	Tutorial_Unk02.lcd	Unknown	0	4.737	14,840,655	0.7
6	Tutorial_Unk03.lcd	Unknown	0	4.699	14,803,802	0.7
7	Tutorial_Unk04.lcd	Unknown	0	4.718	14,238,404	0.6
8	Tutorial_Unk05.lcd	Unknown	0	4.708	14,084,370	0.6

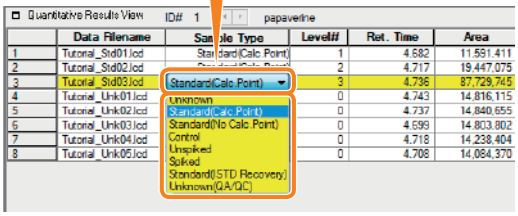
Hint The [Level#] can be edited regardless of the [Sample Type].

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.

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

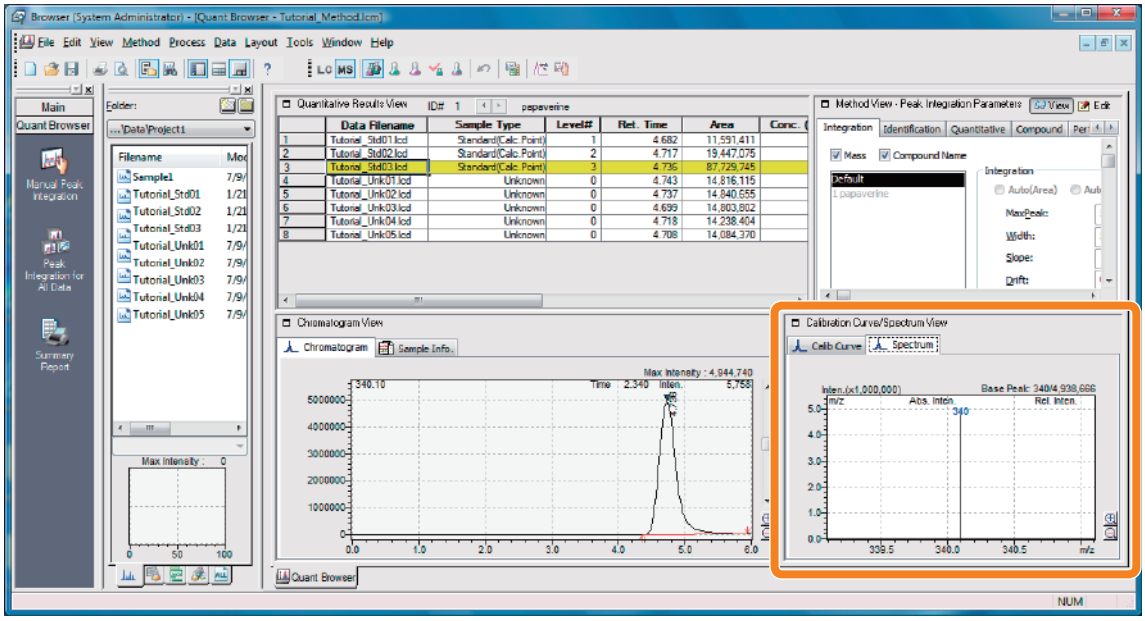


	Data Filename	Sample Type	Level#	Ret. Time	Area
1	Tutorial_Std01.lcd	Standard(Calc.Point)	1	4.682	11,591,411
2	Tutorial_Std02.lcd		2	4.717	19,447,075
3	Tutorial_Std03.lcd	Standard(Calc.Point)	3	4.736	87,729,745
4	Tutorial_Unk01.lcd	Unknown	0	4.743	14,816,115
5	Tutorial_Unk02.lcd	Standard(Calc.Point)	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	0	4.708	14,084,370

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

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.

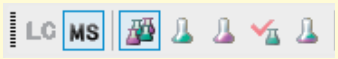
Method File

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.

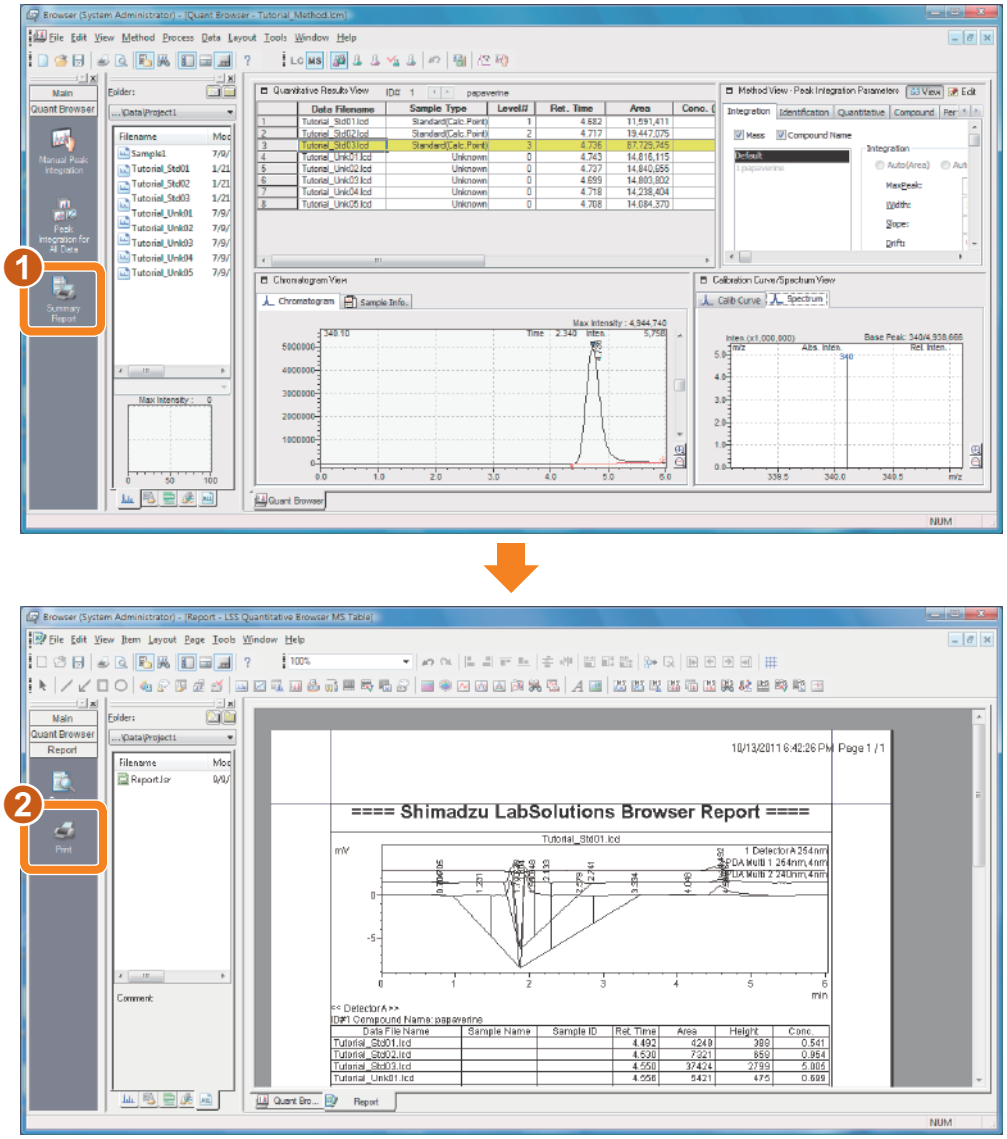
Data Files

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.



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.

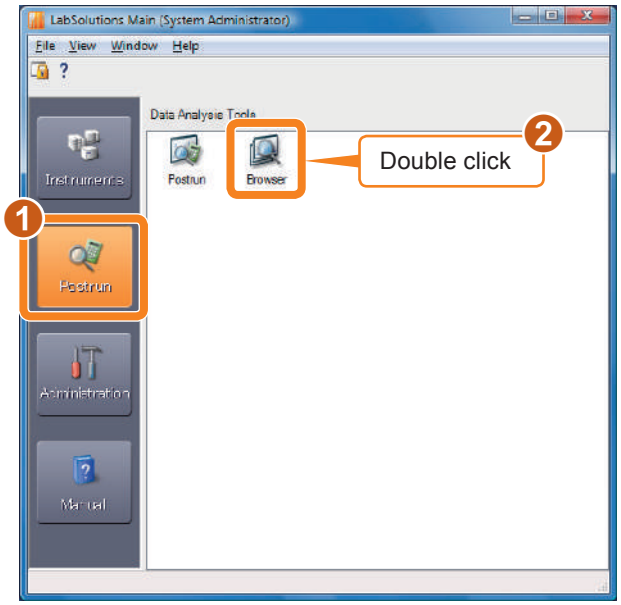
Chapter 6. Qualitative Data Analysis

6.1 Display Data Files in the [Data Browser] Window

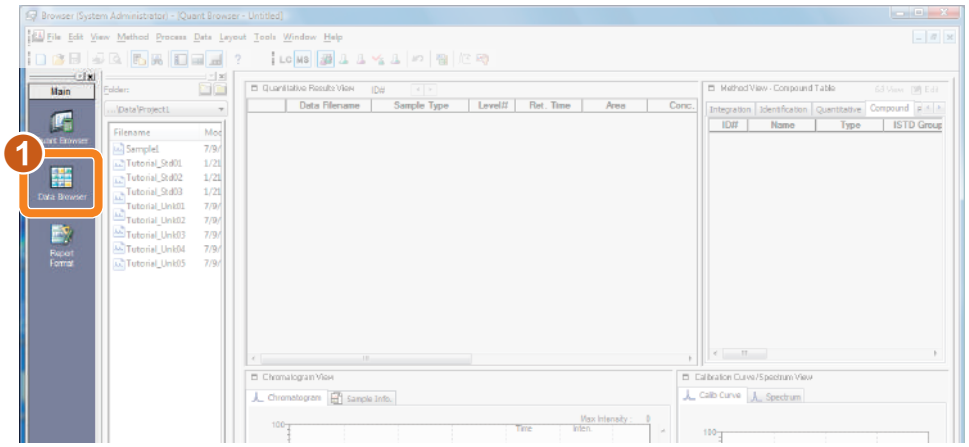
The [Data Browser] window can be used to display chromatograms, spectra and multiple data file information from different detectors, such as MS or PDA, in various formats.

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

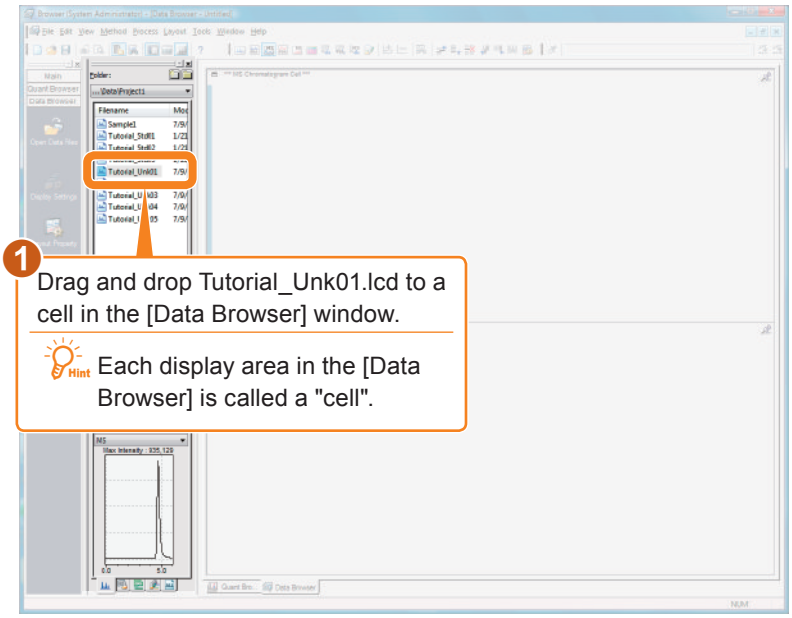
1 Start the [Browser] program.

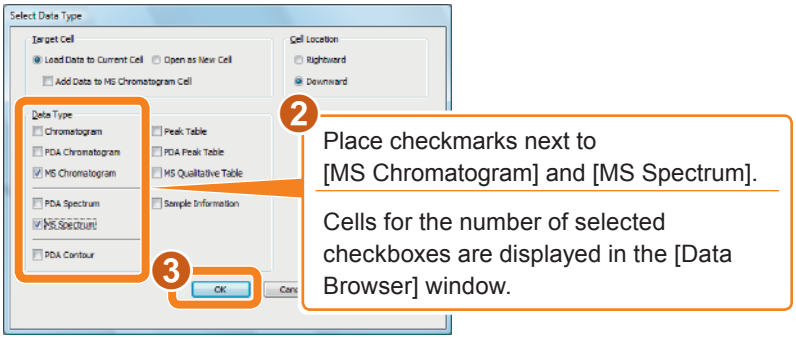


2 Open the [Data Browser] window.

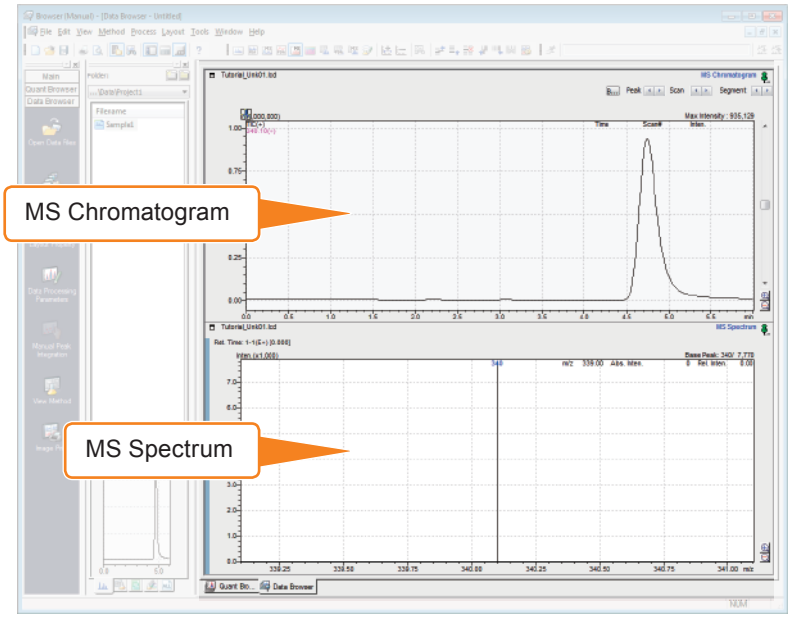


3 Select a data file.





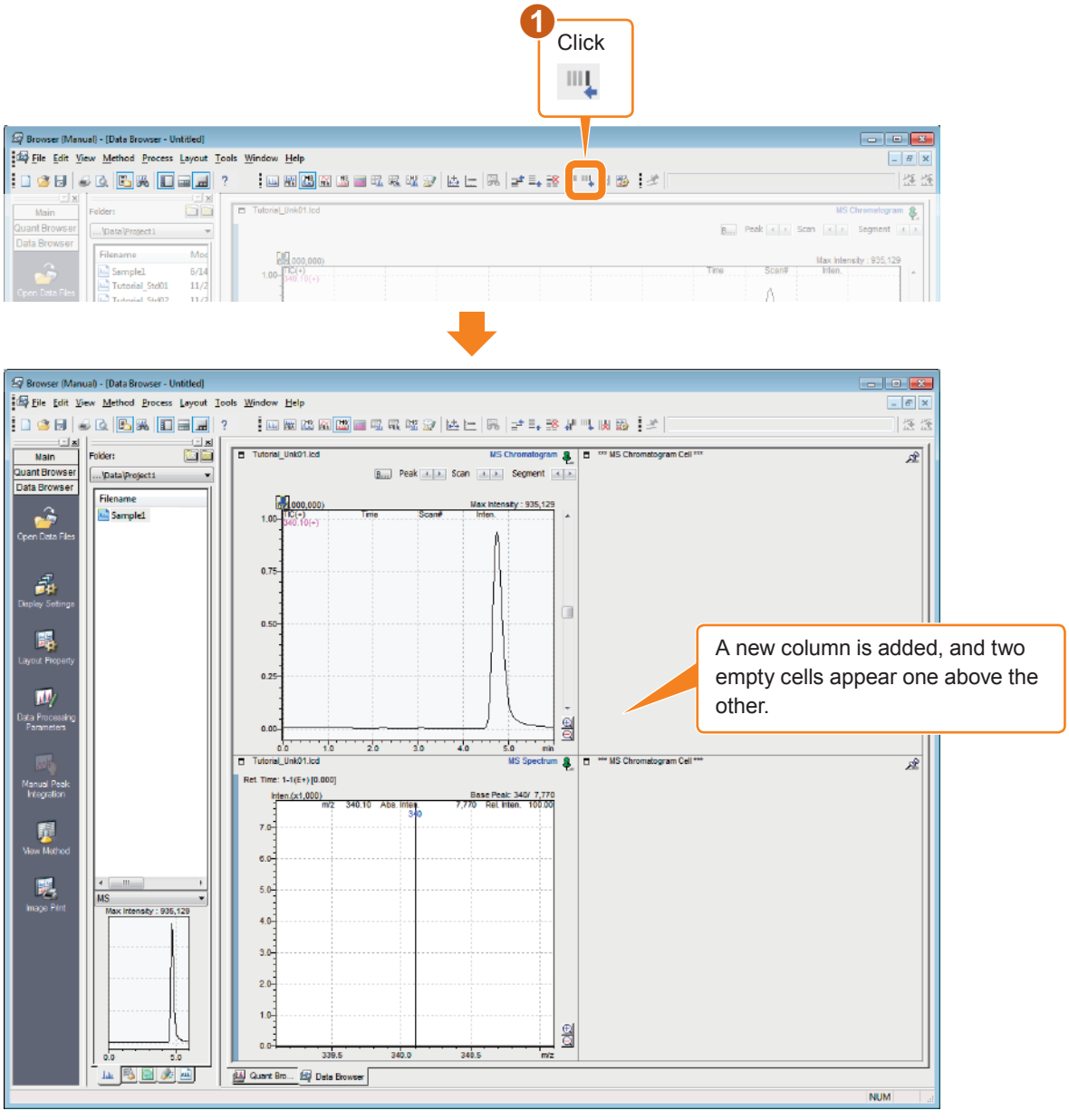
The MS chromatogram and MS spectrum are displayed.
Double click a point on the MS chromatogram to display the MS spectrum at that point.



6.2 Change the Display Layout Settings

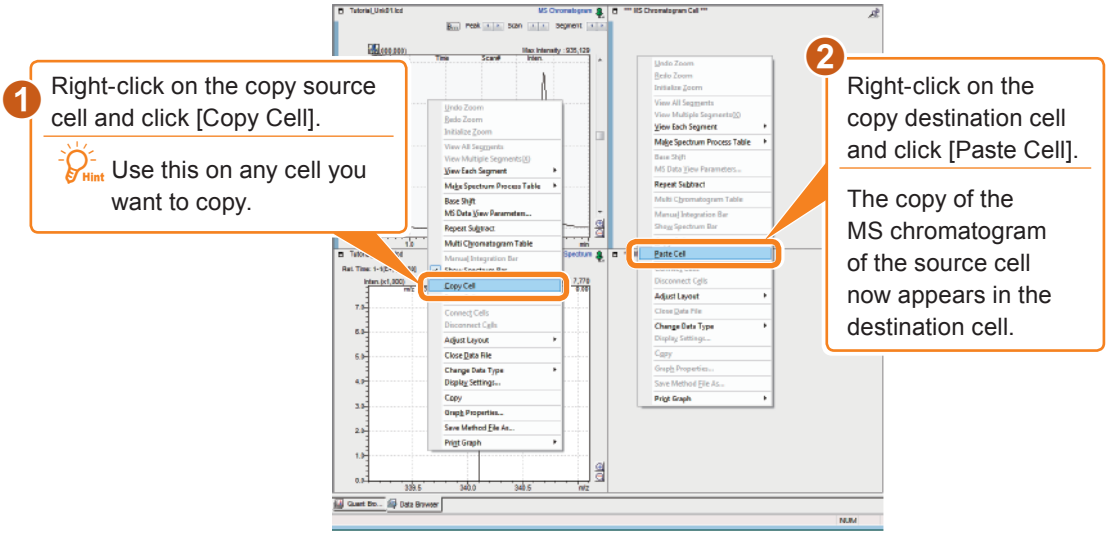
1 Add a column

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.

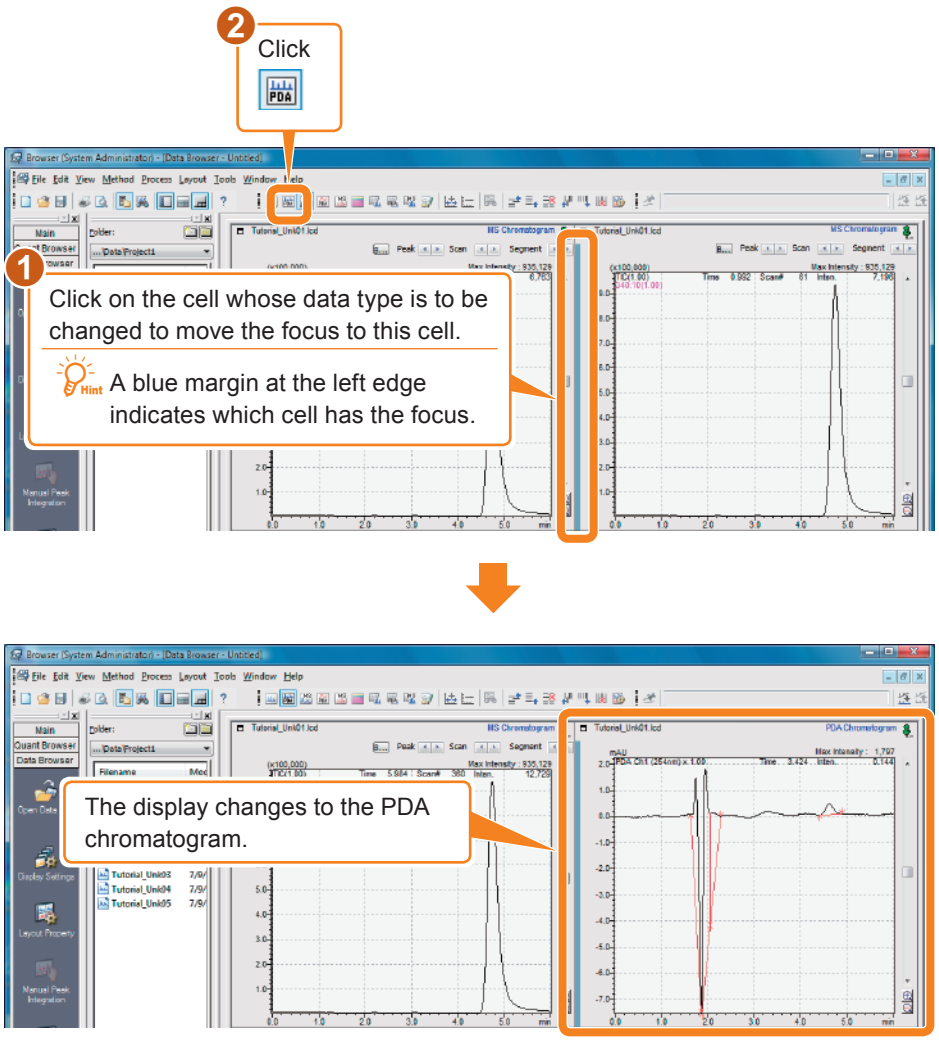


2 Copy and paste cell contents

You can copy information from one cell to another.



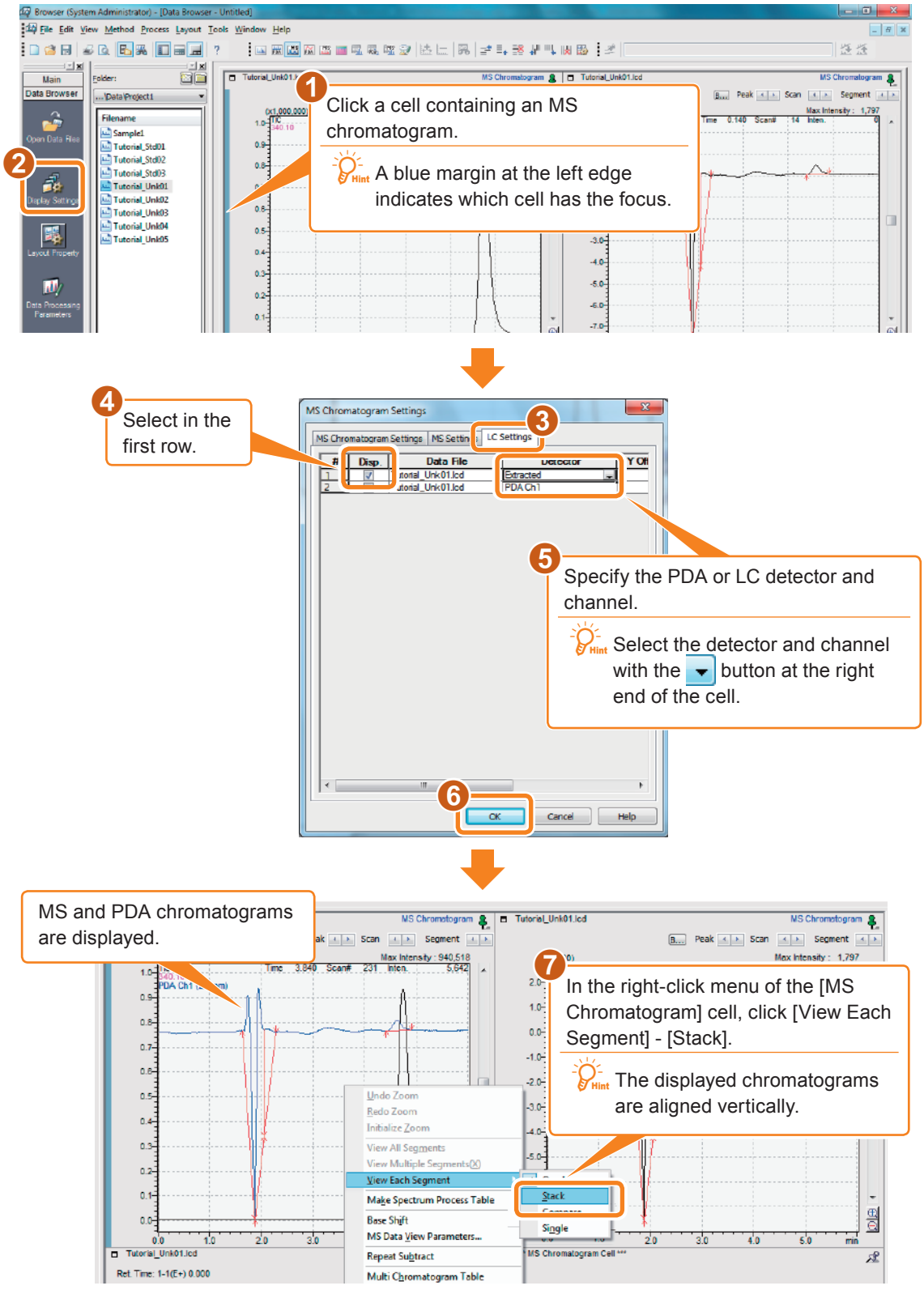
3 Change the data type.



6.3 Compare Different Types of Chromatograms

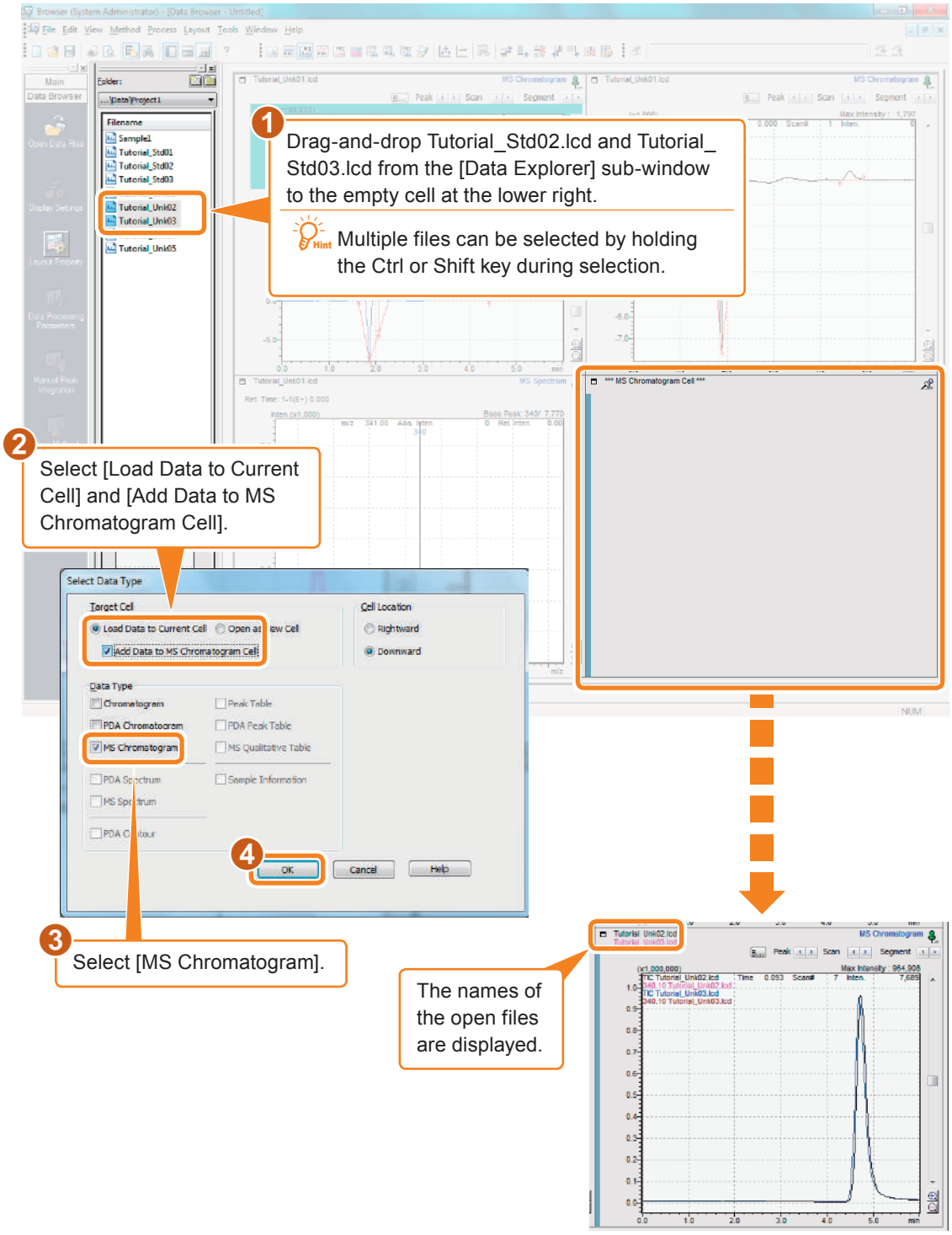
1 Compare MS and PDA chromatograms.

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



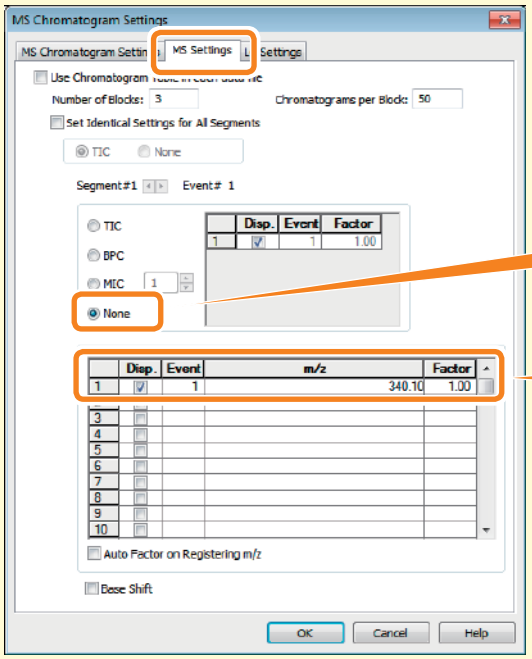
2 Compare the data for different chromatograms.

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



▼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.

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

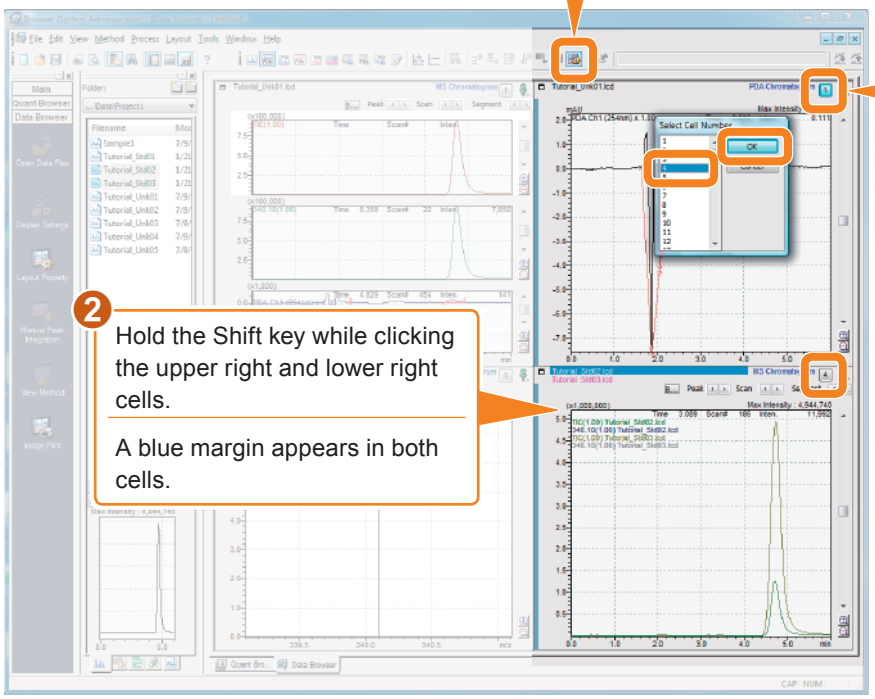
6.4 Use the Cell Fixed Function

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.



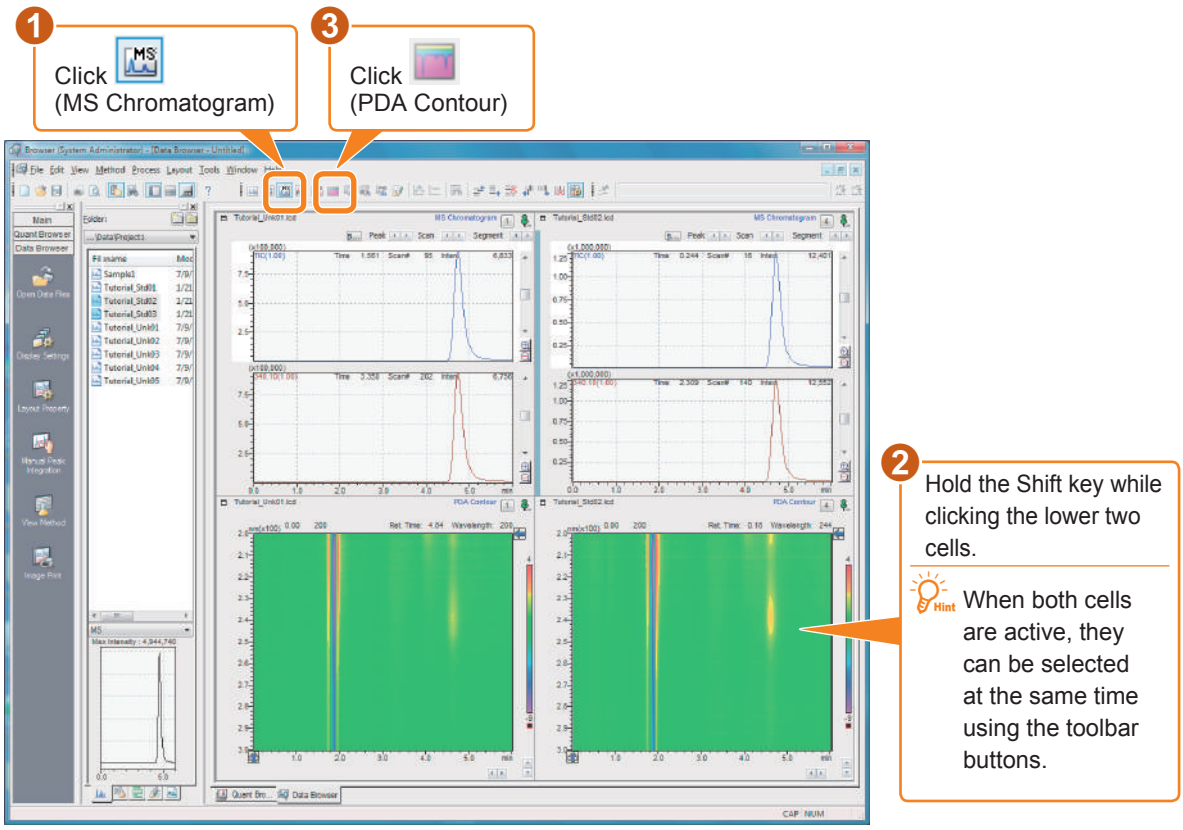
2 Hold the Shift key while clicking the upper right and lower right cells.

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.

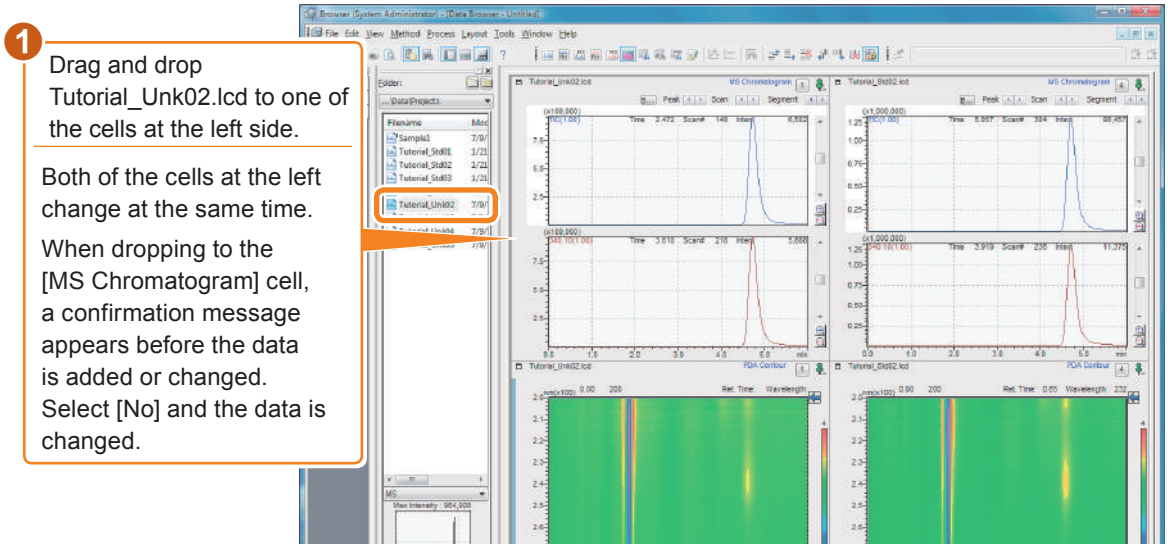
2 Display an MS chromatogram and PDA contour.



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.

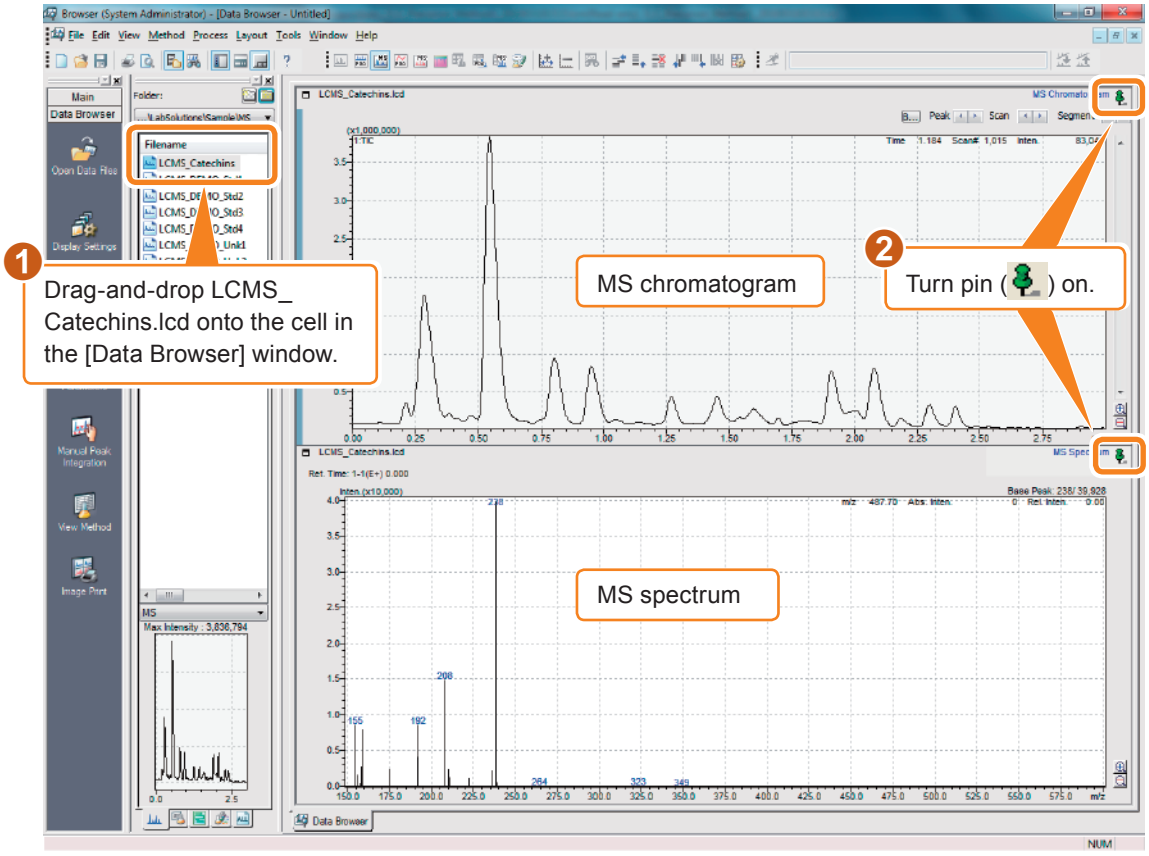
3 Confirm while comparing data.

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



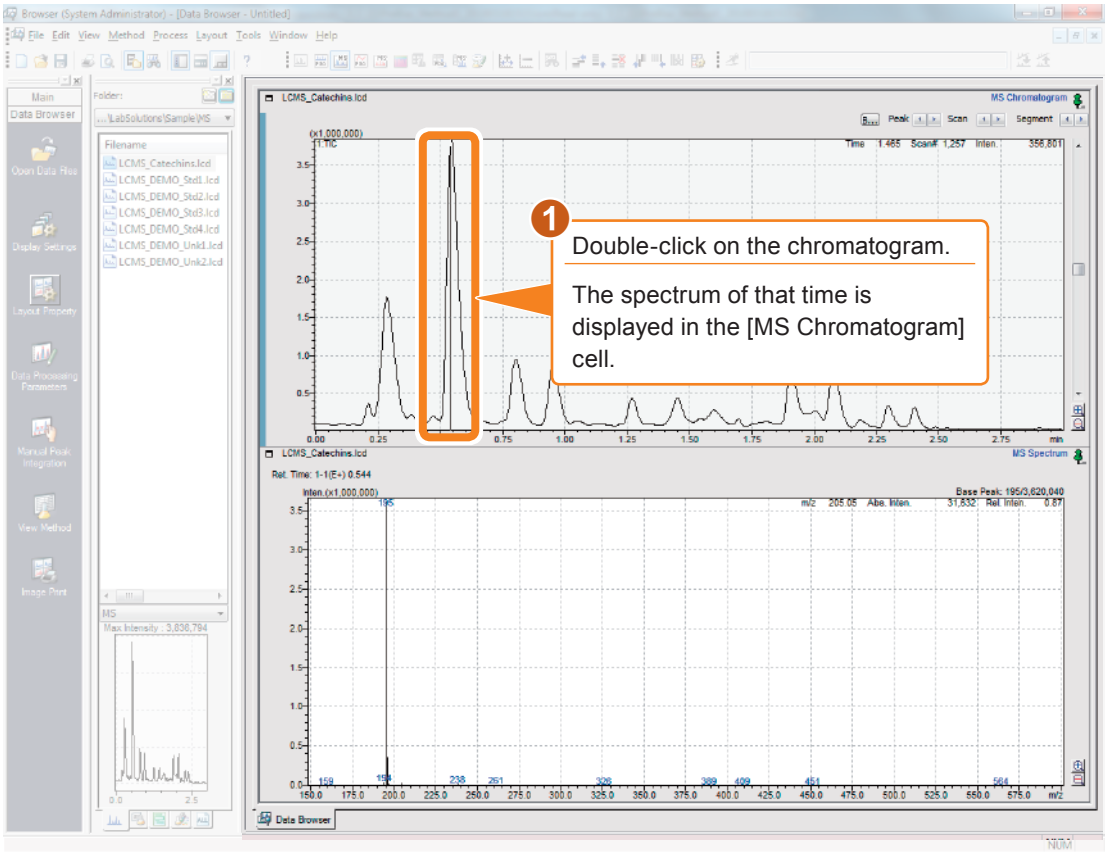
6.5 Qualitative Processing in the [Data Browser] Window

1 Load the data file.



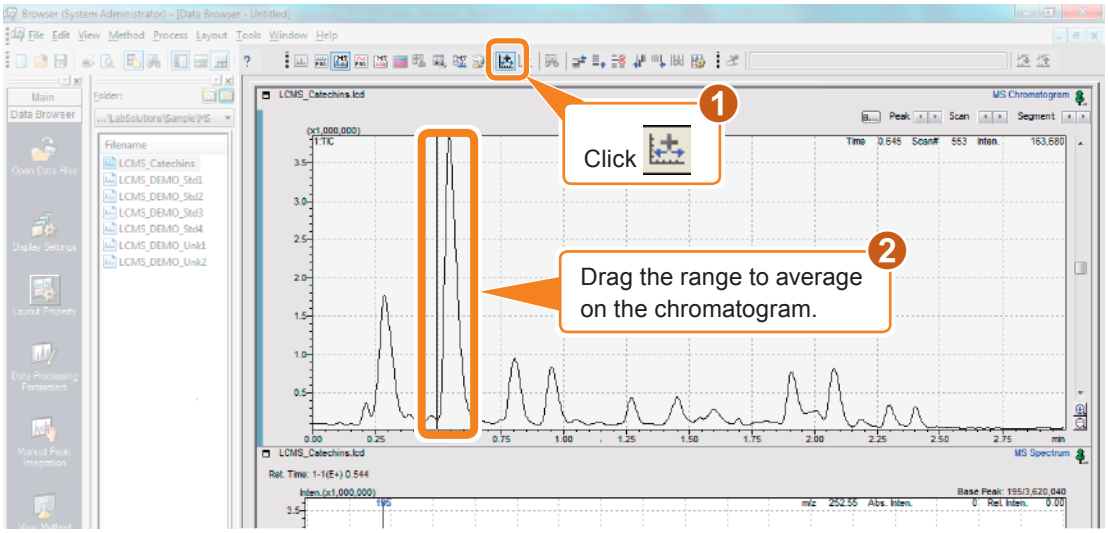
Hint
Clicking the pin switches toggles it on and off. Cells are interlocked when the pin is on. Browser functions applied to one pinned cell are executed in all of the pinned cells.

2 Display the MS spectrum.



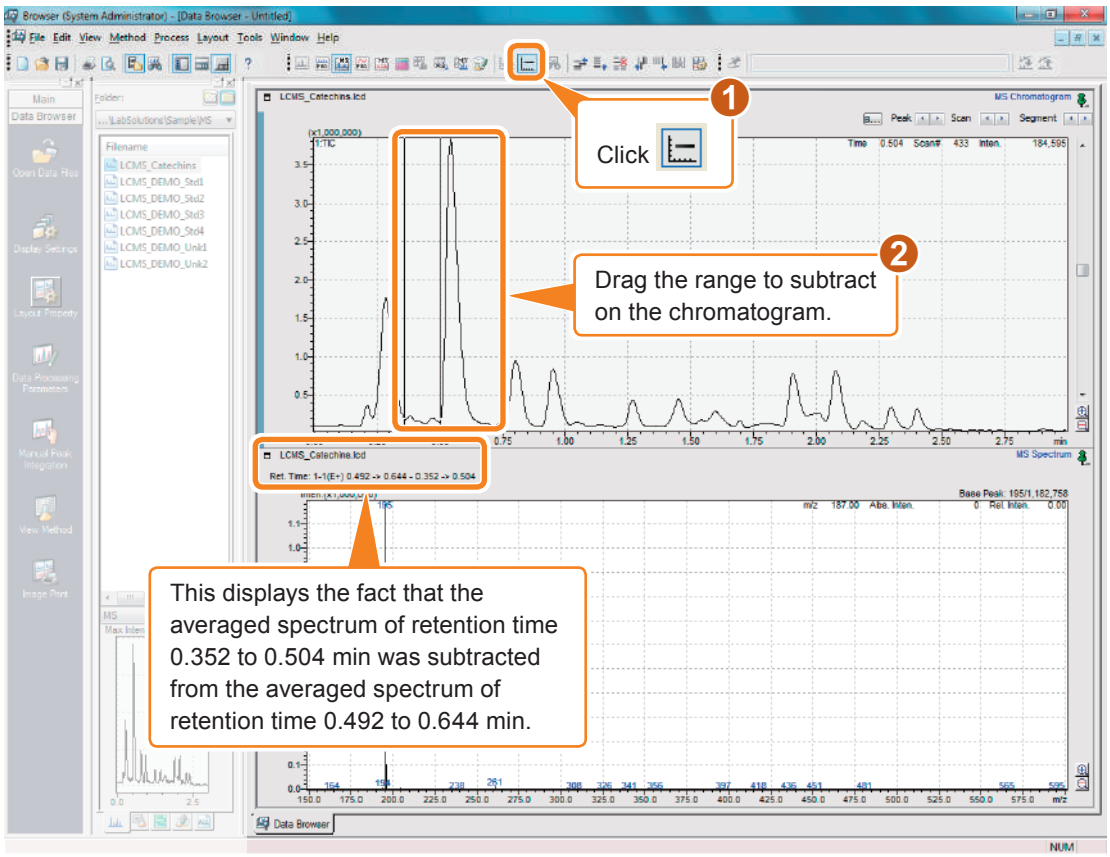
3 Average the MS spectrum.

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



4 Perform subtraction on the MS spectra.

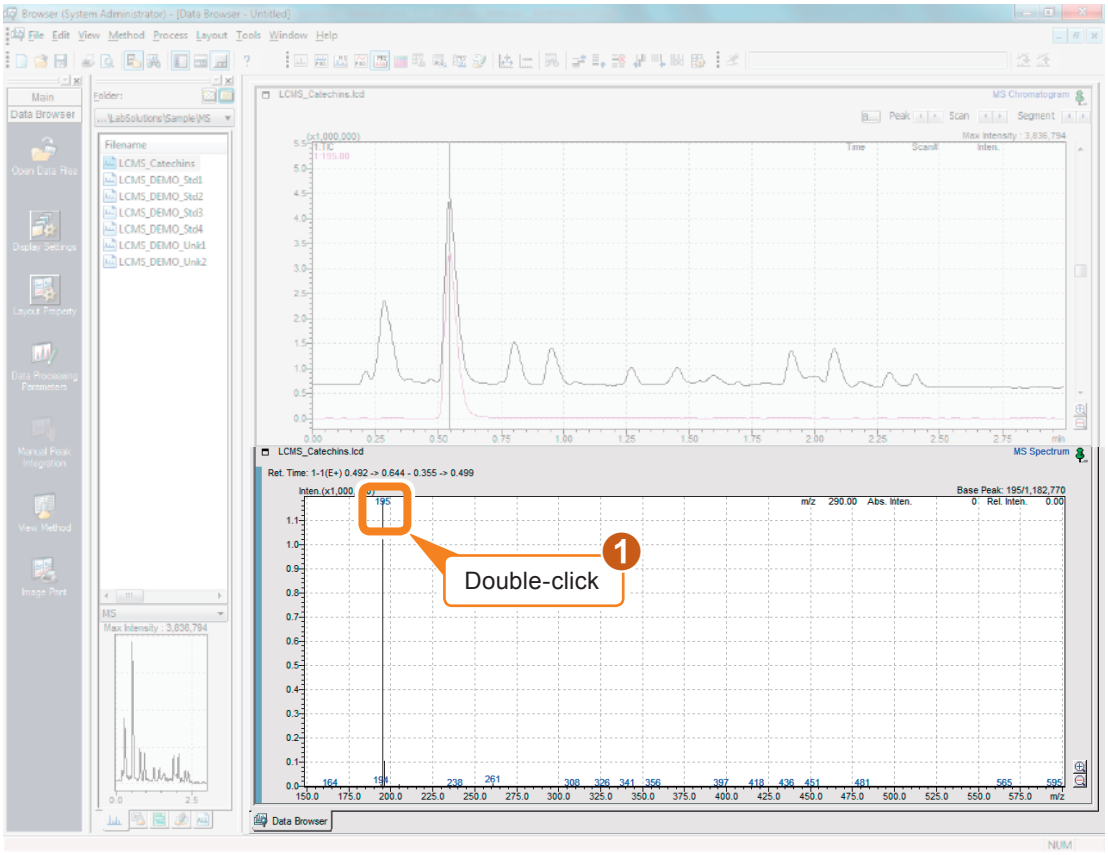
A cleaner-looking spectrum can be displayed by subtracting the background MS spectrum from the averaged spectrum.



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

5 Display the MS chromatogram.

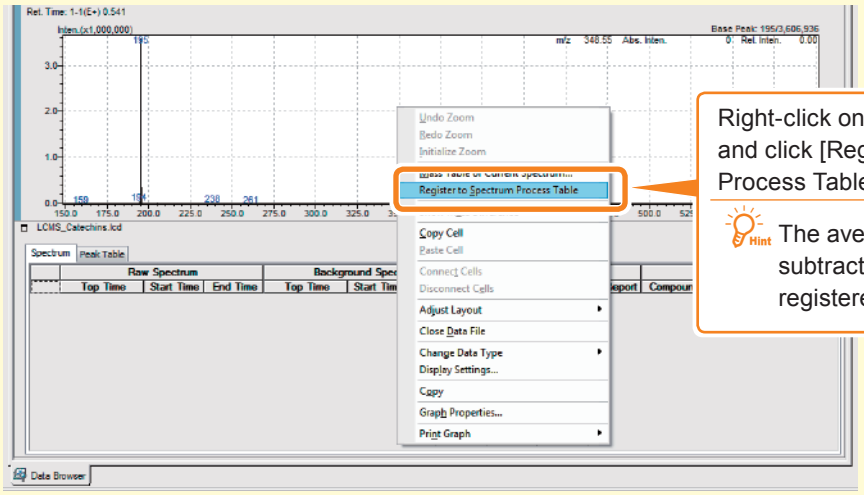
Double-click the MS spectrum peak. The chromatogram of the *m/z* at the position double-clicked in the [MS Chromatogram] cell is added to the display.



▼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.



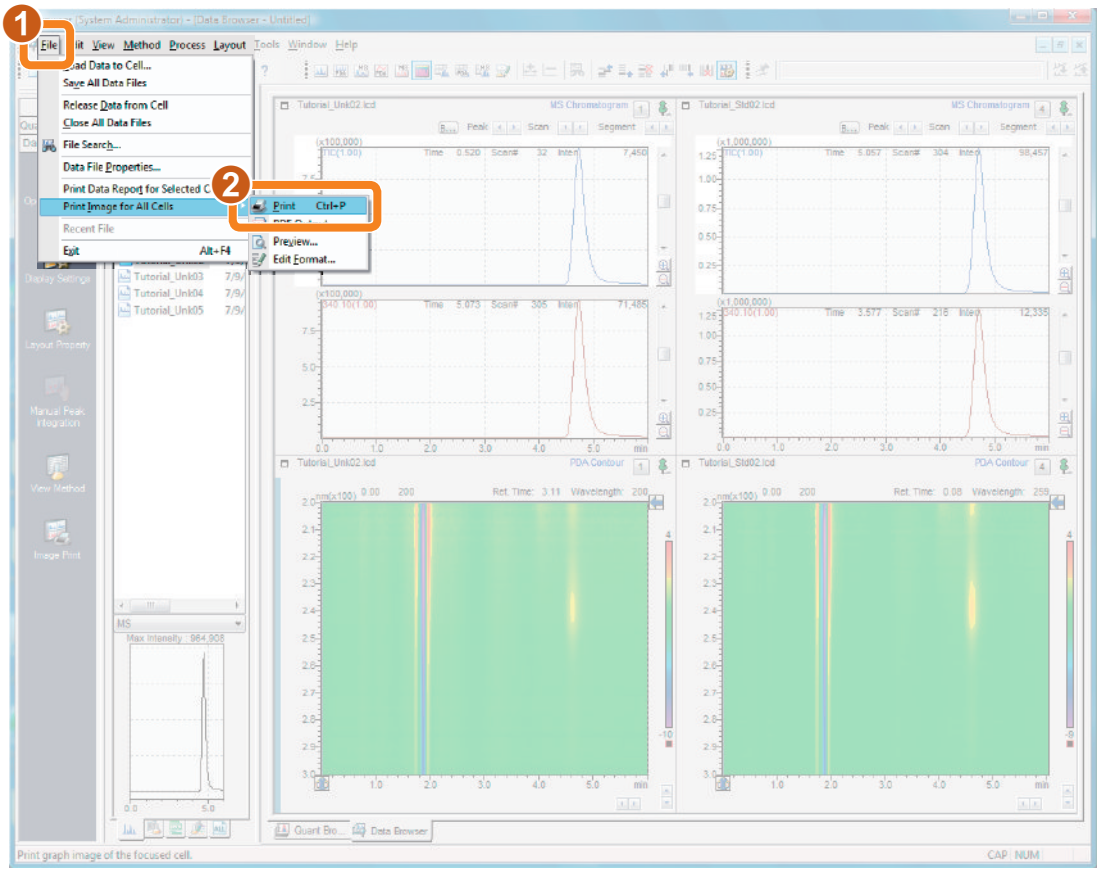
Right-click on the spectrum graph, and click [Register to Spectrum Process Table].

Hint The averaged and/or subtracted MS spectrum is registered.

6.6 Print from the [Data Browser] Window

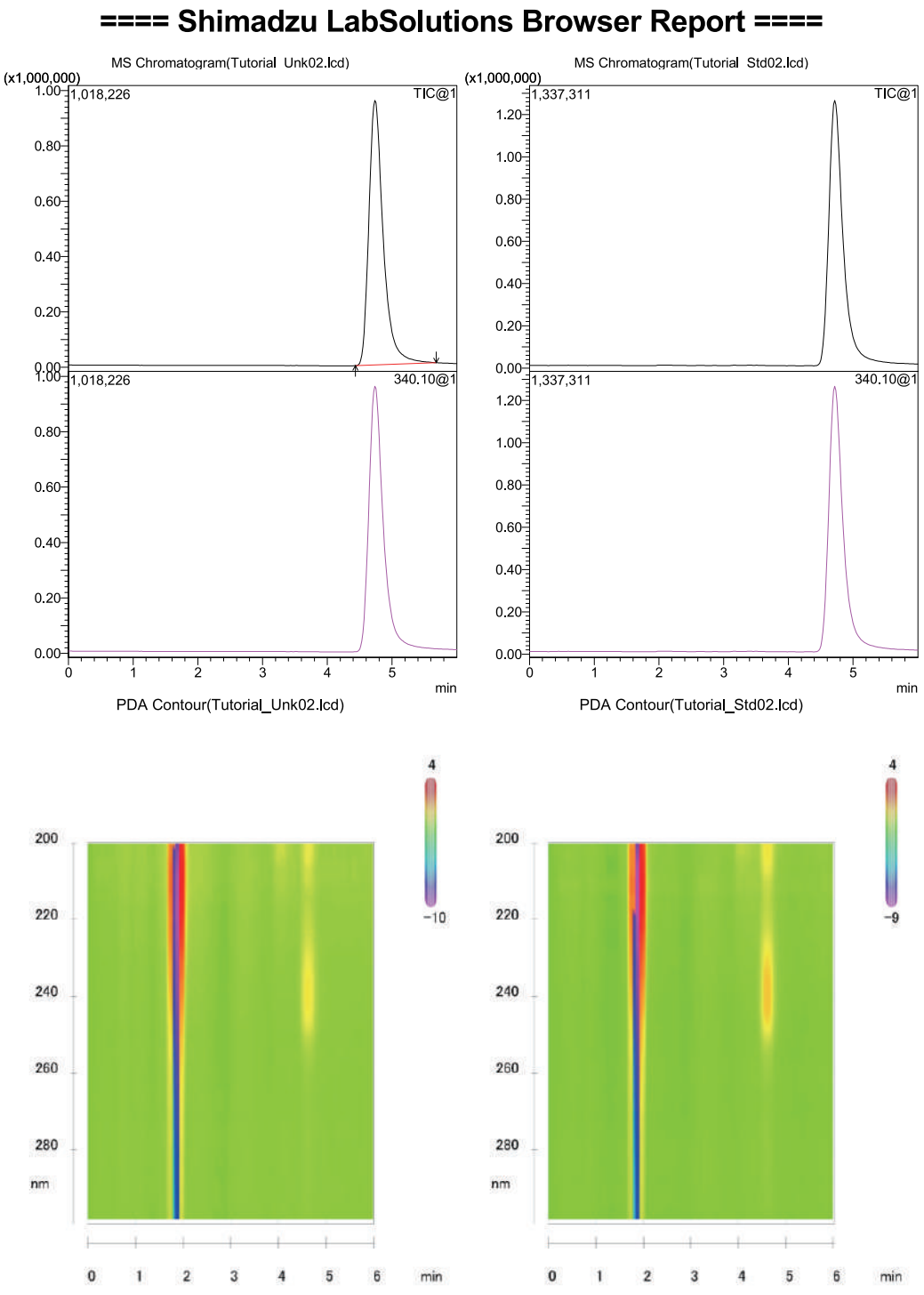
1 Print an image of the display.

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



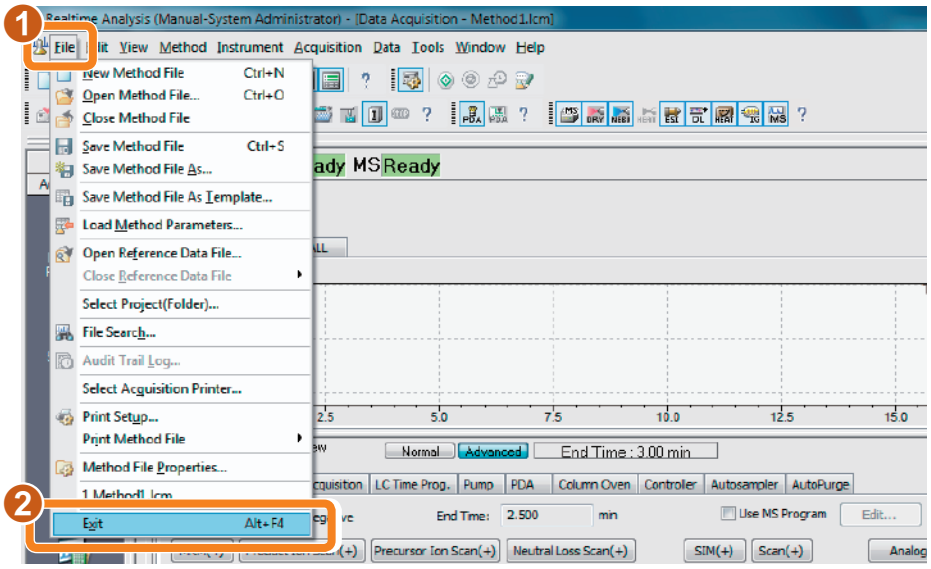
Hint Select [Print Data Report for Selected Cell] from the [File] menu to print using the report format saved in the data file.

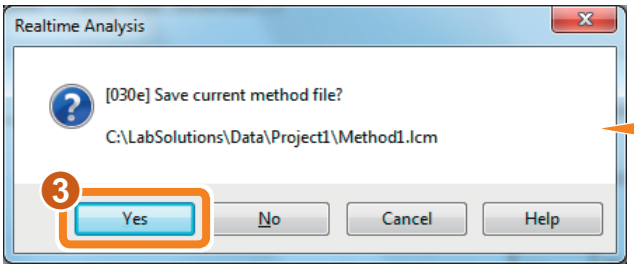
[Data Browser] Window Printout Example



Chapter 7. Shutdown

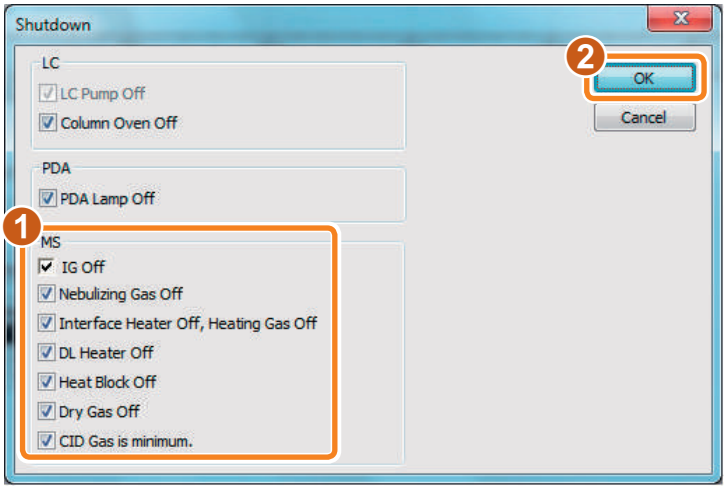
1 Close any open windows.



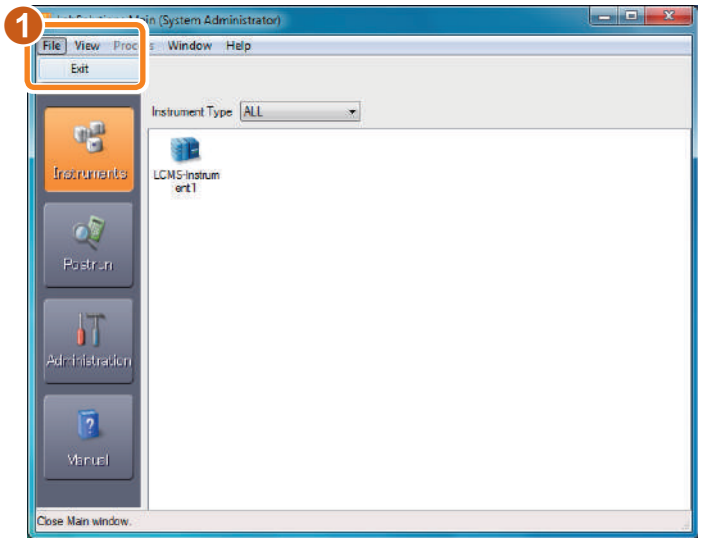


Hint This sub-window appears if there are any unsaved files.

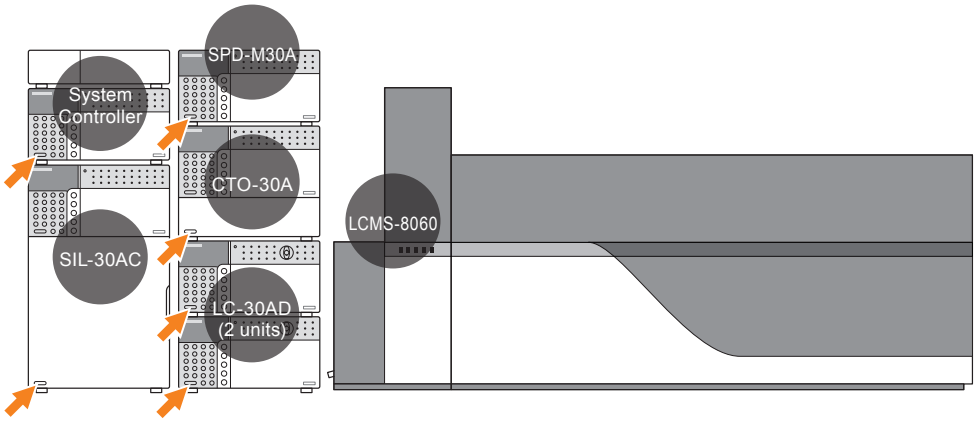
2 Stop the LC pumps, gas flows and heaters from the [Shutdown] sub-window.



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.