SHIMADZU

225-18376D
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LabSolutions LCMS

Getting Started Guide

NOTICES

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- Maintenance parts for this product are provided for seven years after production has stopped. Please note that we may not be able to provide maintenance parts after this period. However, for parts that are not genuine Shimadzu parts, the period of provision is determined by the manufacturer.
- The contents of the hard disk in a PC can be lost due to an accident. Backup your hard disk to protect your important data from accidents.
- If the user or usage location changes, ensure that this Instruction Manual is always kept together with the product.
- If this manual is lost or damaged, immediately contact your Shimadzu representative to request a replacement.

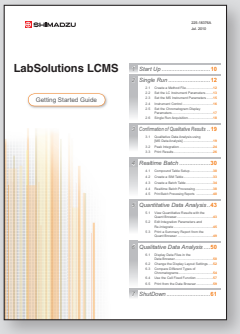
Original version is approved in English.

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 in the *Operators Guide*
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 functions.

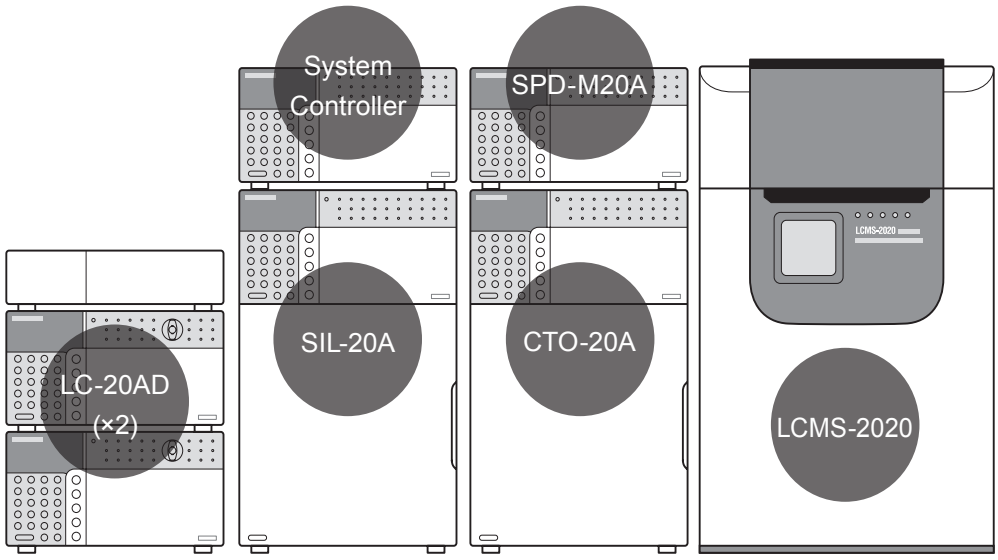
- Data acquisition and control of analytical instruments
- Data analysis and viewing of data
- Creation and printing of various customizable reports

System Structure

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

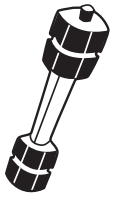
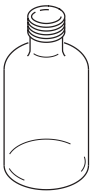
High-pressure gradient LCMS + PDA system

- Pump ····· LC-20AD (×2)
- Detector ····· SPD-M20A
- MS Detector ····· LCMS-2020
- Column Oven ····· CTO-20A
- Autosampler ····· SIL-20A



Acquisition Conditions

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

Column	Shim-pack VP-ODS 150 mm × 2.0 mm, 5 µm ID (Shimadzu P/N 228-34937-94 or equiv.)	
Mobile Phase	Binary Gradient Mode Pump A = Ultra-pure water Pump B = Acetonitrile (HPLC grade)	
Samples	Papaverine 0.5, 1, 5, 25, 50 ng/µL (Shimadzu P/N 225-06613-05)	

File Types

Data file (.lcd)

This file contains all analysis results and acquisition information from the following files.

Method file (.lcm)

Acquisition conditions, analysis conditions, calibration curve information, and etc.

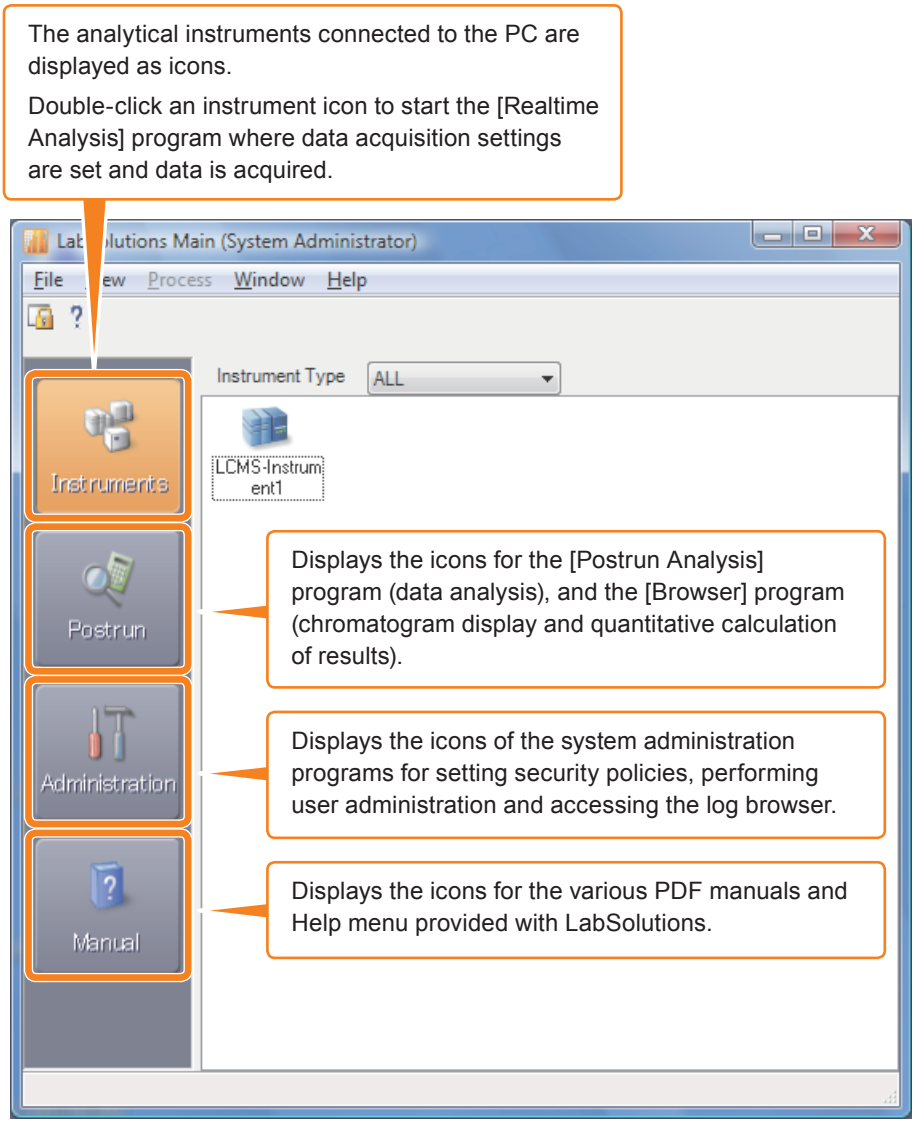
Batch file (.lcb)

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

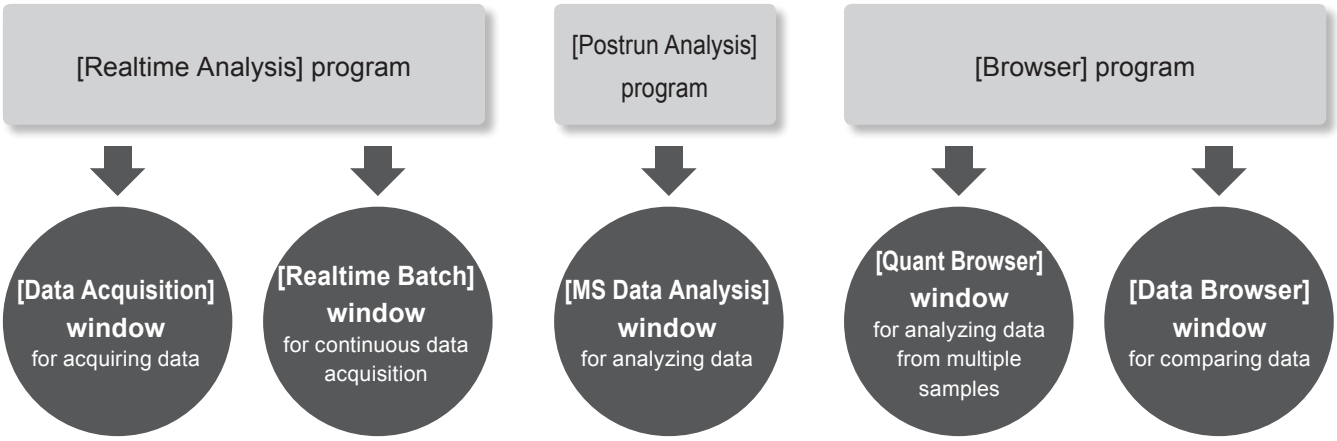
Report format file (.lsr)

This file is used to print data acquisition results.

LabSolutions Main Window

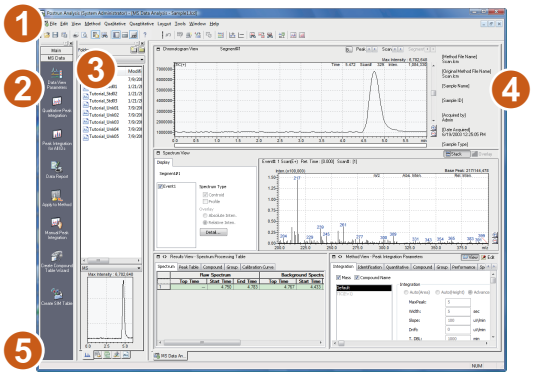


LabSolutions Main Programs and Main Windows



LabSolutions Windows

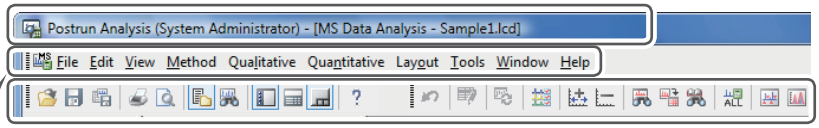
The following example describes the [Postrun Analysis] program window.



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

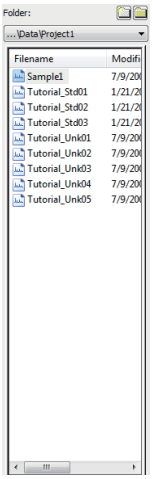
This bar displays icons for frequently used data acquisition operations.

3

Data Explore

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

Click  to change folders.



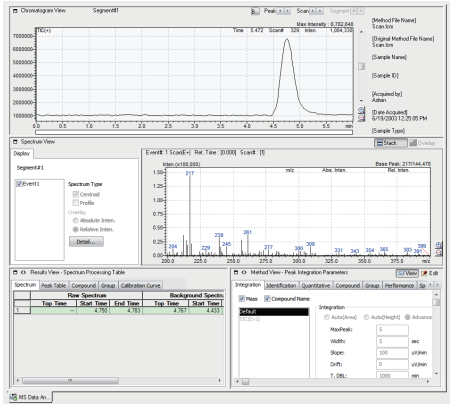
4

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.

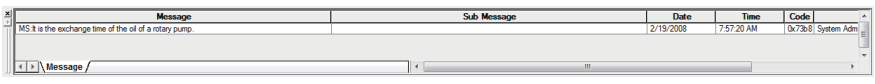
Switch the windows by clicking the icons on the assistant bar.



5

Output Window

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



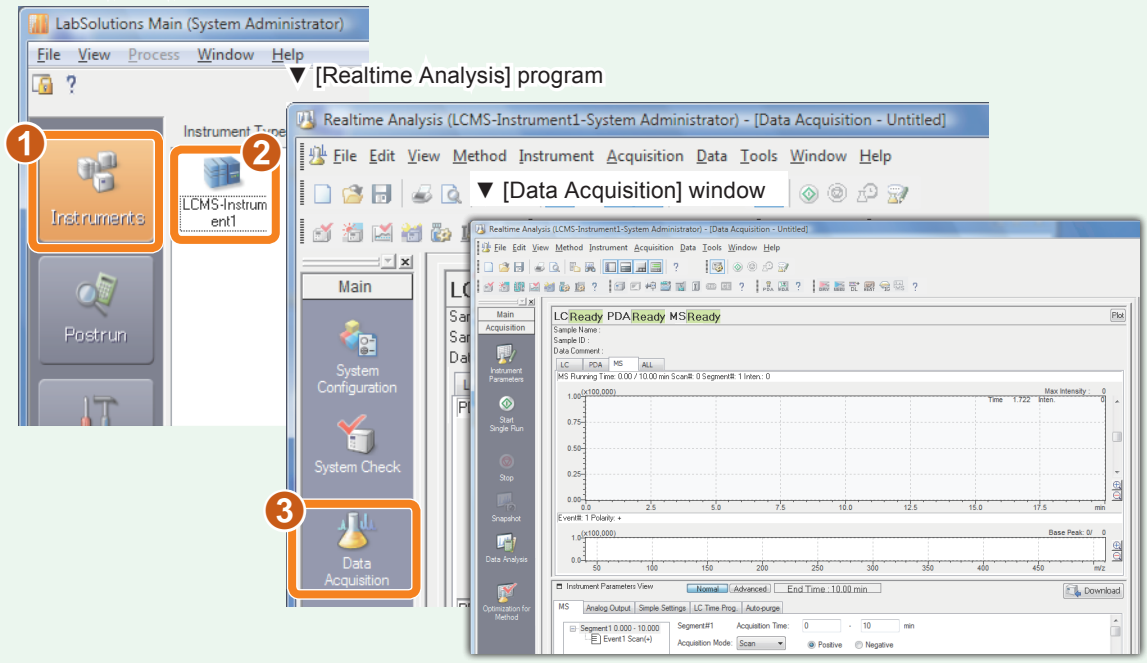
How to Open Windows

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

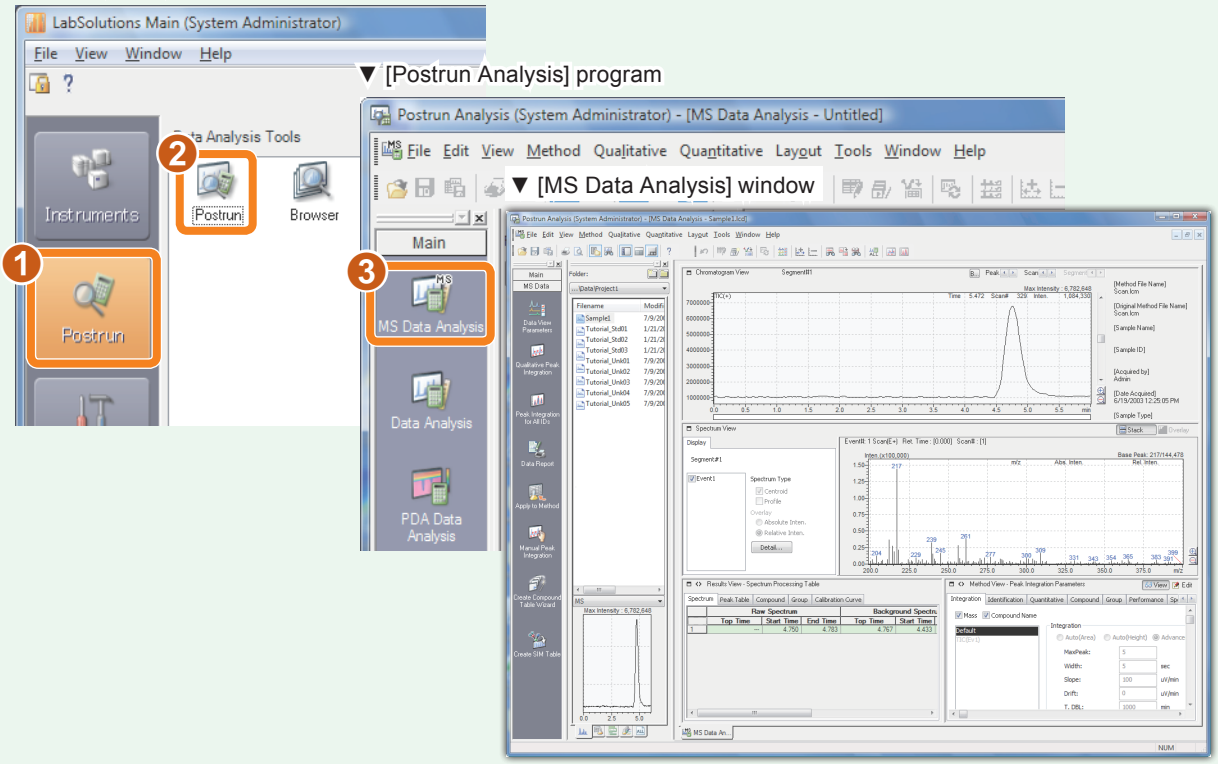


Data Analysis and Qualitative Calculations

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

Reference 3. Confirmation of Qualitative Results

▼ Main window

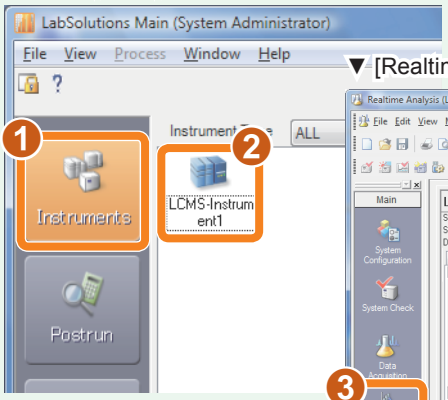


Continuous Data Acquisition of Sequential Samples

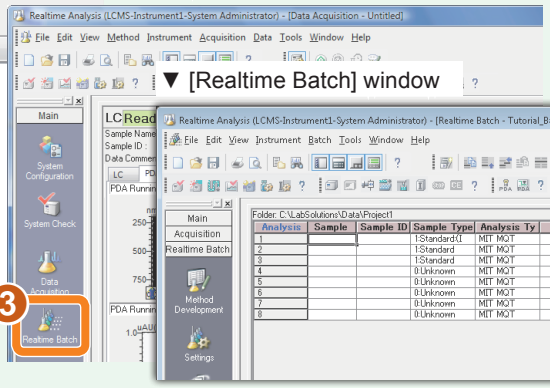
Open the [Realtime Batch] window from the main window.

Reference 4. Realtime Batch

▼ Main window



▼ [Realtime Analysis] program



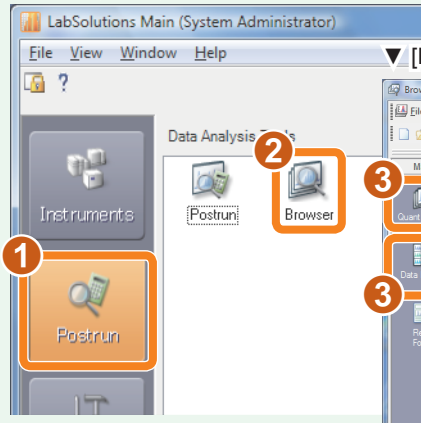
▼ [Realtime Batch] window

Data Analysis and Quantitative Calculations

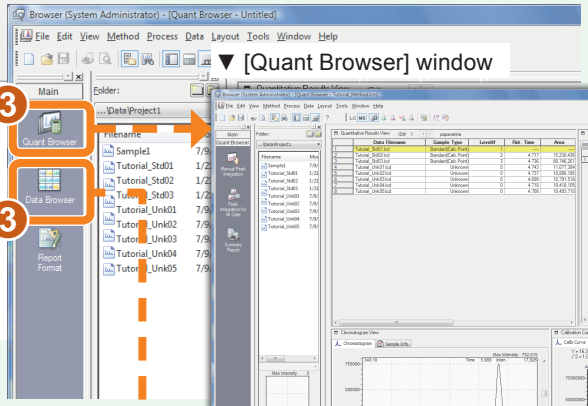
Open the [Quant Browser] window from the main window.

Reference 5. Quantitative Data Analysis

▼ Main window



▼ [Browser] program



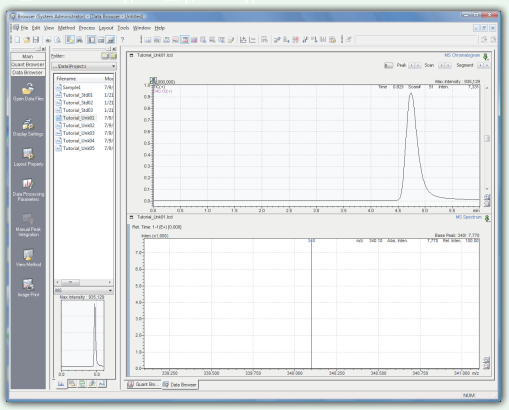
▼ [Quant Browser] window

Compare Data

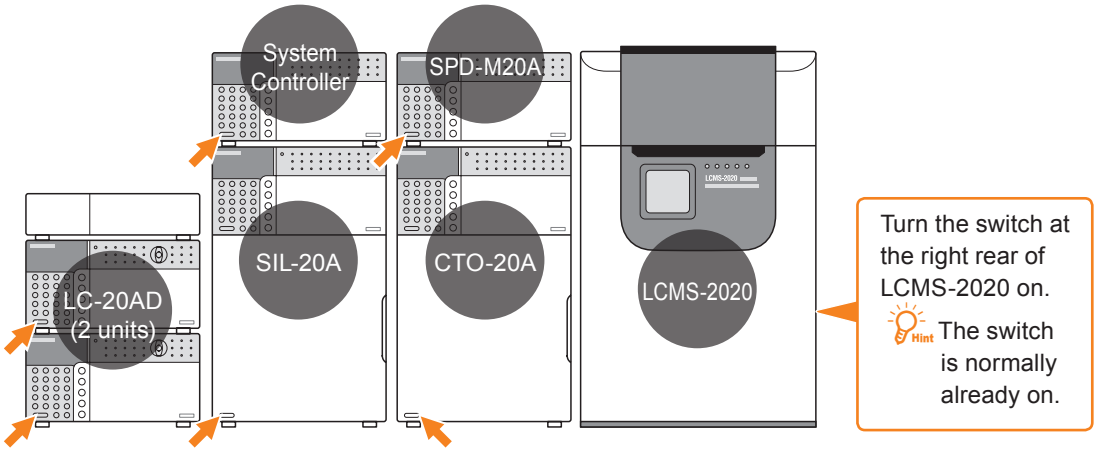
Open the [Data Browser] window from the main window.

Reference 6. Qualitative Data Analysis

▼ [Data Browser] window



1 Turn ON all of the instruments.



2 Confirm that nitrogen gas is being supplied to the MS instrument.

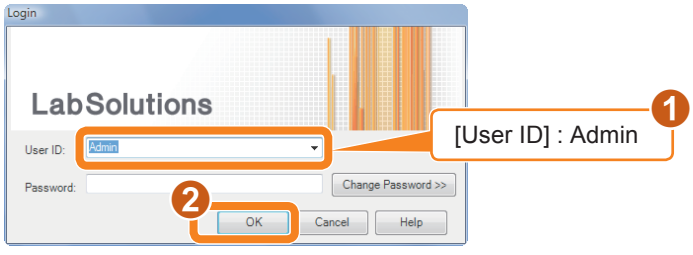
3 Start the PC.

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

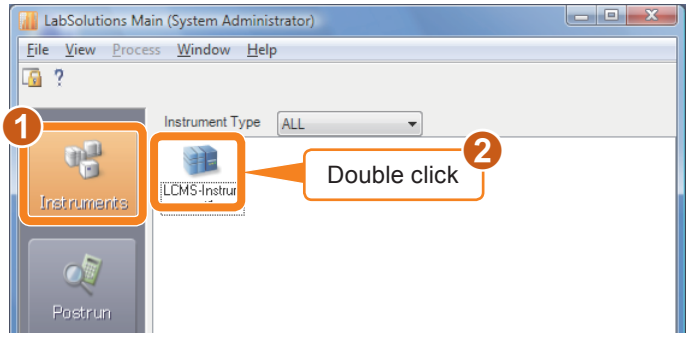
Icon Color	LabSolutions Status	Operation
Green	Normal	
Yellow	Starting up	Please wait
Red	Error	Please restart the PC.

5 Double-click  on the desktop.

6 Log in.



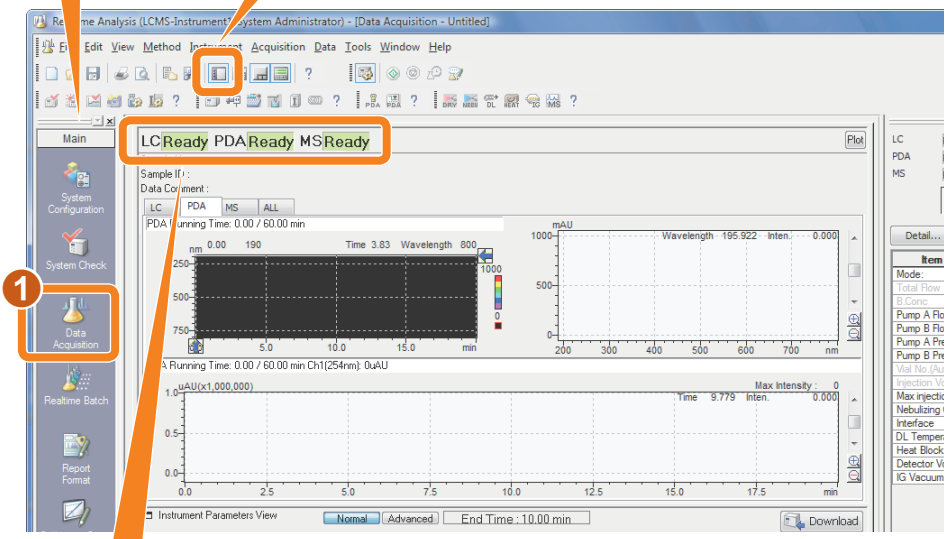
7 Start the [Realtime Analysis] program.



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.



2 [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

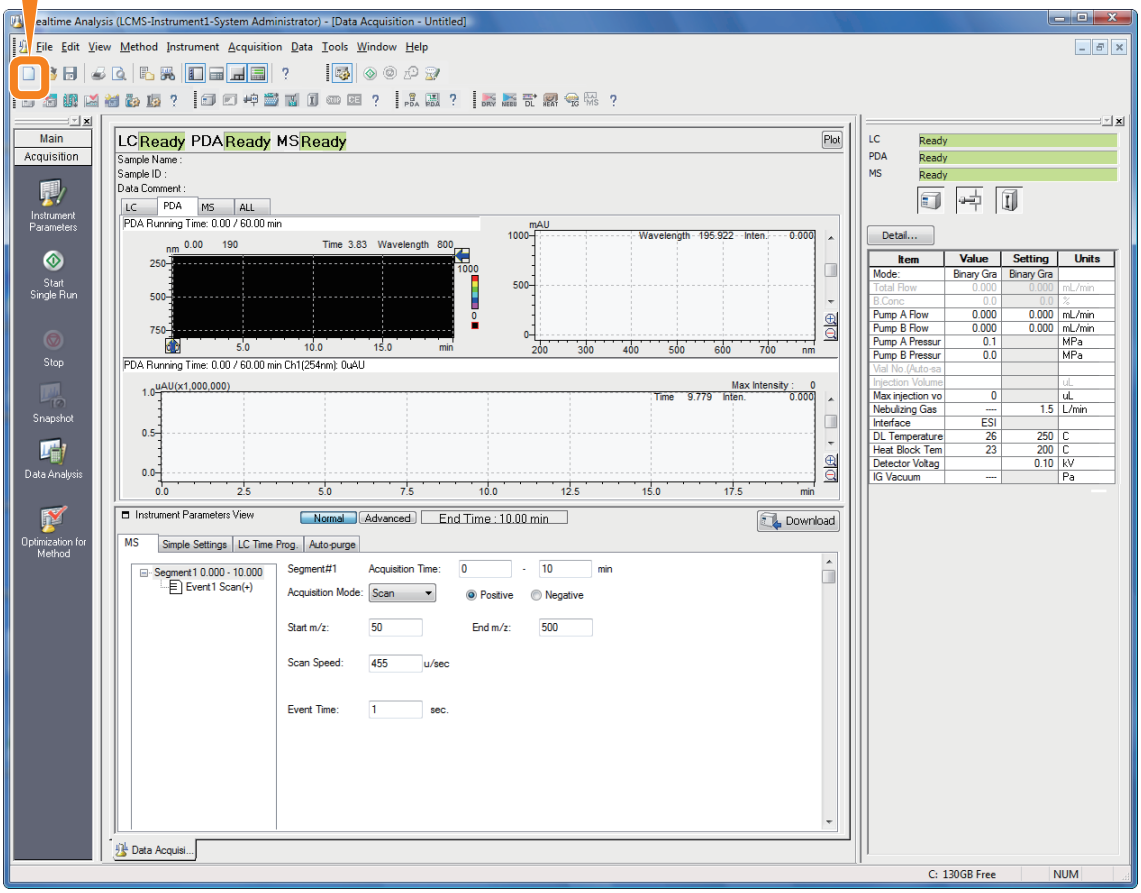
Set the LC instrument parameters and MS instrument parameters (acquisition conditions) in the [Data Acquisition] window, and acquire data.

2.1 Create a Method File

1 Click the [New] button on the toolbar.

Click 

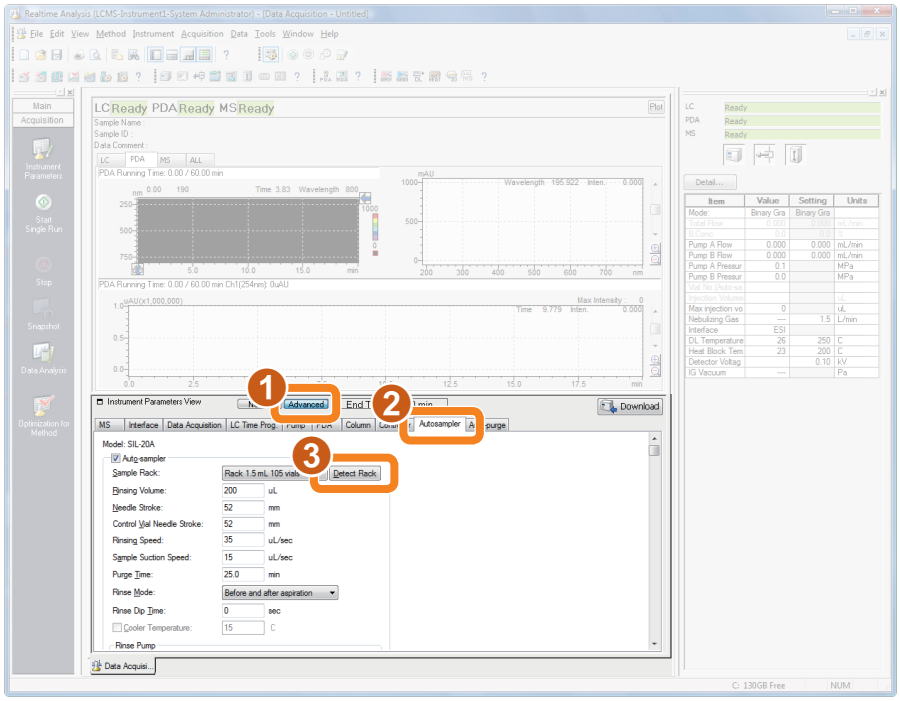
Hint When asked to "Save current Method File?", select [No].



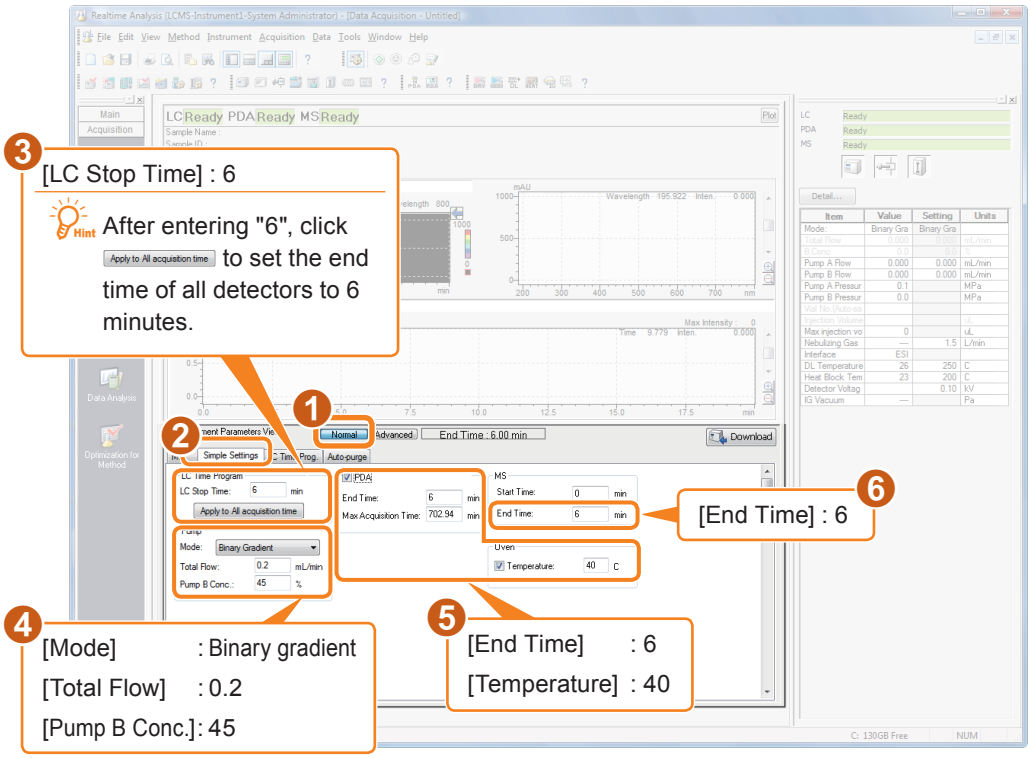
2.2 Set the LC Instrument Parameters

Reference "2.2 Enter Data Acquisition Parameters" in *Operators Guide*.

1 Detect the type of autosampler rack.

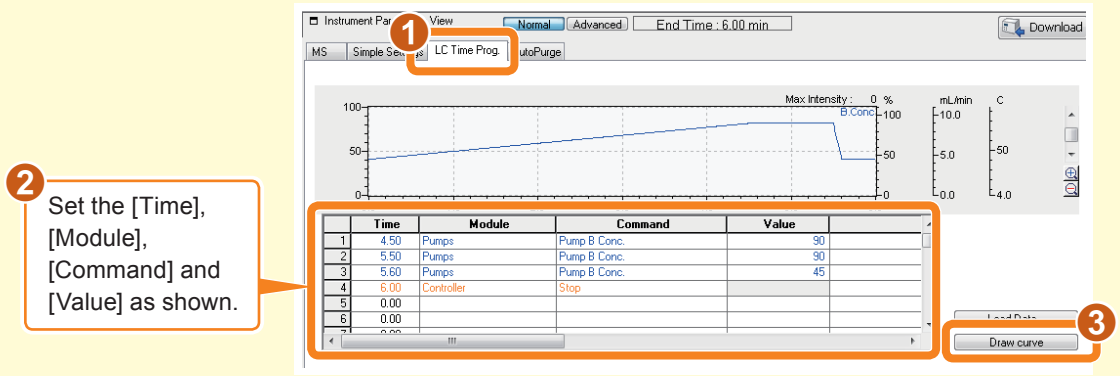


2 Set the LC instrument parameters.



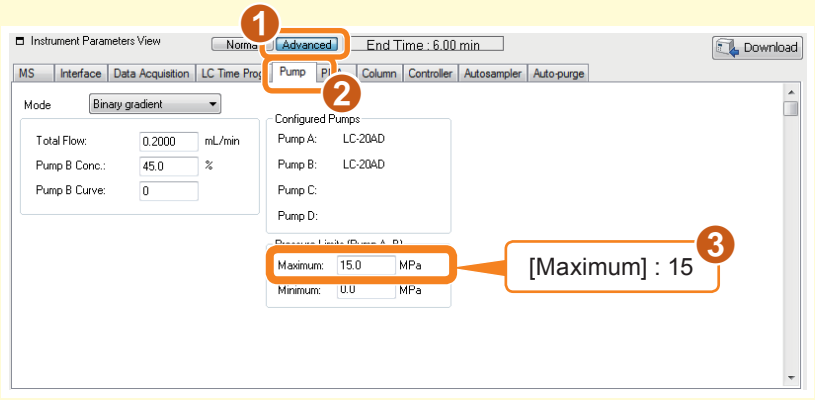
▼Tips Gradient Conditions

Go to the [LC Time Prog.] Tab Gradient mode to change the mobile phase mixture ratio, and set with the following procedure.



▼Tips Pump Pressure Limits

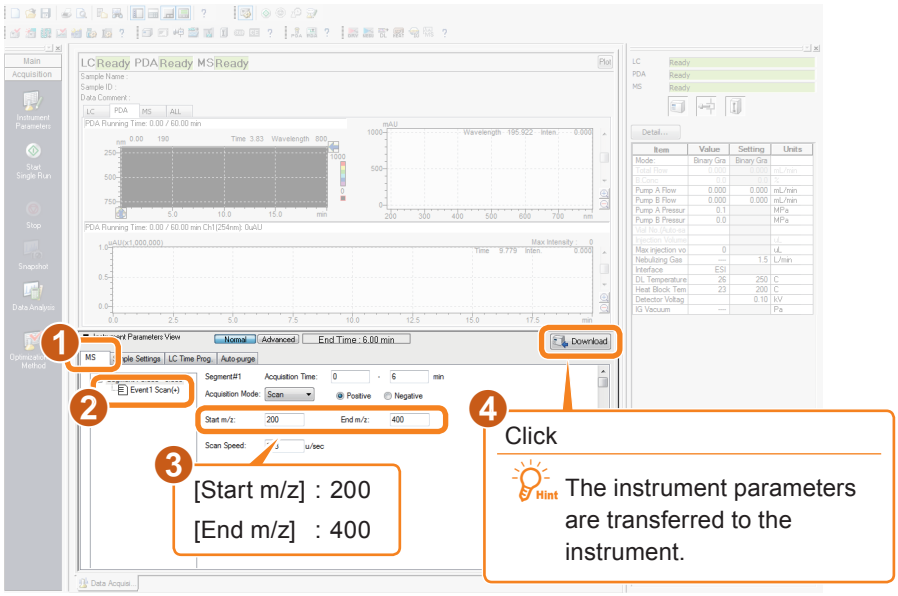
The maximum column pressure (pressure resistance) value is specified in the column's instruction manual. Use the following procedure to set the pressure threshold (typically, the column's pressure resistance) at which the pump automatically stops to protect the column. This procedure changes the upper pressure value to 15 MPa, as an example.



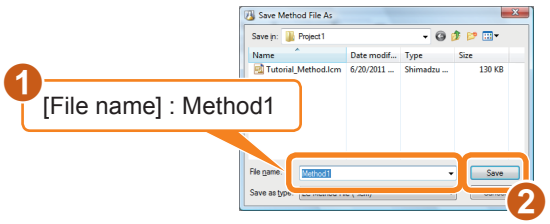
2.3 Set the MS Instrument Parameters

Reference "2.2 Enter Data Acquisition Parameters" in *Operators Guide*.

1 Set the MS instrument parameters.



2 Save the method file.



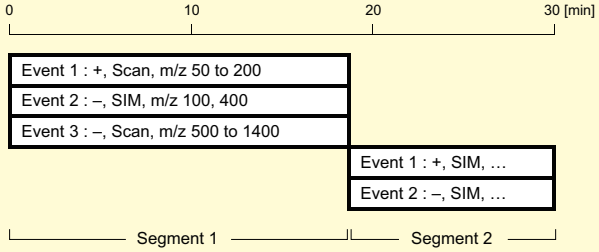
Hint This sub-window is not displayed when a method file is already saved.

▼Tips Segments and Events

During each acquisition with the LCMS-2020, acquisition conditions are switched at a specified interval. The interval is called a "segment". Multiple MS conditions can be set for each segment. Each set of MS conditions is called an "event".
Segments and events can be combined to configure complex MS acquisition conditions.
In this guide, only one event is used for data acquisition.

When multiple events are set for the same segment, the events change when the event acquisition time elapses. After the last event in a segment, the first event is repeated. This cycle (in the diagram to the right, Segment 1, Event 1 → Event 2 → Event 3 → Event 1 ...) is repeated for the specified segment time.

When the time specified for the segment has elapsed, the same actions are repeated in the next segment.



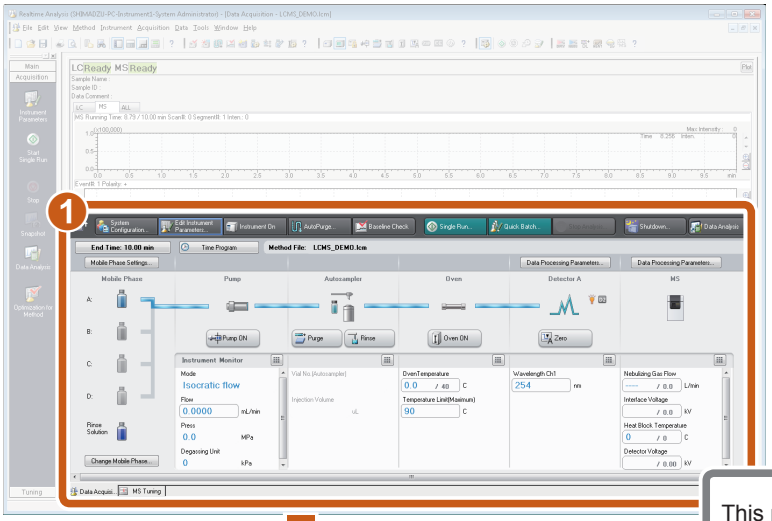
Hint Switching polarities between positive and negative modes requires 15 msec. Therefore, the length of an event following one where polarity was switched is actually 15 msec shorter than the set time. Adjust the event time as necessary.

LabSolutions

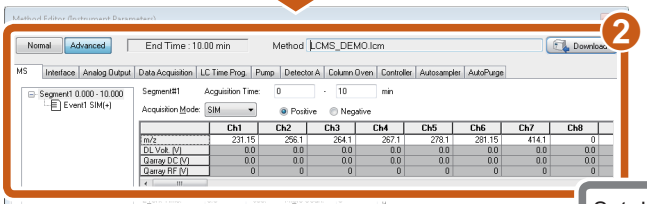
SUPPLEMENT

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.



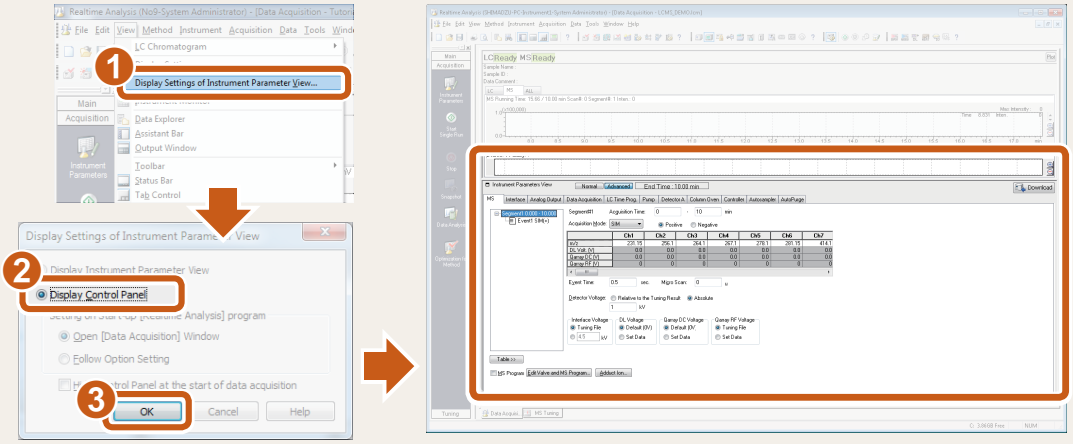
Set data acquisition conditions (instrument parameters).

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.

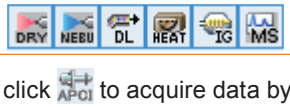


2.4 Instrument Control

1 Take control of the instrument.

The DL plug must be removed before starting analysis.

1. To take control of the MS instrument

   Click each 

.

   Hint Also click 

to acquire data by atmospheric pressure chemical ionization (APCI).

2. Click 

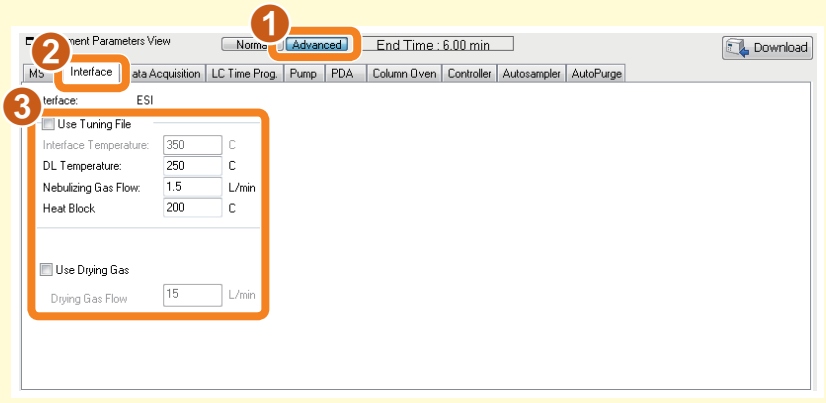
   To take control of the LC instrument

2 Purge the LC pump and autosampler.

Always purge after changing the mobile phase.

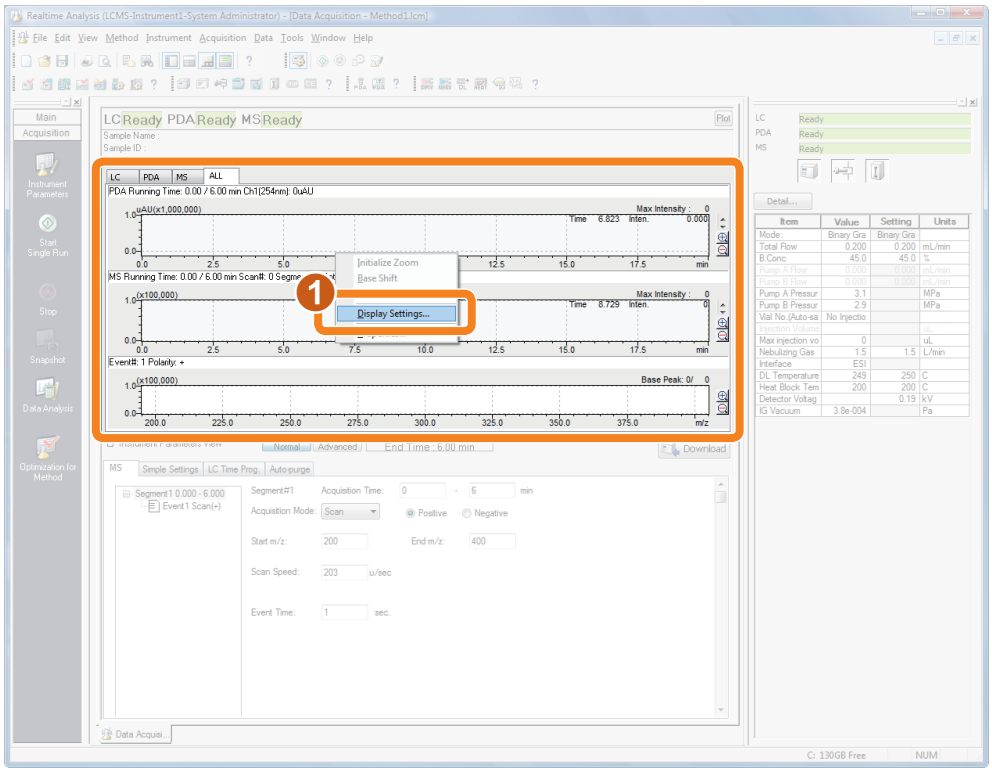
▼Tips Set the interface temperature and the gas flow

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



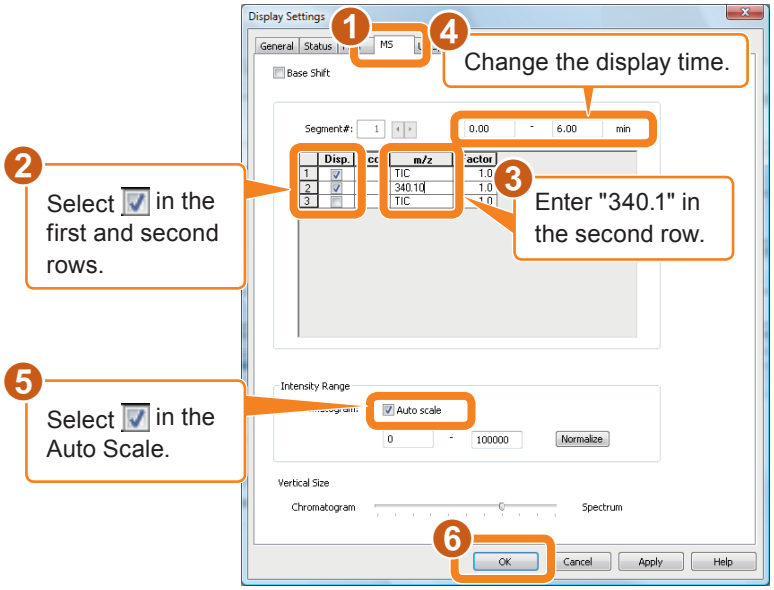
2.5 Set the Chromatogram Display Parameters

1 Right click on the chromatogram to open the [Display Settings] sub-window.



2 Select the type and range for the graph to display.

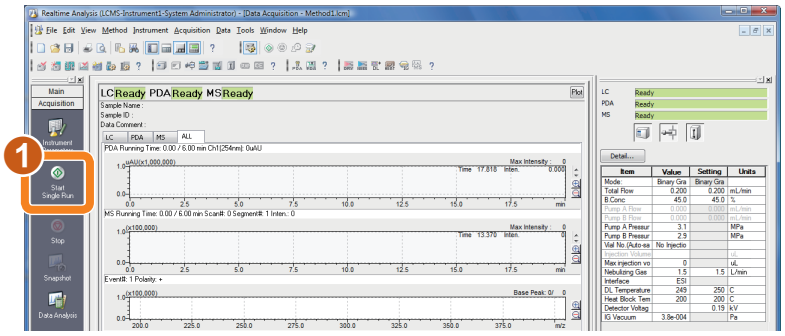
For example, configure settings to display a TIC and a m/z 340.1 MS chromatogram.



2.6 Single Run Acquisition

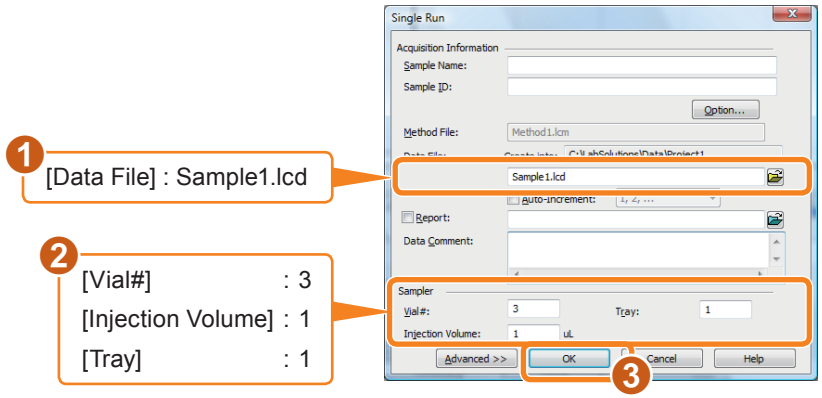
Conduct a single run with the settings made in "2.2 Set the LC Instrument Parameters" and "2.3 Set the MS Instrument Parameters".

1 Open the [Single Run] sub-window.

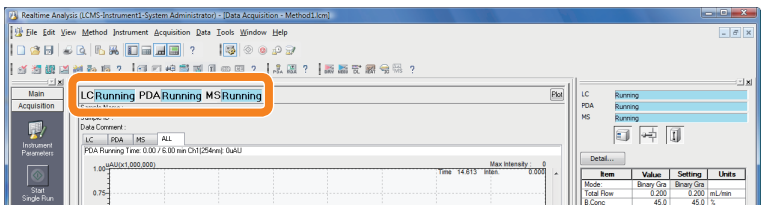


2 Set the conditions for a single run.

For this example, prepare 5 ng/µL of papaverine in autosampler vial #3, and inject 1 µL.



❸ Click [OK] to start the acquisition.

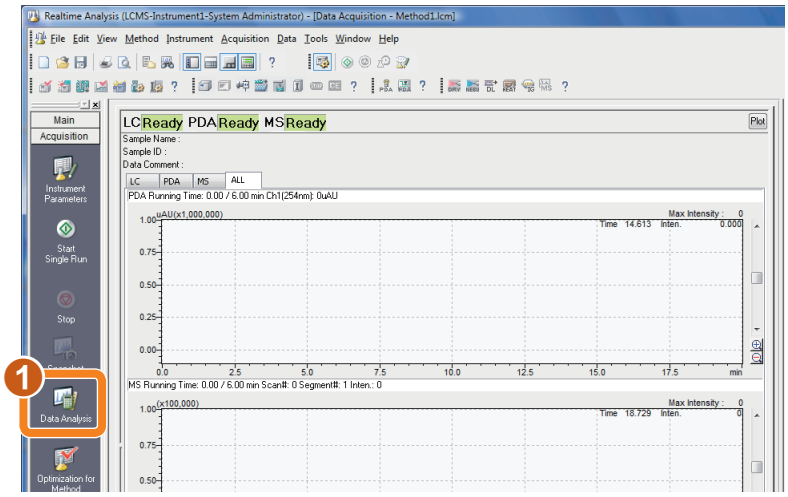


Data acquisition ends when the [Acquisition Time] set in the method file has elapsed.

Chapter 3. Confirmation of Qualitative Results

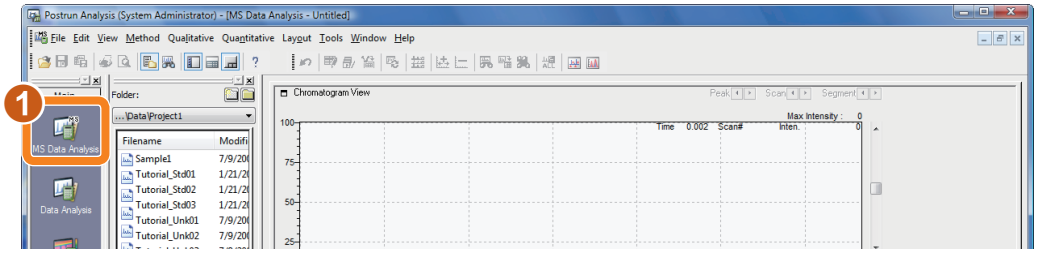
3.1 Qualitative Data Analysis using [MS Data Analysis] window

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

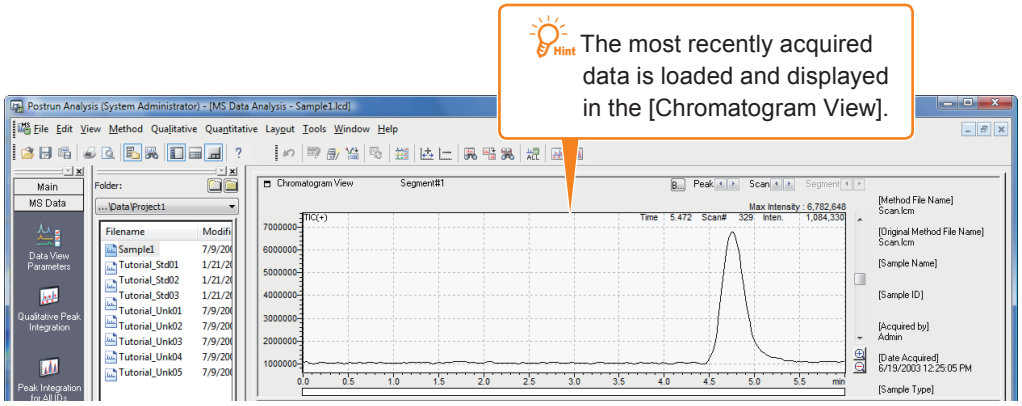


The [Postrun Analysis] program starts.

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

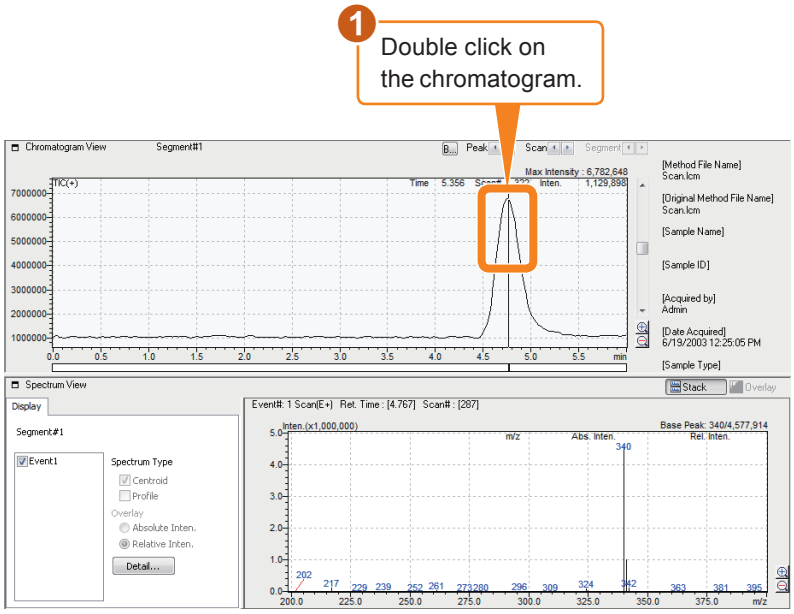


The [MS Data Analysis] window opens.



Hint The most recently acquired data is loaded and displayed in the [Chromatogram View].

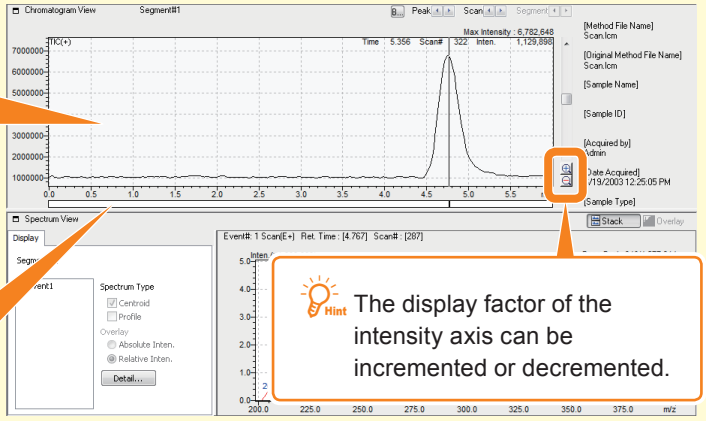
3 Display the MS spectrum.



▼Tips About viewing operations

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

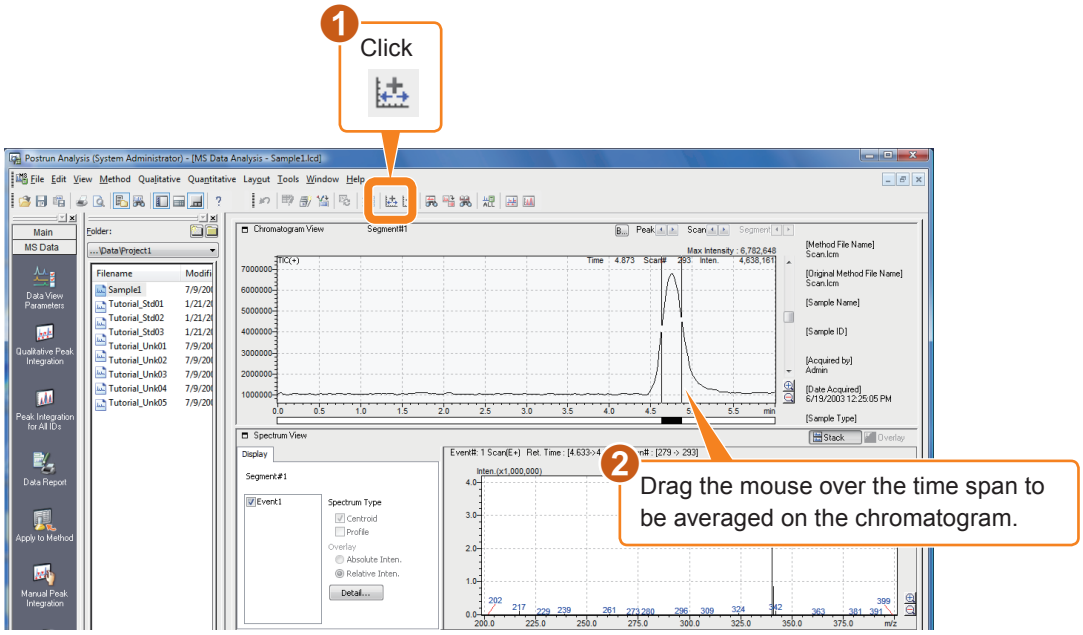
Hint Drag the frame border to change the relative size of each view.



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

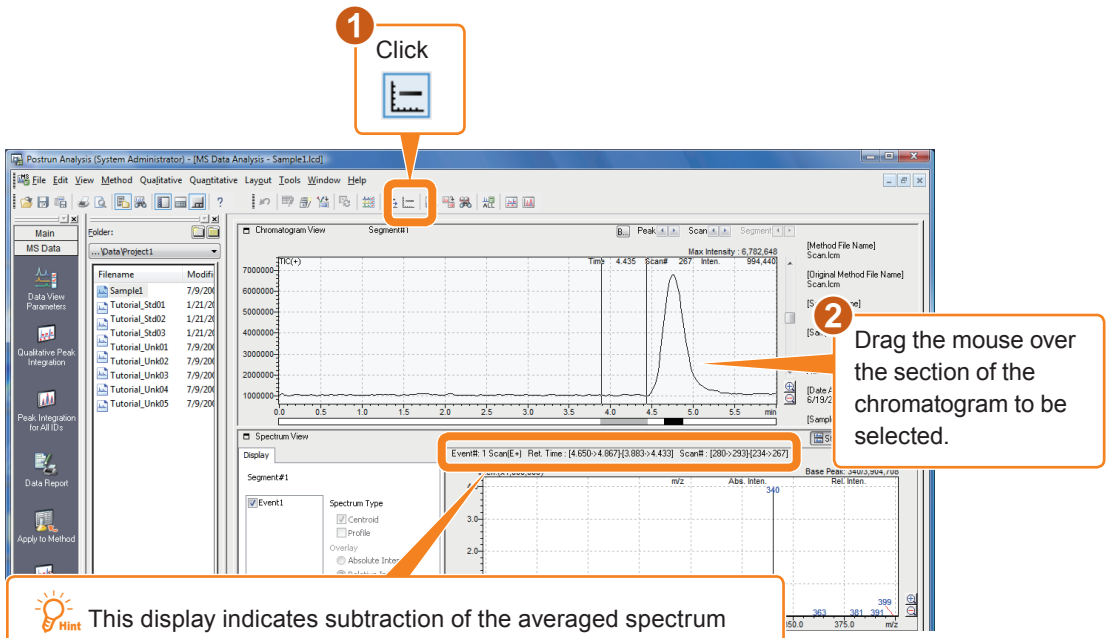
4 Average the MS spectrum.

A stable spectrum display can be obtained by accumulating and averaging the spectrum over a specified time span.



5 Subtract the background MS spectrum.

The spectrum display can be improved by subtracting the background MS spectrum from the averaged spectrum.

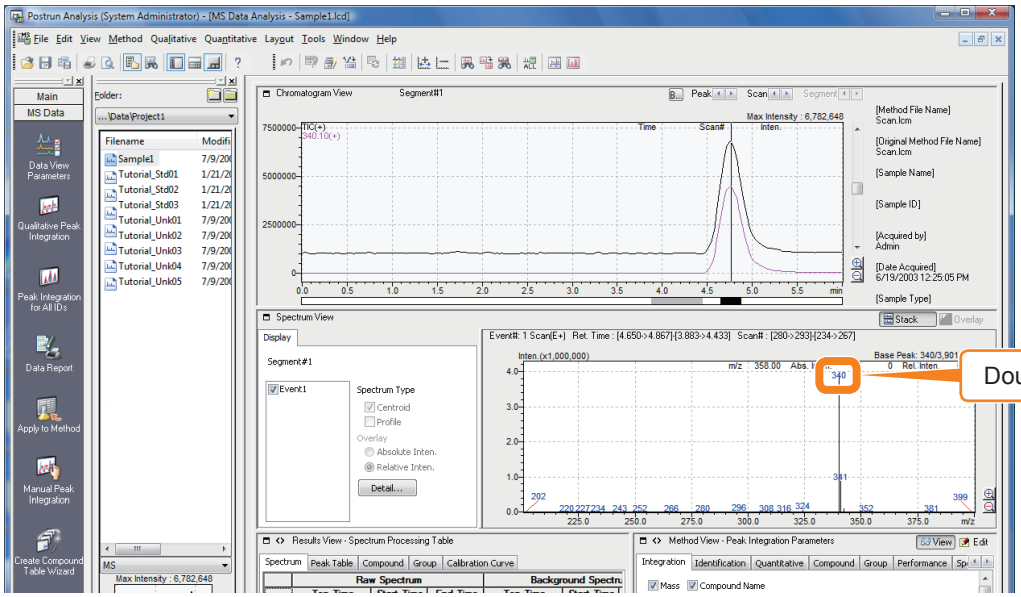


Hint This display indicates subtraction of the averaged spectrum between 3.883 and 4.433 minutes from the averaged spectrum between the retention times of 4.650 and 4.867 minutes.

Hint Double click on the chromatogram to subtract the spectrum at that position.

6 Display the MS chromatogram.

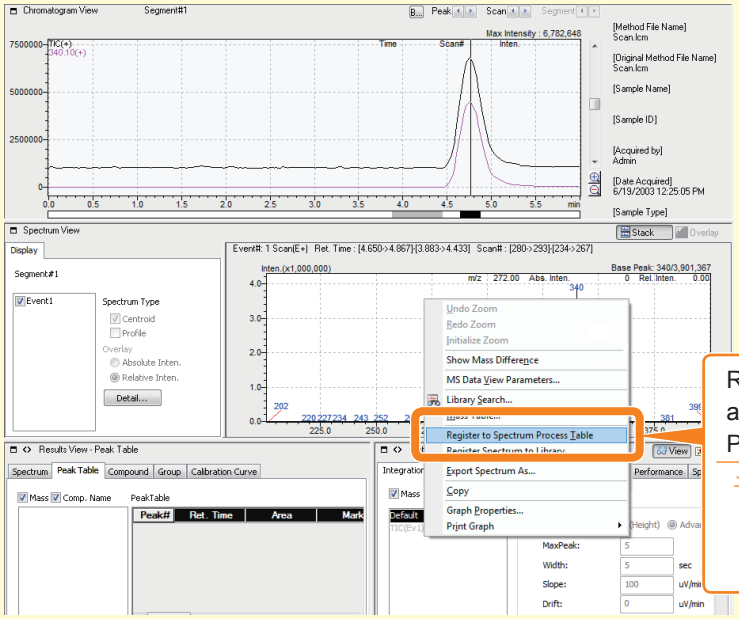
Double click the MS spectrum peak. The m/z chromatogram at the double-clicked position is overlaid on the [Chromatogram View].



▼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 from the [Report] window.



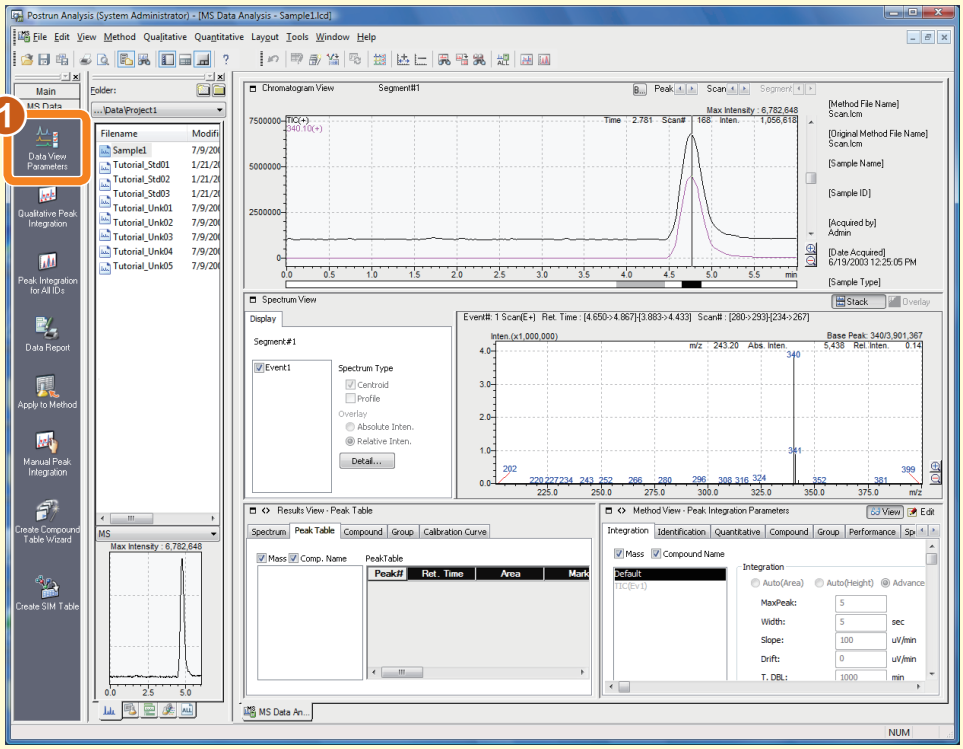
Right click on the spectrum graph, and select [Register to Spectrum Process Table].

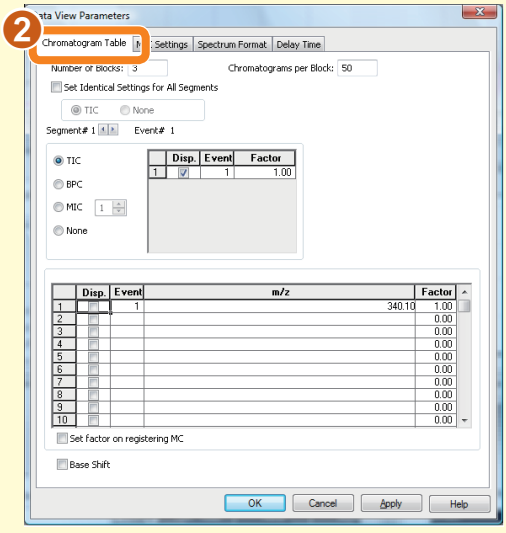
Hint The averaged and/or subtracted MS spectrum is registered.

Hint Registration is also available by clicking in the toolbar.

▼Tips　Change the MS chromatogram settings

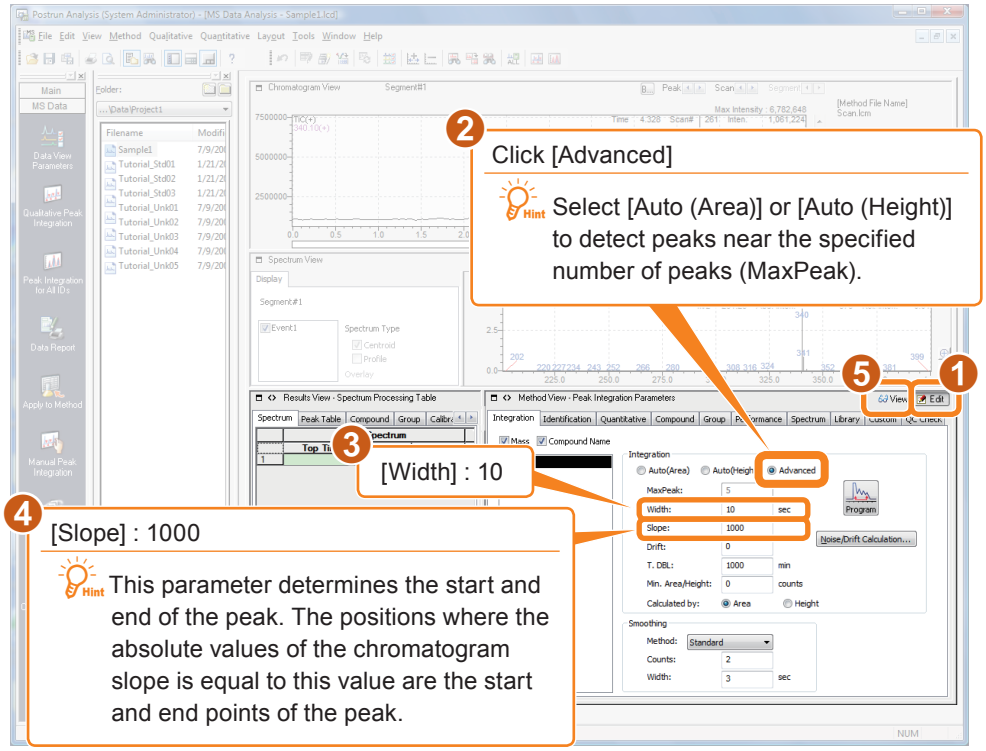
To change the *m/z* of the MS chromatogram to be displayed in the [Chromatogram View], use the [MS Data View Parameters] sub-window.
The [MS Data View Parameters] sub-window is displayed according to the following procedure.





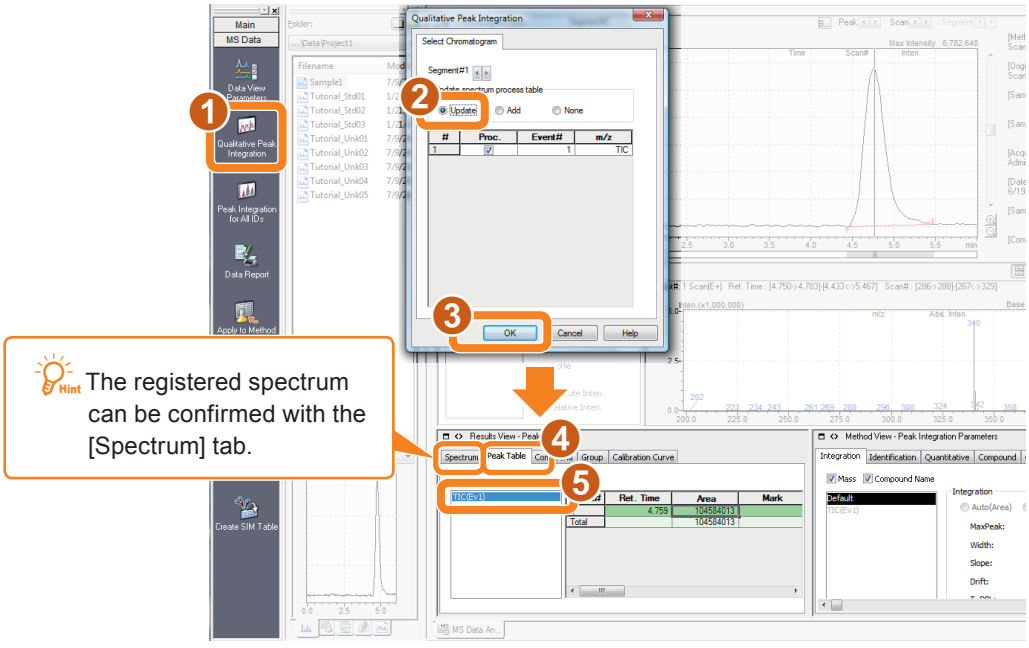
3.2 Peak Integration

1 Reset the peak integration parameters.



2 Detect the peaks.

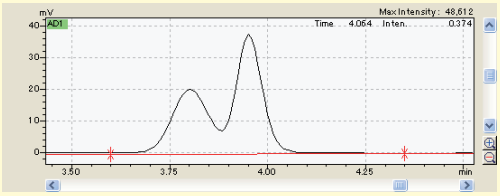
Click [Qualitative Peak Integration] in the [MS Data] assistant bar.
The results of integration are listed on the [Peak Table] tab of the [Results View].



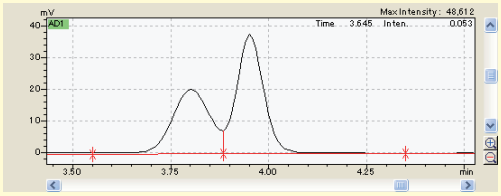
▼Tips Simple Peak Integration Parameters

First set the 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 surplus peaks are detected, then use those settings as the peak integration parameters.

Width Setting Example

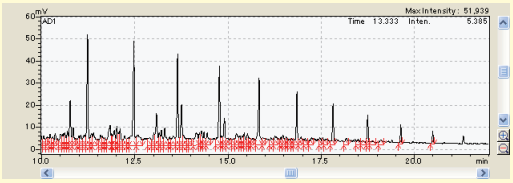


With the [Width] set to 30, the data is processed as one peak.

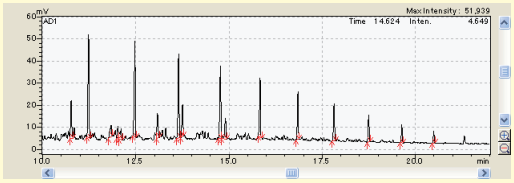


With the [Width] set to 10, the data is processed as two peaks.

Slope Setting Example



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

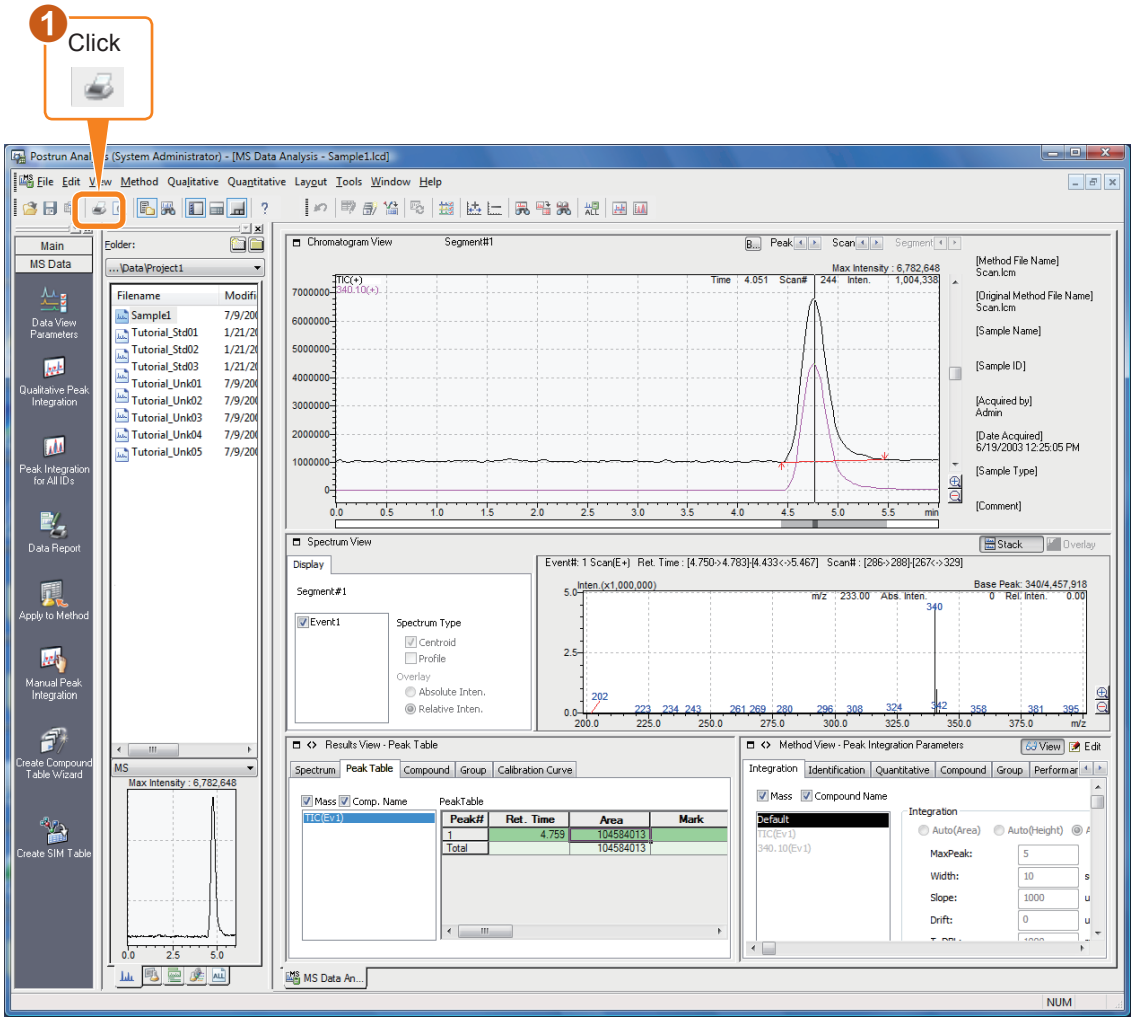


When the [Slope] is set to 100000, only those peaks larger than the Slope setting are detected.

3.3 Print Results

Print the results of qualitative analysis.

Print the information displayed in the window

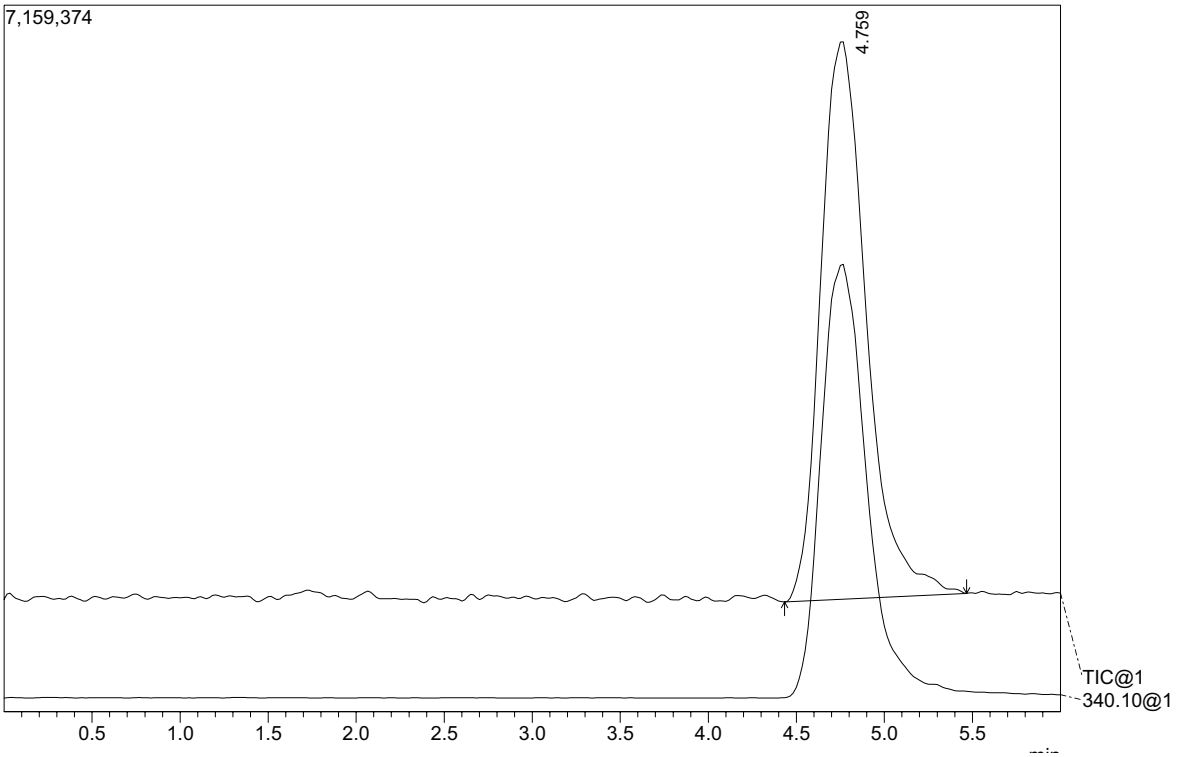


Graphic Image Printout Example

==== Shimadzu LabSolutions Data Report ====

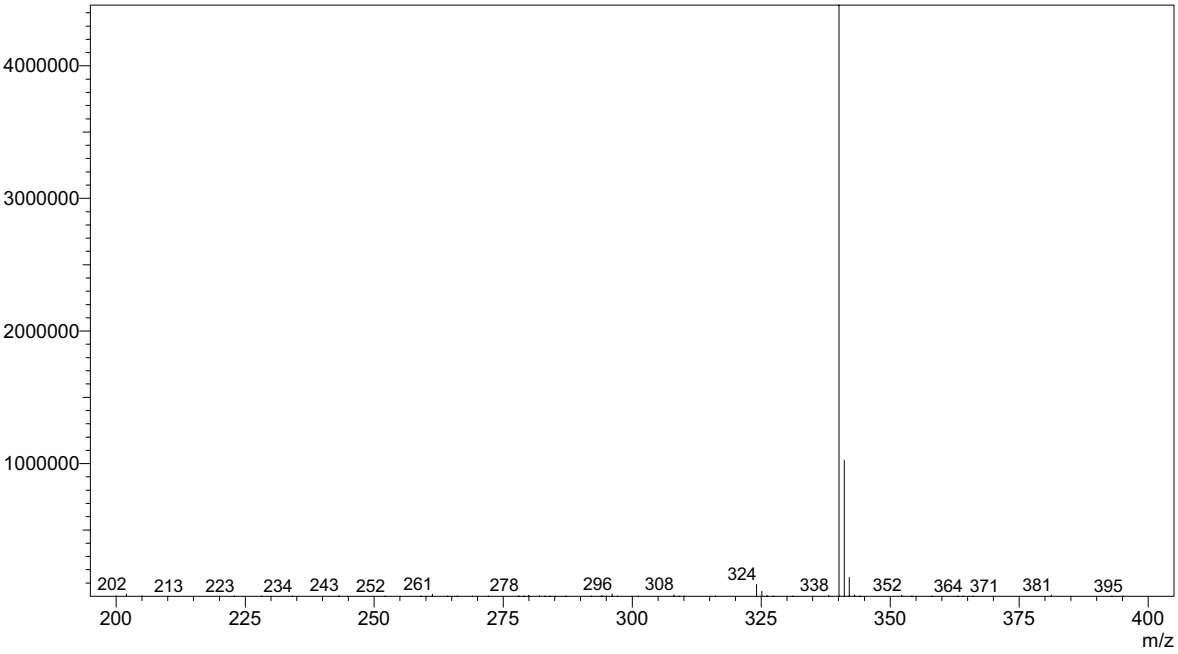
Sample ID : **Date Acquired** : **1/19/2008 9:25:05 PM**
Data Name : **Sample1.lcd**

<Chromatogram>



<Spectrum>

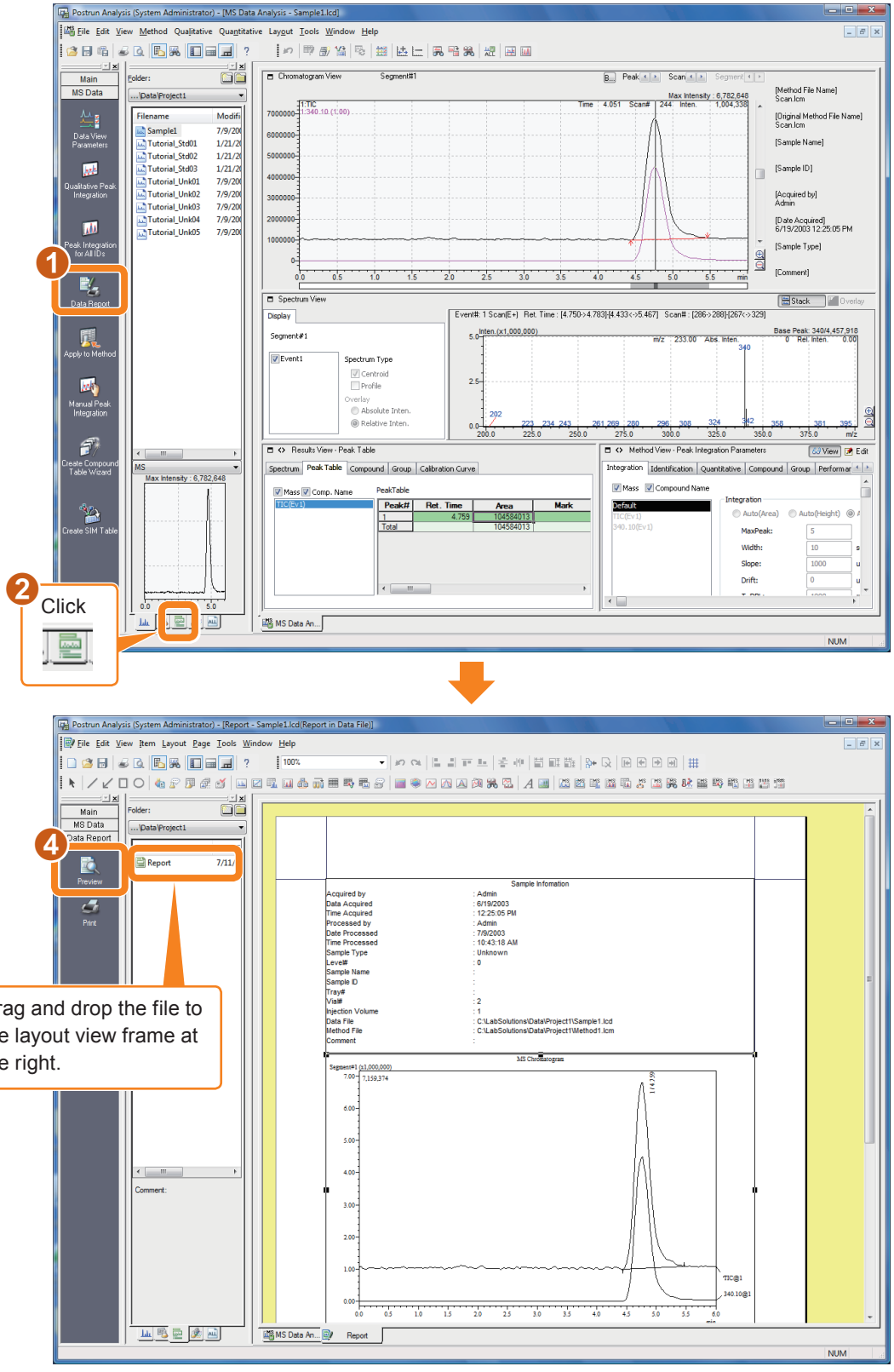
Line#:1 R.Time:4.767(Scan#:287)
MassPeaks:106
RawMode:Averaged 4.750-4.783(286-288) BasePeak:340(4457918)
BG Mode:Calc Segment 1 - Event 1



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.

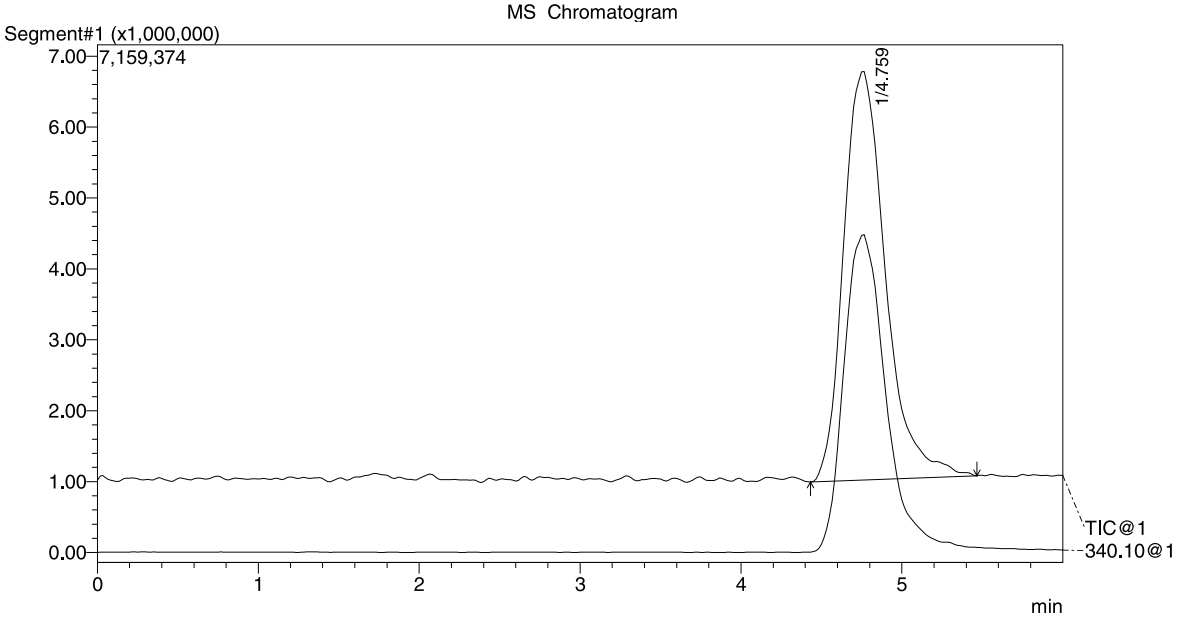


Report Format Printout Example

Sample Infomation

Acquired by	: Admin
Data Acquired	: 1/19/2008
Time Acquired	: 9:25:05 PM
Processed by	: System Administrator
Date Processed	: 4/3/2008
Time Processed	: 12:17:52 PM
Sample Type	: Unknown
Level#	: 0
Sample Name	:
Sample ID	:
Tray#	:
Vial#	: 2
Injection Volume	: 1
Data File	: C:\LabSolutions\Data\Project1\Sample1.lcd
Method File	: C:\LabSolutions\Data\Project1\Method1.lcm
Comment	:

MS Chromatogram



MS Peak Table TIC

Peak#	Ret. Time	m/z	Area	Mark	Compound Name	A/H	Event#
1	4.759	TIC	104584013			18.153	1-1
Total			104584013				

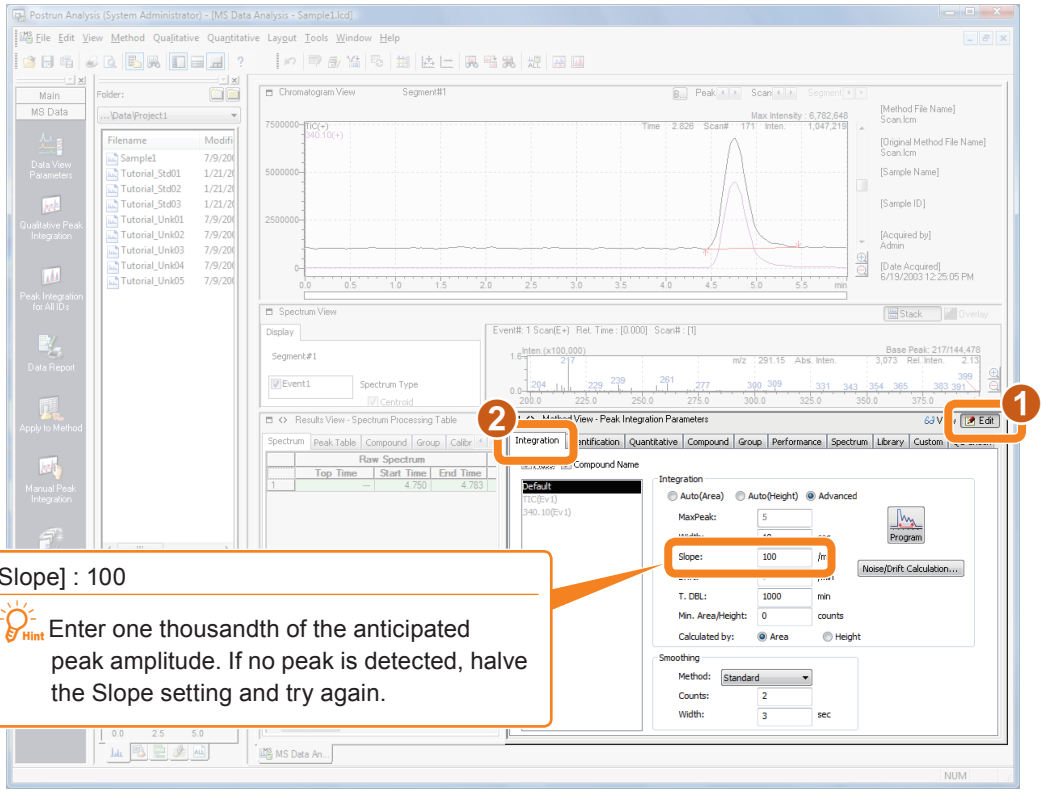
Chapter 4. Realtime Batch

4.1 Compound Table Setup

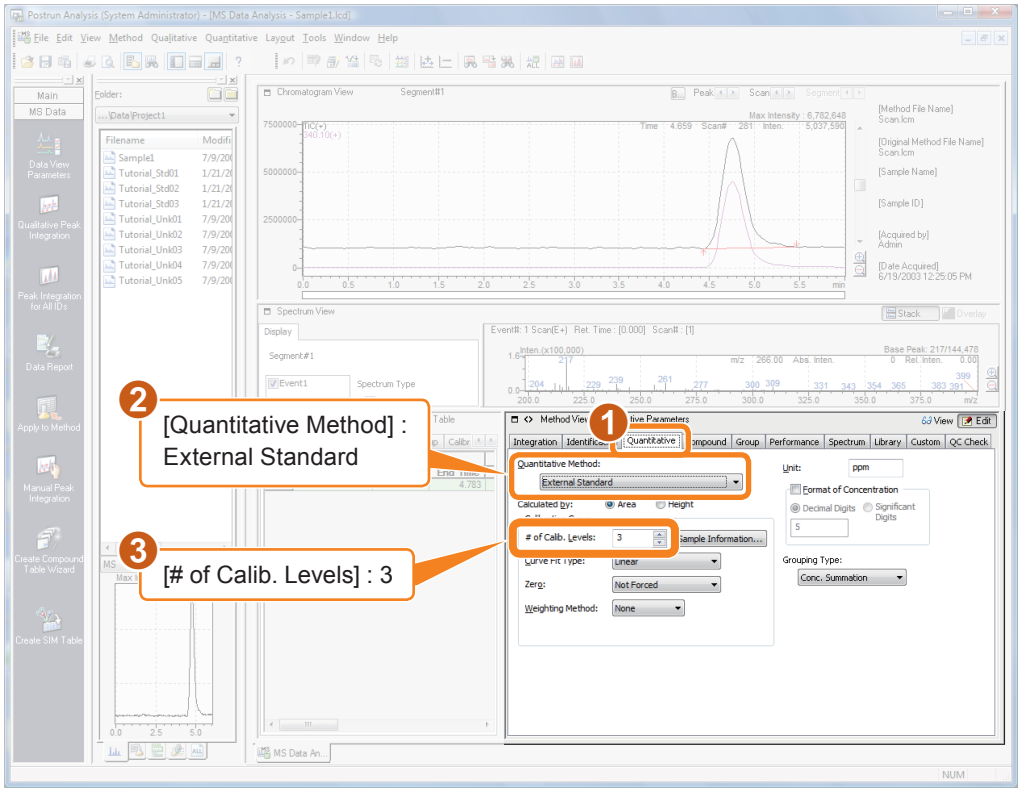
For quantitative processing, use a "standard sample" with a known concentration to create a "calibration curve".
Using this calibration curve to calculate the concentration of the components in the unknown data source.
In this example, we create a calibration curve by injecting 1 µL of papaverine at 0.5, 1 and 5 ng/µL. Measure 0.7 ng/µL papaverine as a presumed unknown, and calculate quantitatively.

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

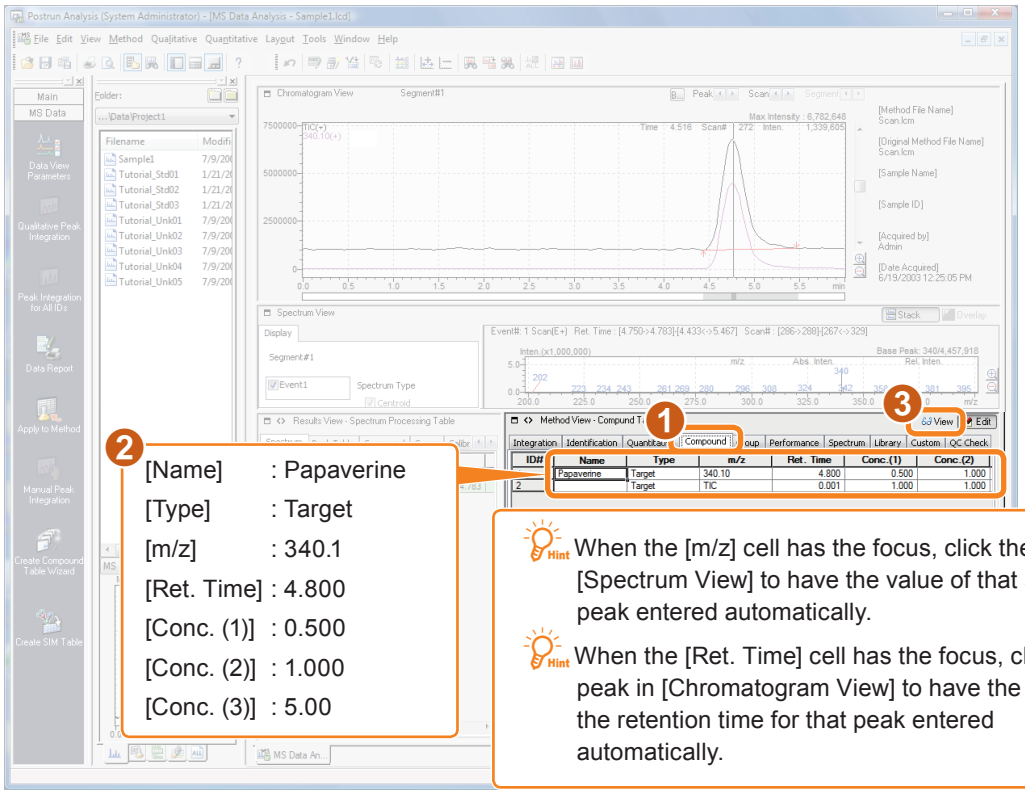
Use the Sample1.lcd papaverine data that was loaded in [MS Data Analysis] in the previous chapter.



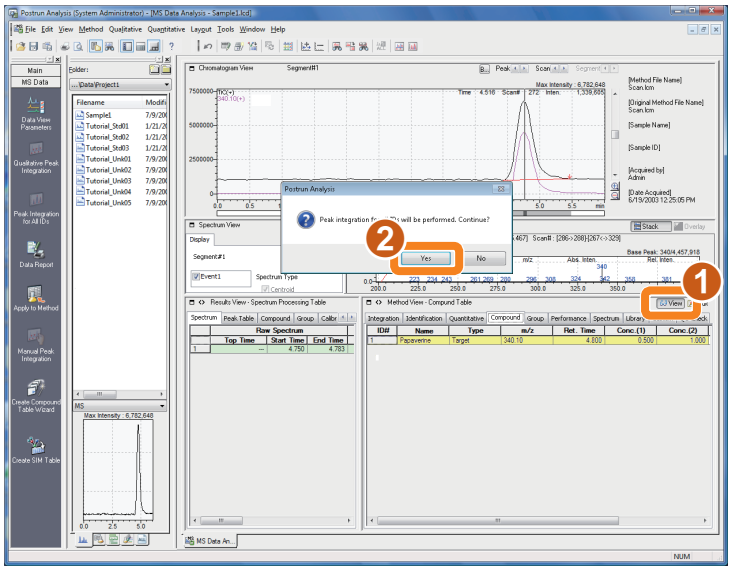
2 Enter the quantitative parameters.



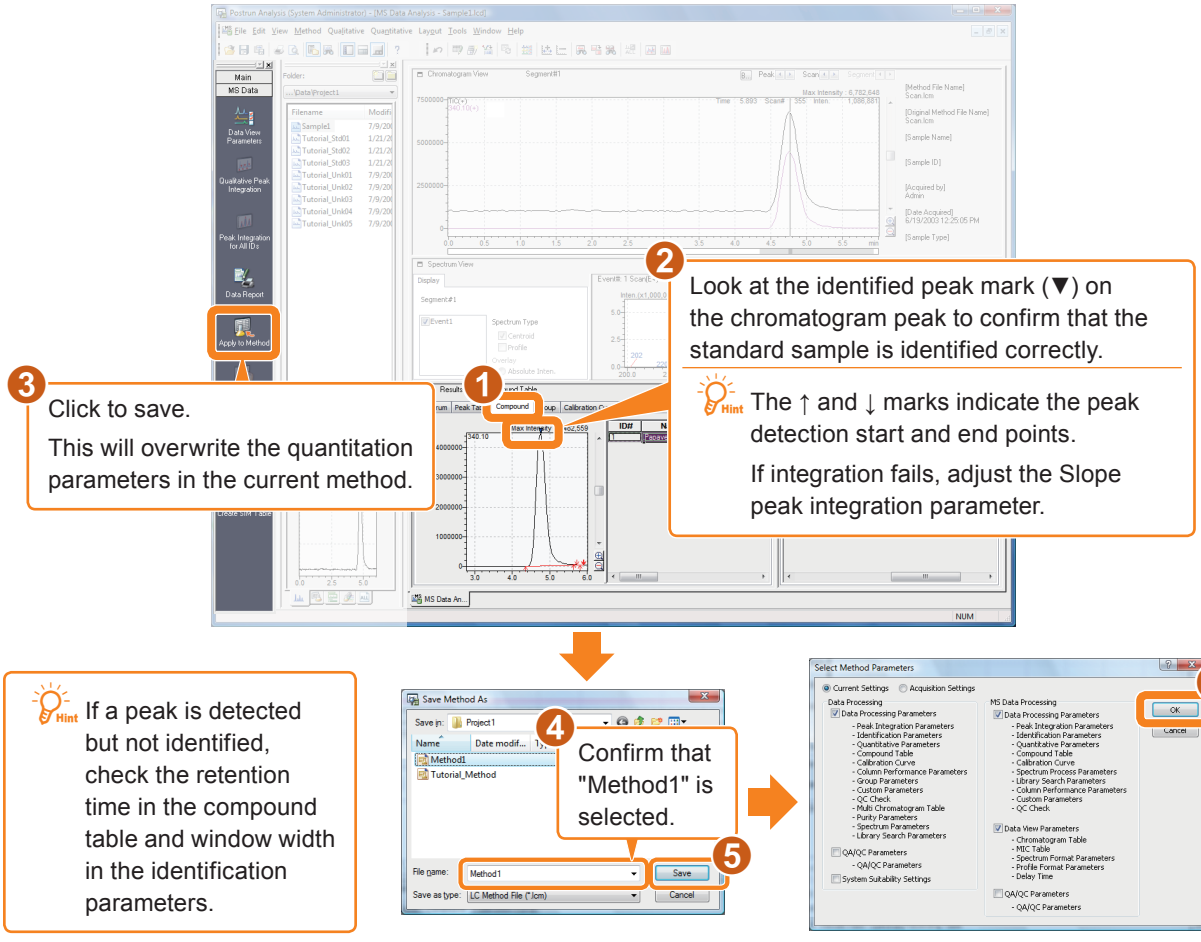
3 Fill in the Compound Table.



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



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



3 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.

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

4 Confirm that "Method1" is selected.

5 Save

6 OK

The method file is overwritten and saved.

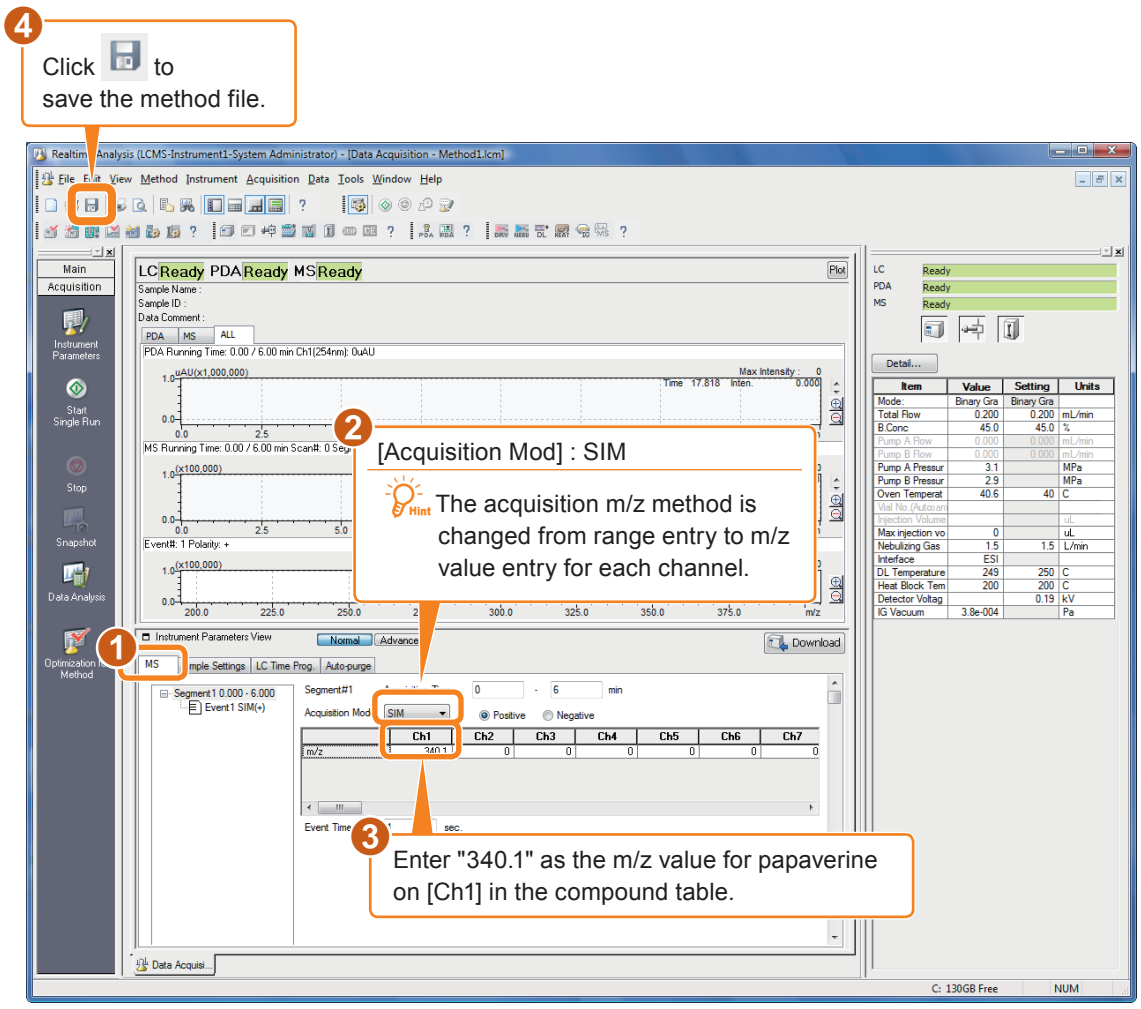
4.2 Create a SIM Table

SIM (Selected Ion Monitoring) is the acquisition mode where only the intensity changes of a specific ion are tracked.
Because detection data is only retained for a specified ion, sensitivity is higher than when the scan mode is used to scan a wide m/z range.
For this quantitative analysis, we use the m/z value set in "4.1 Compound Table Setup" to change the parameter obtained through the acquisition.

1 Click the [Realtime Analysis] program on the task bar.

Return to the [Data Acquisition] window of the [Realtime Analysis] program.

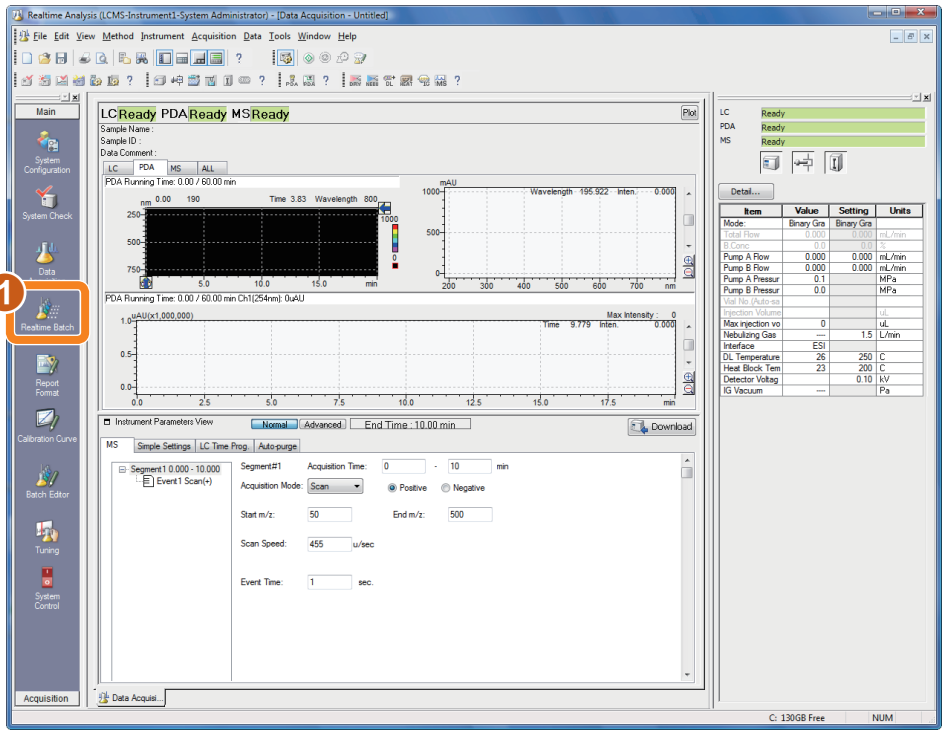
2 Select the [Instrument Parameters View].



4.3 Create a Batch Table

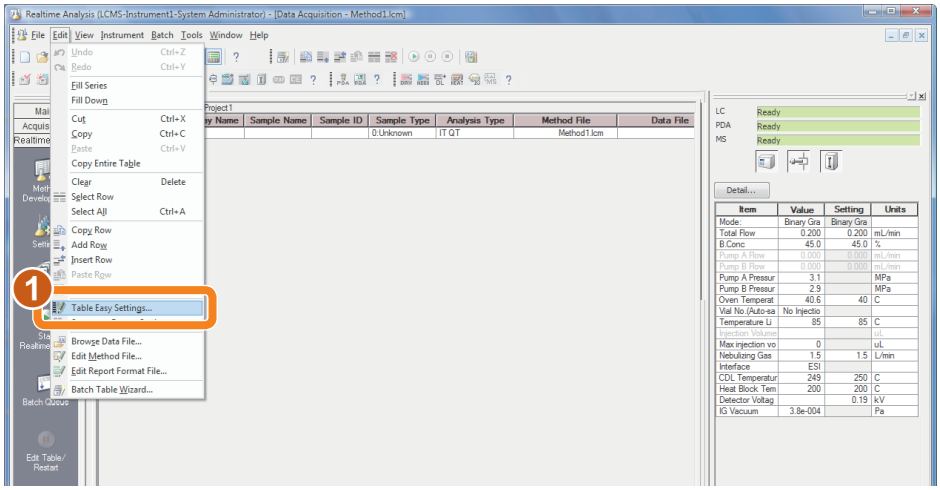
Select a batch table using the method file created for realtime sequential batch analysis.

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

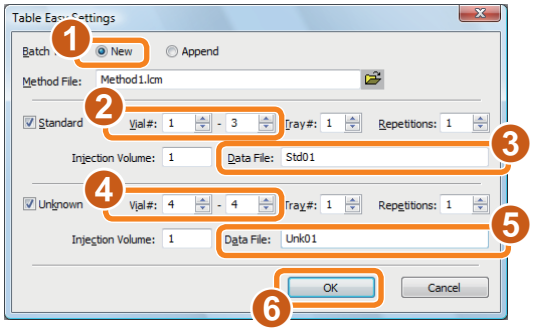


The [Batch Table] window is displayed.
Follow the next steps to create a Batch Table. Use the first three rows for the standard sample and leave the fourth row as unknown.

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

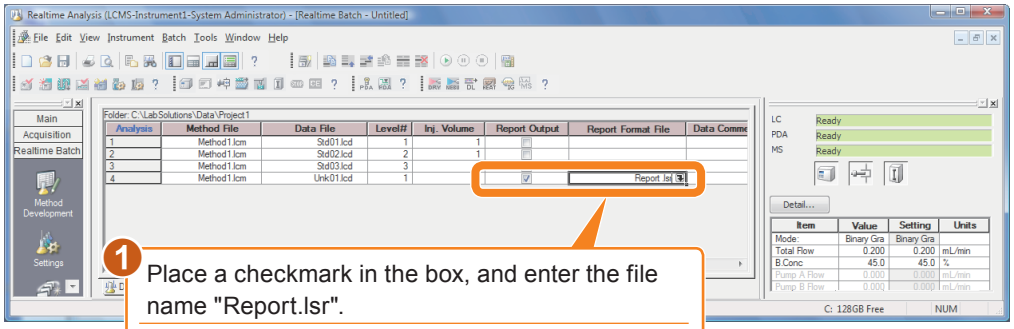


3 Make the following settings on the [Table Easy Settings] sub-window.



A four-row Batch Table is created.

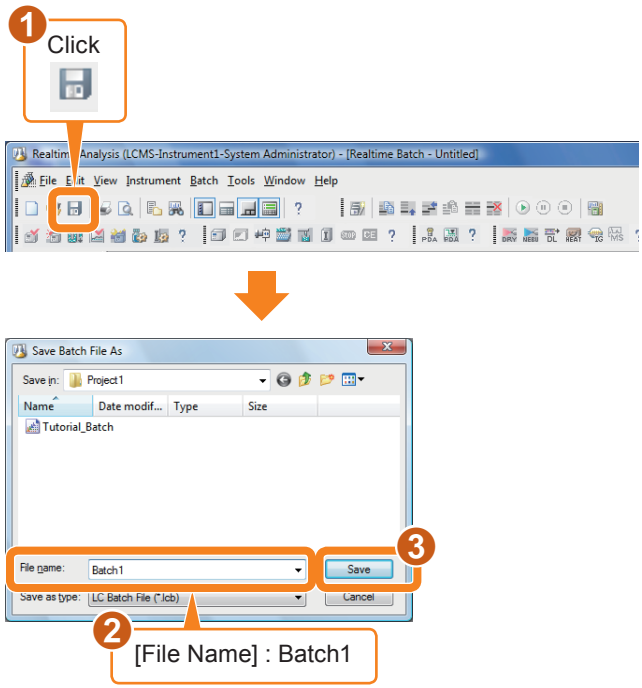
4 Specify the fourth (unknown) row for report output.



1 Place a checkmark in the box, and enter the file name "Report.lsr".

Hint If a path is not specified for the file name, the report will be stored in the folder that is open in the [Data Explorer].

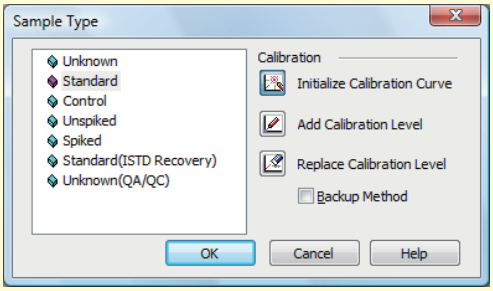
5 Save the Batch Table settings.



▼Tips Batch Table Settings

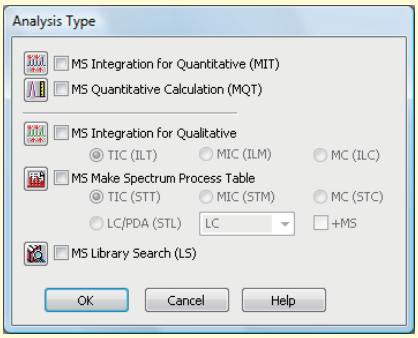
Sample Type

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

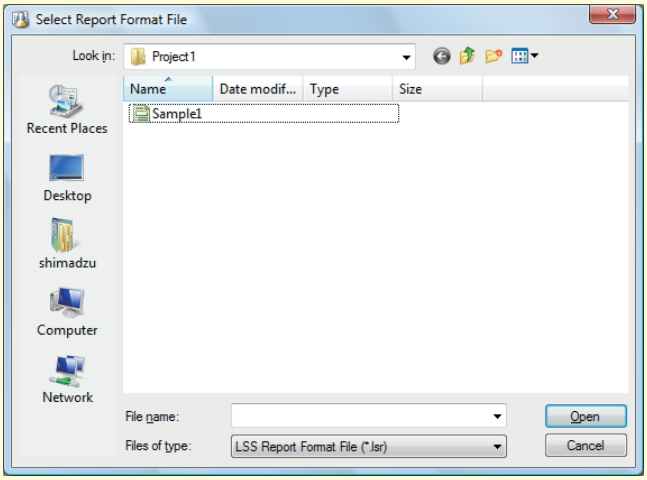
Enter a level number for all of the standard samples.

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.

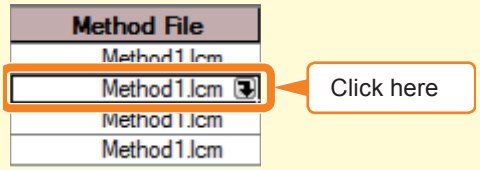


Reference *Help*

▼Tips Table Entries

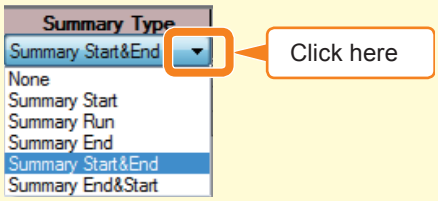
Popup Windows (for complex settings)

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



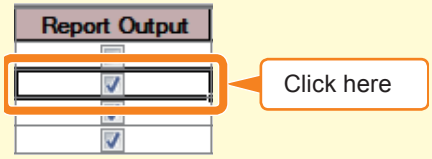
Drop-Down List (to select from a list of choices)

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.



Checkbox (to select on/off)

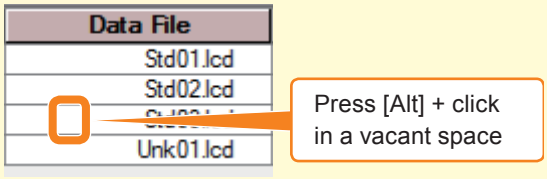
Click the displayed checkbox to select or clear a checkmark.



[Alt] + click (to open a file)

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

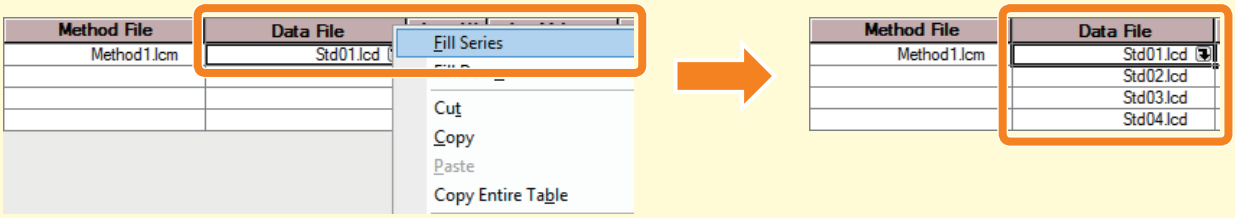
The data or method file for the selected row in a Batch Table can also be opened from the [Edit] menu.



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

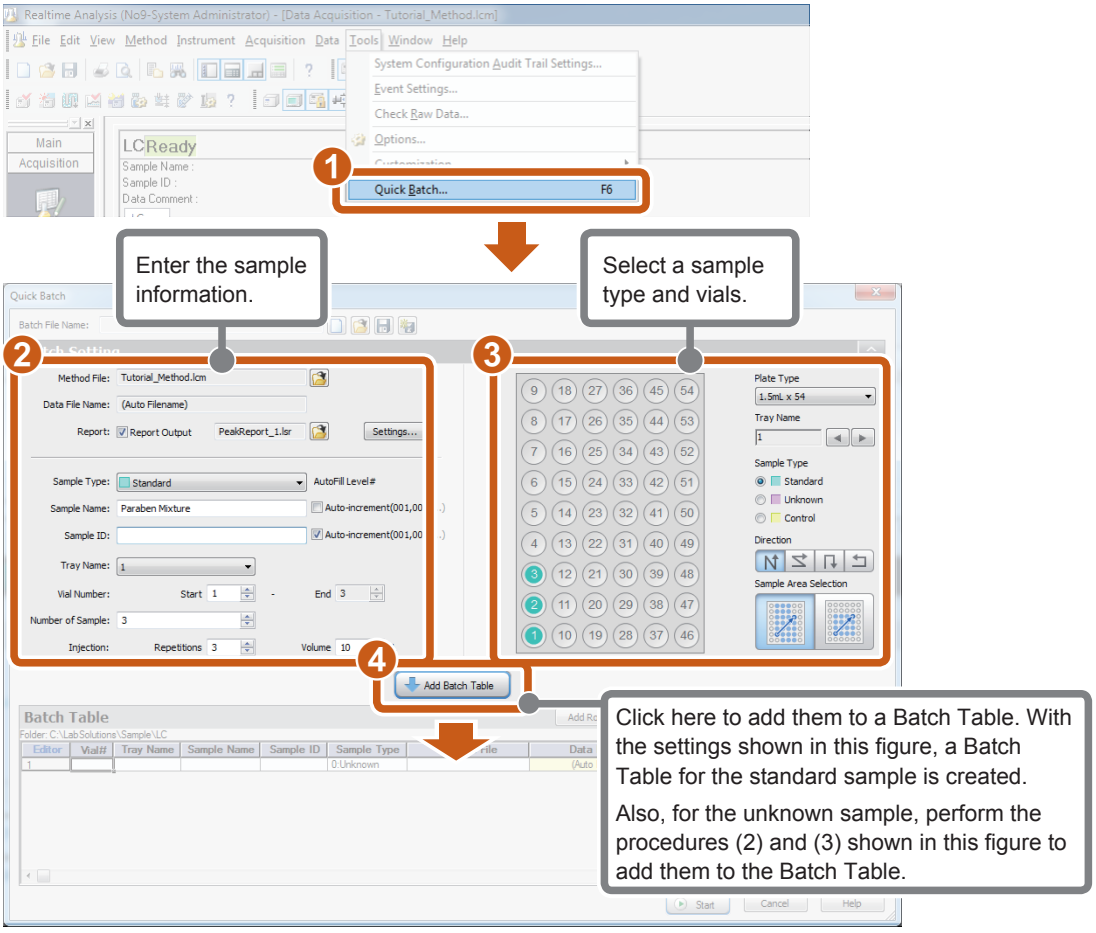
Hint To add rows, select [Add Row] from the right-click menu of the batch table.

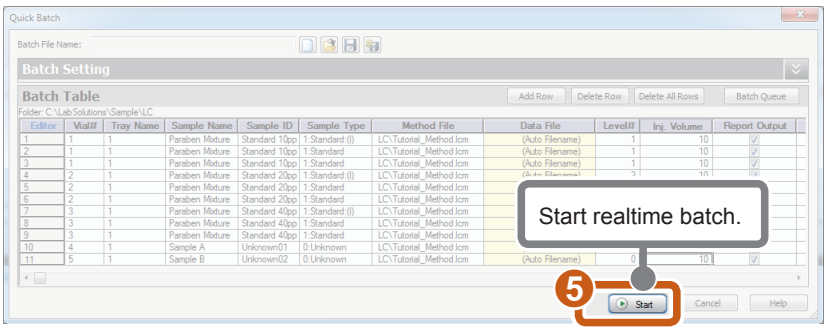
LabSolutions

SUPPLEMENT

Create a Batch Table Using Quick Batch

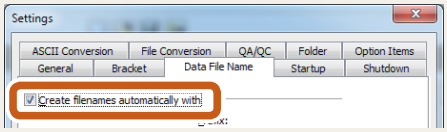
You can also create a Batch Table using quick batch.





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.



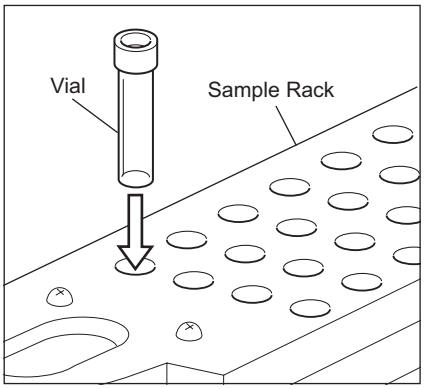
Chapter 4

4.4 Realtime Batch Processing

Execute a batch process using a Batch Table created as described in "4.3 Create a Batch Table".

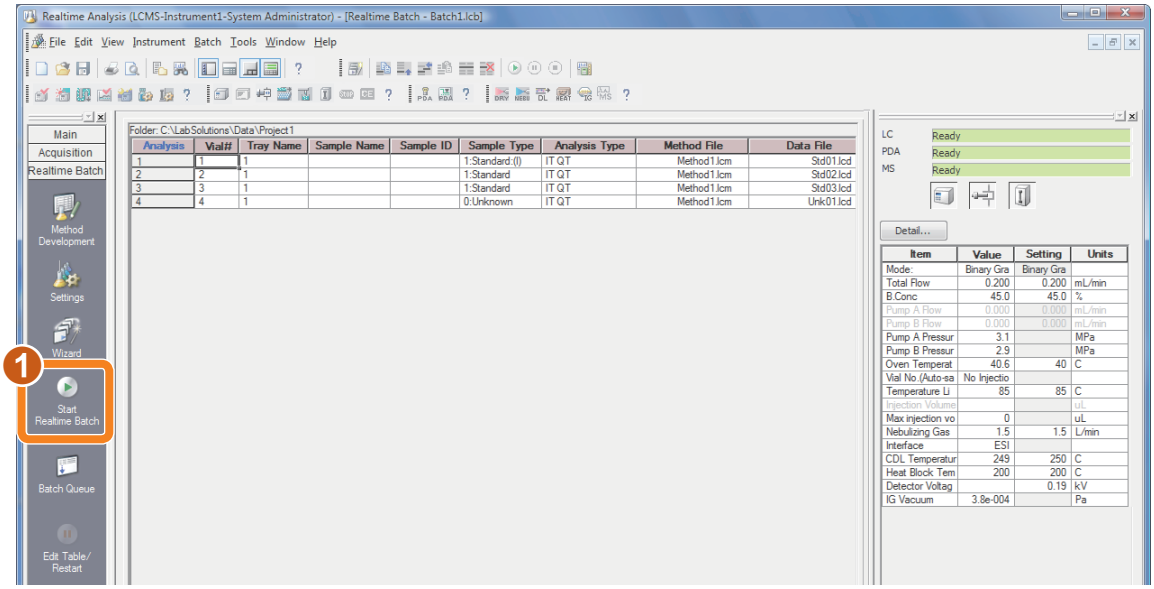
1 Place the samples in the autosampler.

Vial 1 0.5 ng/μL papaverine liquid (standard sample)
Vial 2 1 ng/μL papaverine liquid (standard sample)
Vial 3 5 ng/μL papaverine liquid (standard sample)
Vial 4 Unknown sample (for quantitation)
* The unknown sample is a 0.7 ng/μL papaverine solution.



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 continues.

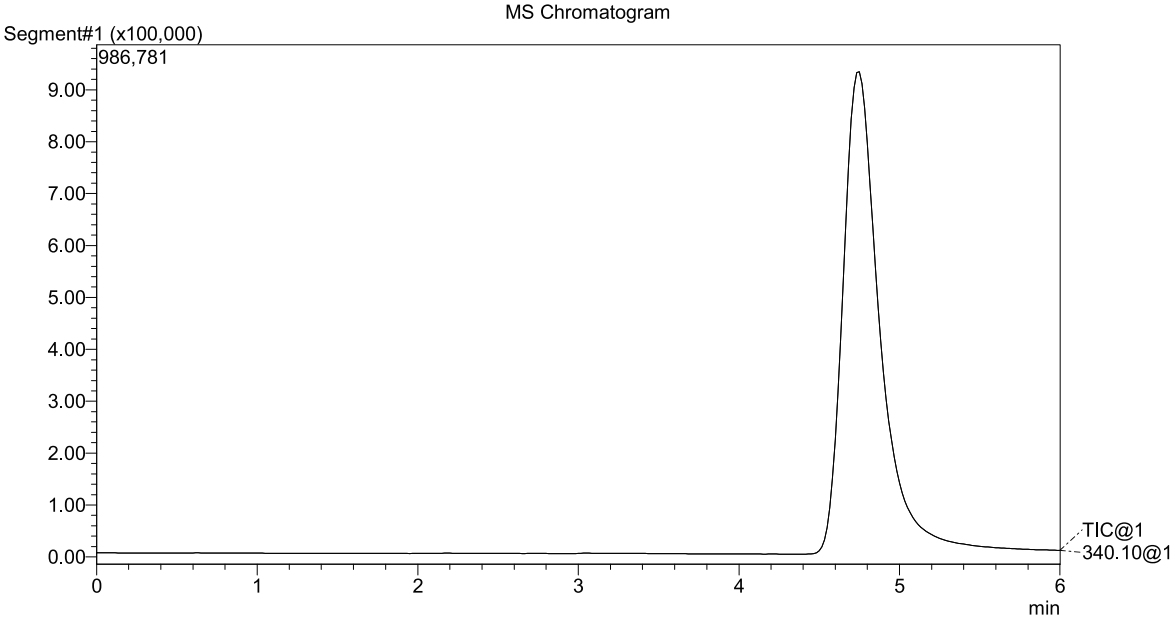
Hint You can take a snapshot to view the data during acquisition. To take a snapshot, click Snapshot in the [Data Acquisition] assistant bar during acquisition.

Realtime Batch Report Printout Example

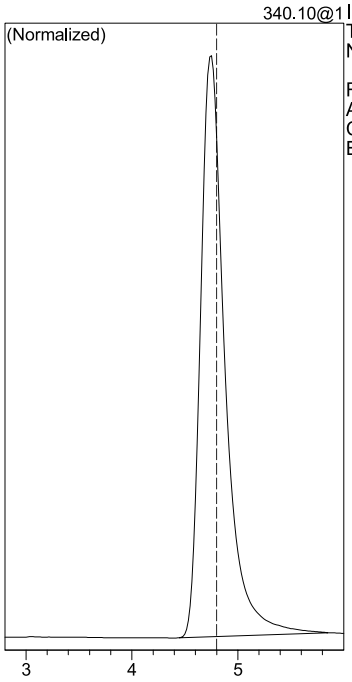
Sample Infomation

Acquired by	: Admin
Data Acquired	: 1/19/2008
Time Acquired	: 9:01:05 PM
Processed by	: System Administrator
Date Processed	: 4/3/2008
Time Processed	: 1:02:22 PM
Sample Type	: Unknown
Level#	: 0
Sample Name	:
Sample ID	:
Tray#	:
Vial#	: 10
Injection Volume	: 1
Data File	: C:\LabSolutions\Data\Project1\Unk01.lcd
Method File	: C:\LabSolutions\Data\Project1\Method1.lcm
Comment	:

MS Chromatogram



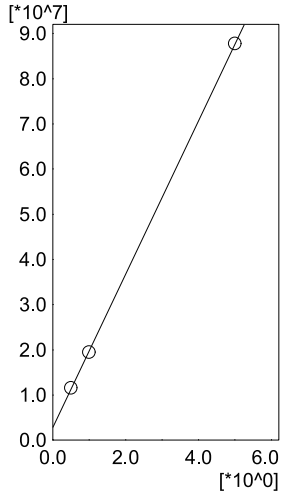
Mass Quant Graph



ID#: 1		m/z: 340.10
Type:		Trgt
Name:		papaverine
Ret.Time:		4.743
Area:		14816115
Conc.:		0.707ppm
Event:1		

Calibration Curve

ID#	: 1	m/z : 340.00
Name	: papaverine	
Function	: f(x)=1.697756e+007*x+2.804693e+006	
Rr1=0.9999711	Rr2=0.9999423	
FitType	: Linear	
ZeroThrough	: Not Through	
Weighted Regression		: None
Quantitation Method	: External Standard	

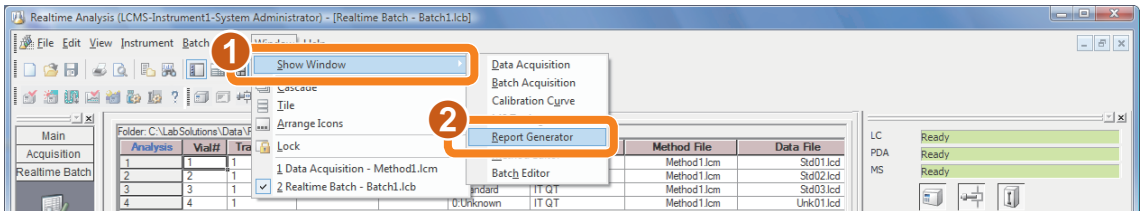


#	Conc.(Ratio)
1	0.500
2	1.000
3	5.000

4.5 Print Batch Processing Reports

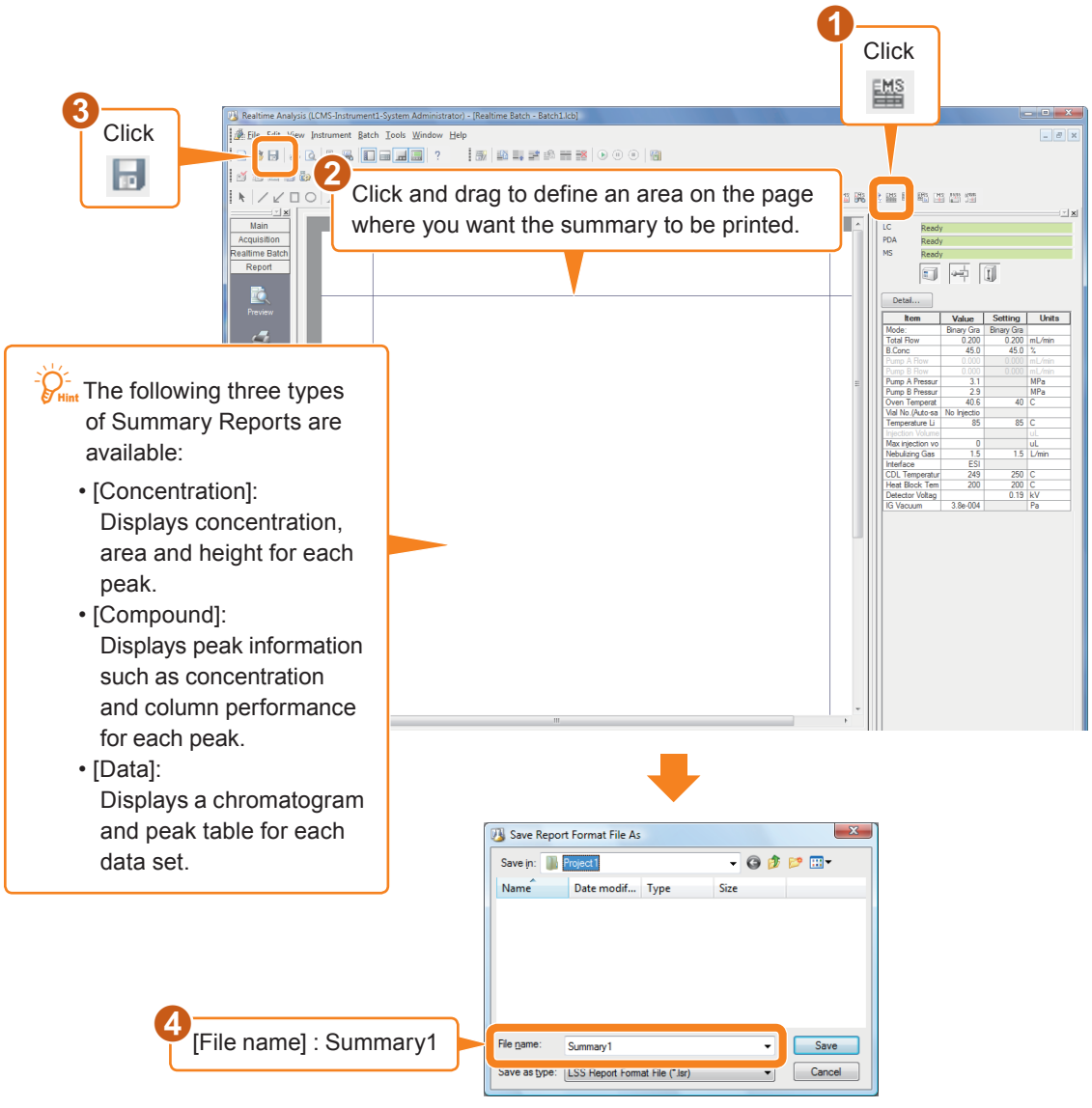
Prints a batch processing summary report (a simple combined report of two or more sets of analysis results).

1 Open the [Report] window.



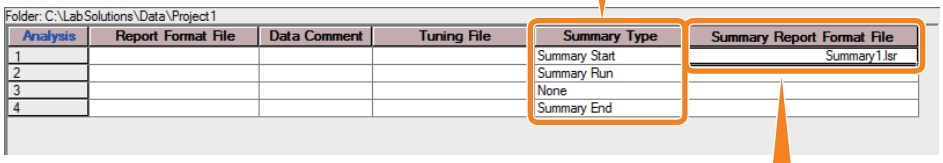
2 Create a summary report format with the [MS Summary (Compound)] report item.

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



3 Set up the summary report.

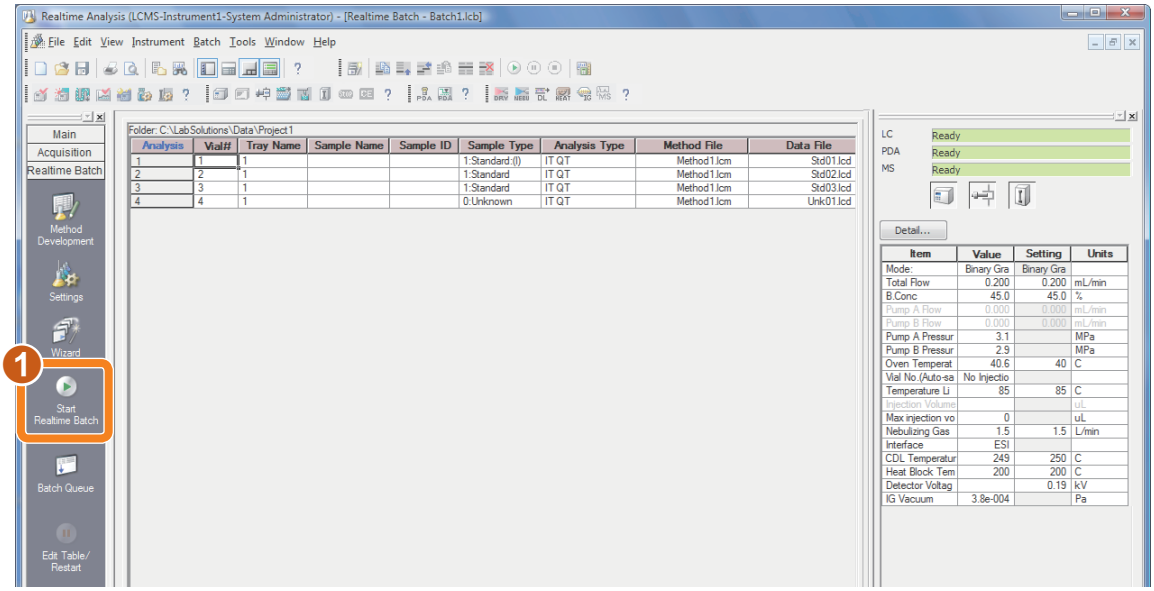
1. Enter [Summary Start] in the first data line to be included in the summary report.
   Enter [Summary Run] in all of the subsequent data lines to be included in the summary report.
   Enter [Summary End] in the last data line to be included in the summary report.



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

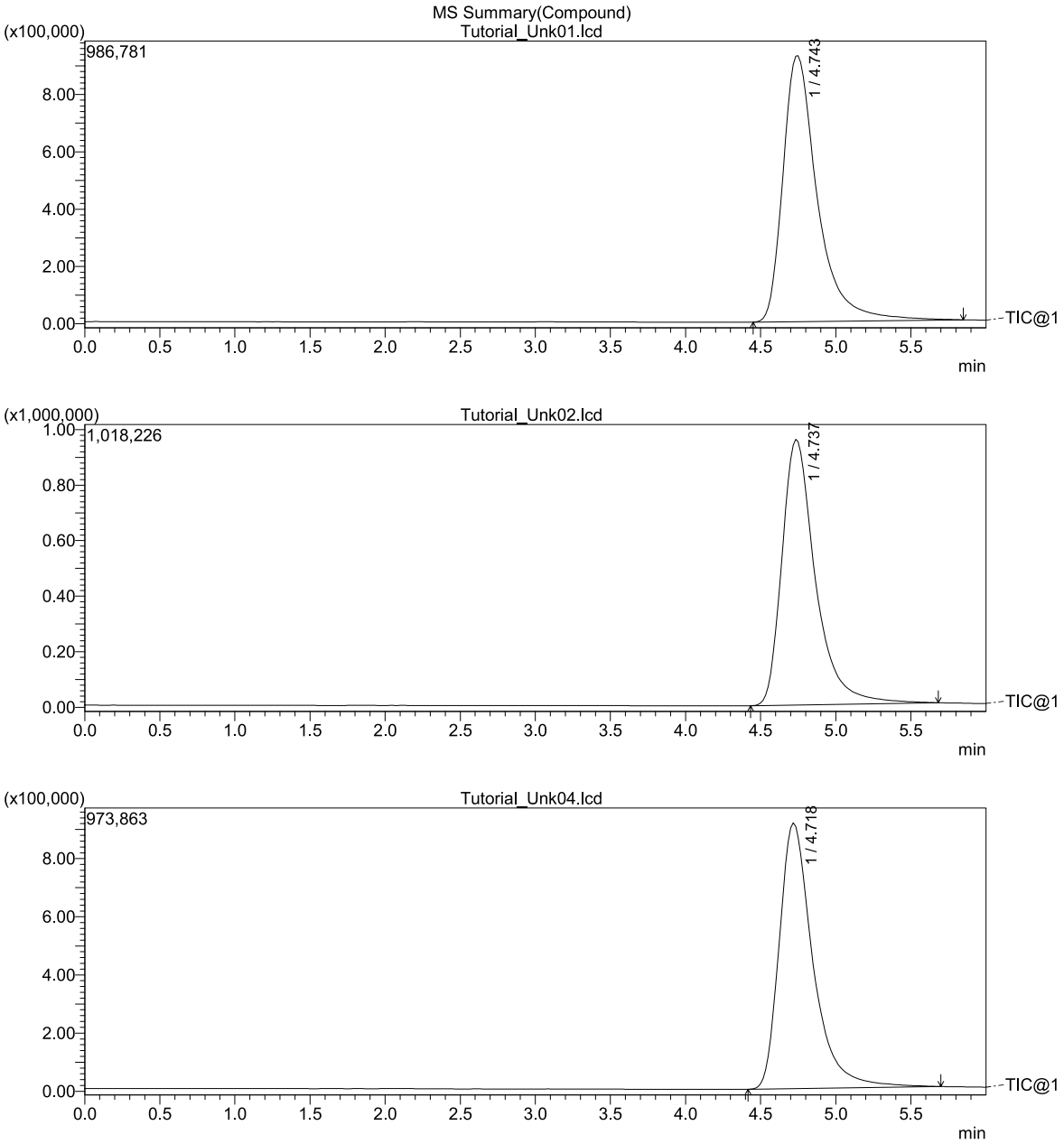
Hint If [Summary Type] and [Summary Report Format File] are not displayed in the Batch Table, use the right-click menu to select [Table Style] and enable display of these items.

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: papaverine

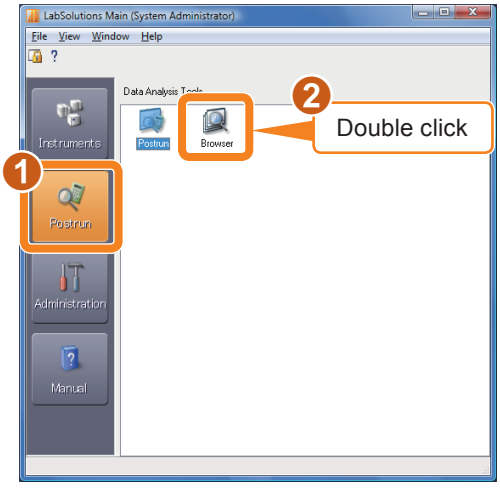
Title	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Tutorial_Unk01.lcd			4.743	11077384	835152	0.746
Tutorial_Unk02.lcd			4.737	10886185	846829	0.735
Tutorial_Unk04.lcd			4.718	10418105	807638	0.706
Average			4.733	10793891	829873	0.729
%RSD			0.274	3.142	2.425	2.840
Maximum			4.743	11077384	846829	0.746
Minimum			4.718	10418105	807638	0.706
Standard Deviation			0.013	339191	20122	0.021

Chapter 5. Quantitative Data Analysis

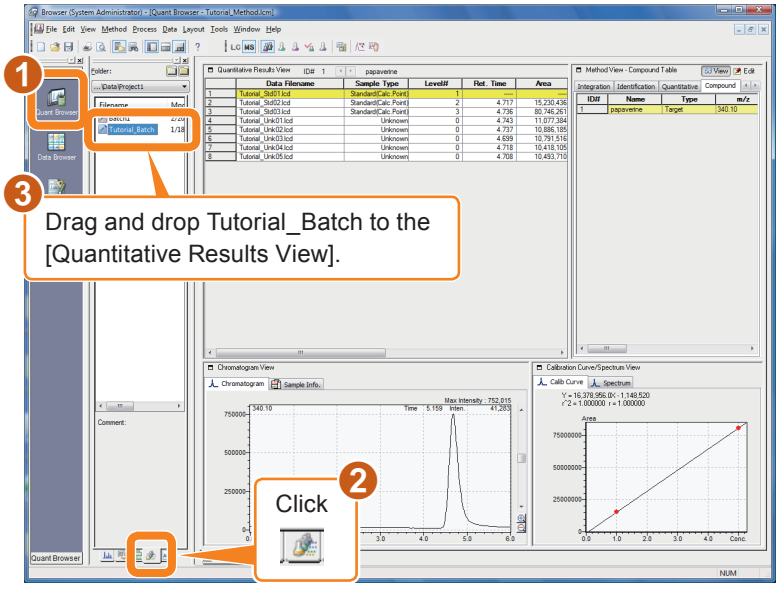
5.1 Confirm Quantitative Results in the [Quant Browser] Window

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

1 Open the [Browser] program.



2 Load the sample data.



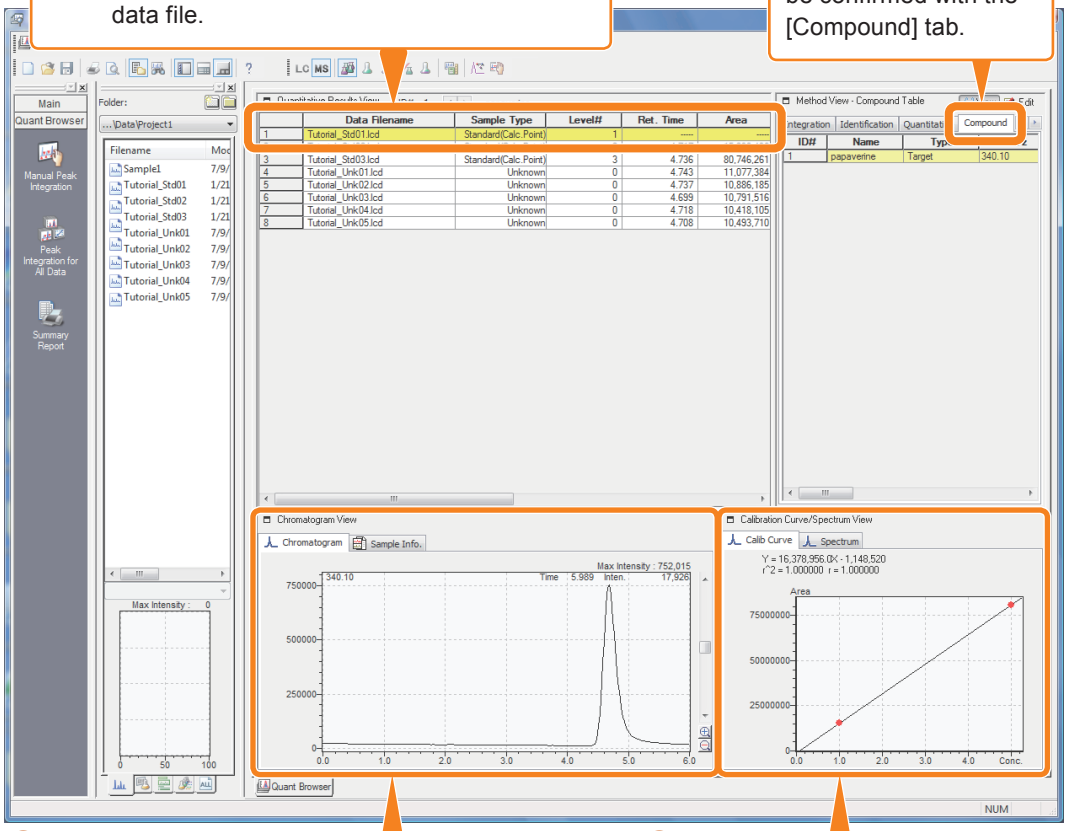
Sample data (Tutorial_Std01.lcd to Tutorial_Std03.lcd and Tutorial_Unk01.lcd to Tutorial_Unk05.lcd) registered in the batch file are opened.
You can select multiple data files with the [Data Explorer] sub-window to drag-and-drop them simultaneously.

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 with the [Compound] tab.



3 Confirm the chromatogram.

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

4 Confirm the calibration curve.

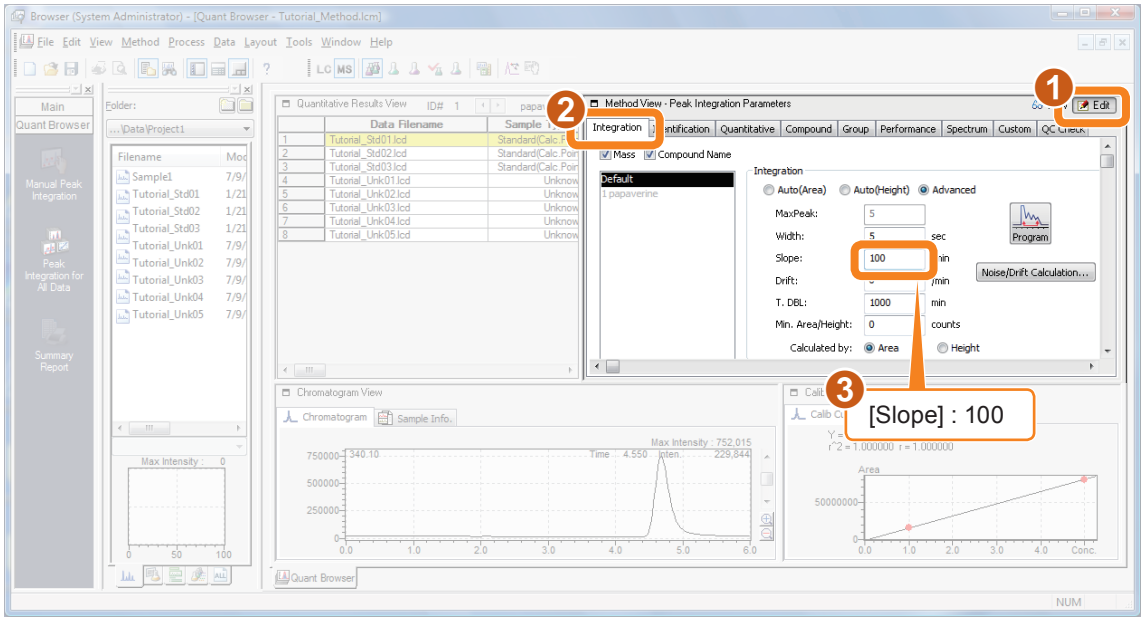
Hint The calibration curve of the selected compound in the [Method View] is displayed.

5.2 Edit Integration Parameters and Re-Integrate

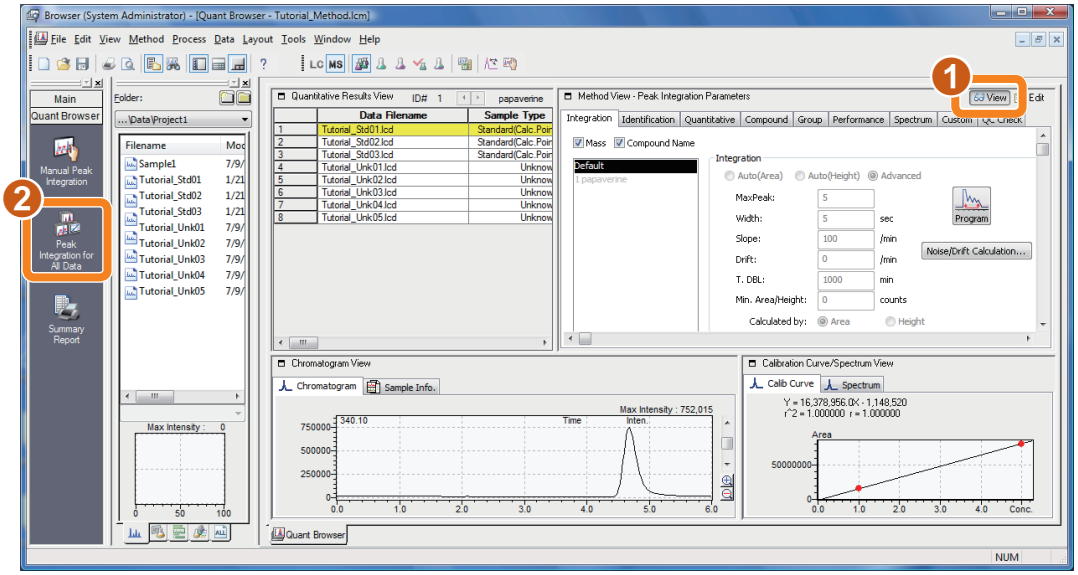
The sample data on the previous page is quantitative data for a three-point absolute calibration curve. However, if the area value for the first line of data (Tutorial_Std01.lcd) in the [Quantitative Results View] is found to be "----", or if confirming the [Chromatogram View] reveals that peak integration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

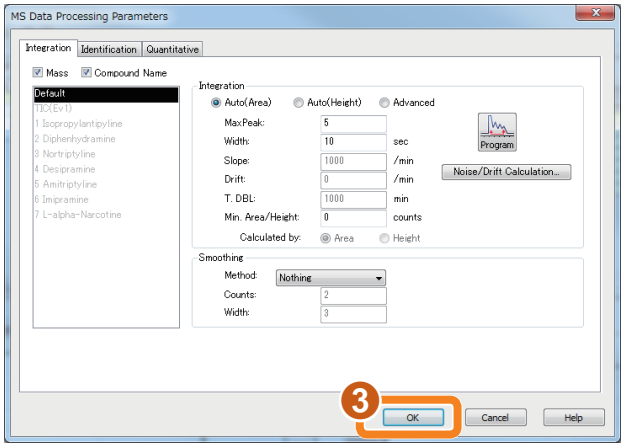
1 Edit the quantitative parameters.

Reference "11.3 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

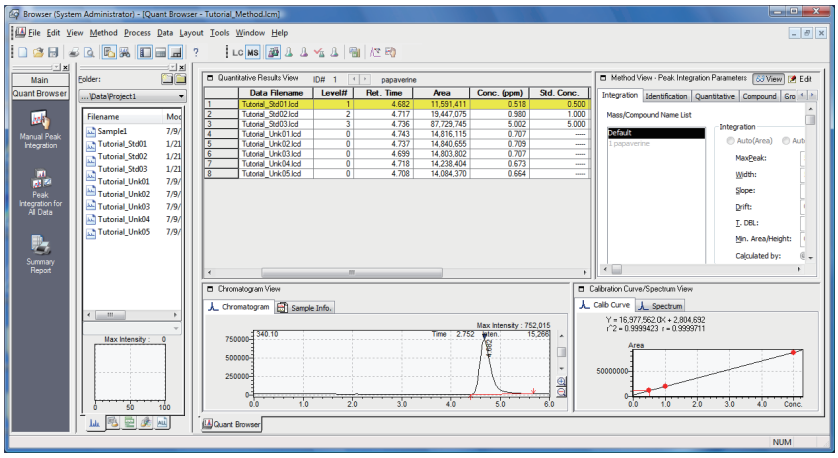
	Data Filename	Sample Type	Level#	Area	Conc. (ppm)	Std. Conc.
1	Tutorial_Std01.lcd	Standard(Calc.Point)	1	11,591.4	0.518	0.500
2	Tutorial_Std02.lcd	Standard(Calc.Point)	2	19,447.0	0.980	1.000
3	Tutorial_Std03.lcd	Standard(Calc.Point)	3	87,729.7	5.002	5.000
4	Tutorial_Unk01.lcd	Unknown	0	14,816.1	0.707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

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

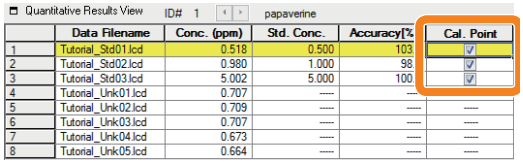
Reference "7.4.6 Manual Quantitative Peak Integration" in *Operators Guide*.

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



Invalidate a Calibration Point

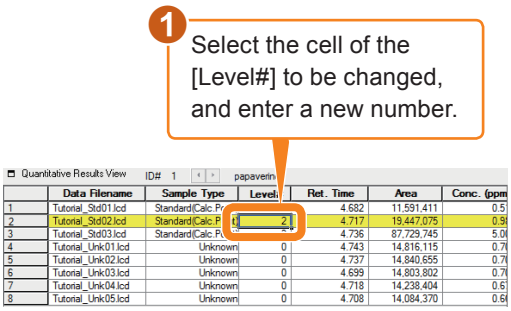
If a standard sample cannot be analyzed properly, the calibration point can be invalidated.
Remove the [Cal. Point] checkmark from the [Quantitative Results View] to invalidate the calibration point. The results are immediately recalculated.
You can enable/disable the calibration point for each compound registered in the [Compound Table].



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.

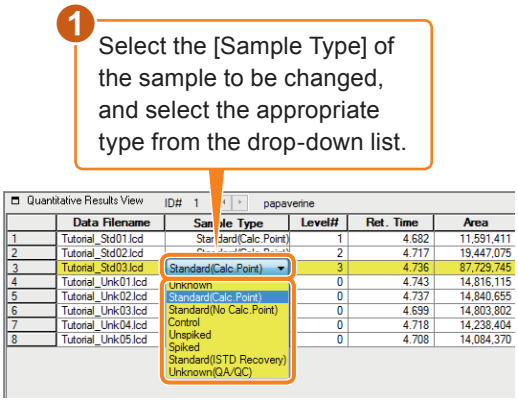


Hint The [Level#] can be edited regardless of the [Sample Type].

Change the Sample Type

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

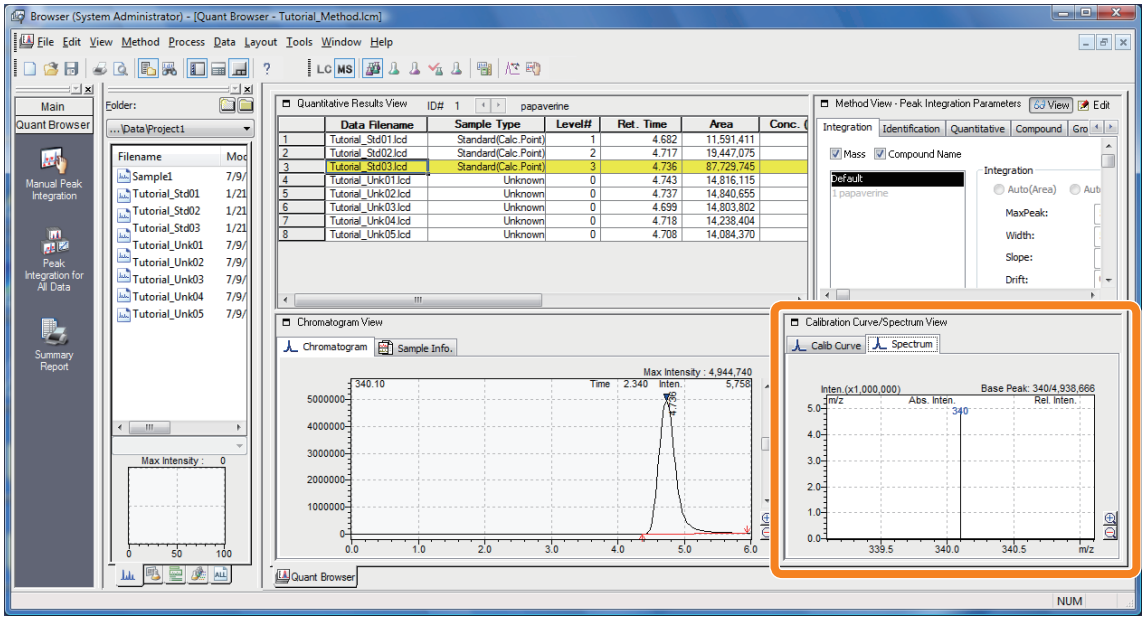
When changes are applied, quantitative results are immediately recalculated.



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

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 File Management with the Quant Browser

The [Quant Browser] window is an application for editing a single method file, and reforming postrun analysis on multiple loaded data sets using the data processing parameters of that method.
Files are loaded according to the following rules.

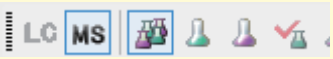
Method File

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 used.

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

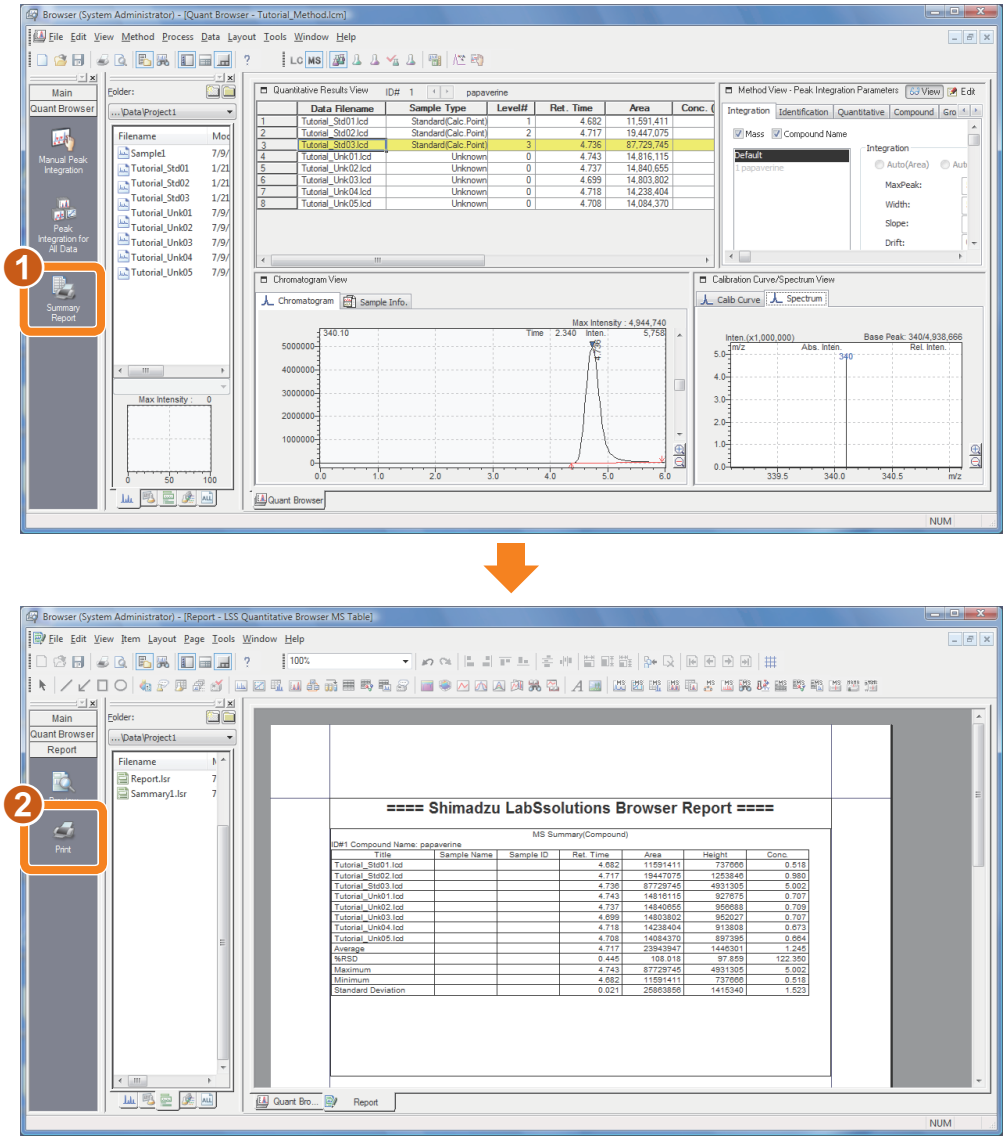
Data Files

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 is printed about each compound.

Quant Browser Printout Example

==== Shimadzu LabSsolutions Browser Report ====

MS Summary(Compound)

ID#1 Compound Name: papaverine

Title	Sample Name	Sample ID	Ret. Time	Area	Height	Conc.
Tutorial_Std01.lcd			4.682	11591411	737666	0.518
Tutorial_Std02.lcd			4.717	19447075	1253846	0.980
Tutorial_Std03.lcd			4.736	87729745	4931305	5.002
Tutorial_Unk01.lcd			4.743	14816115	927675	0.707
Tutorial_Unk02.lcd			4.737	14840655	956688	0.709
Tutorial_Unk03.lcd			4.699	14803802	952027	0.707
Tutorial_Unk04.lcd			4.718	14238404	913808	0.673
Tutorial_Unk05.lcd			4.708	14084370	897395	0.664
Average			4.717	23943947	1446301	1.245
%RSD			0.445	108.018	97.859	122.350
Maximum			4.743	87729745	4931305	5.002
Minimum			4.682	11591411	737666	0.518
Standard Deviation			0.021	25863856	1415340	1.523

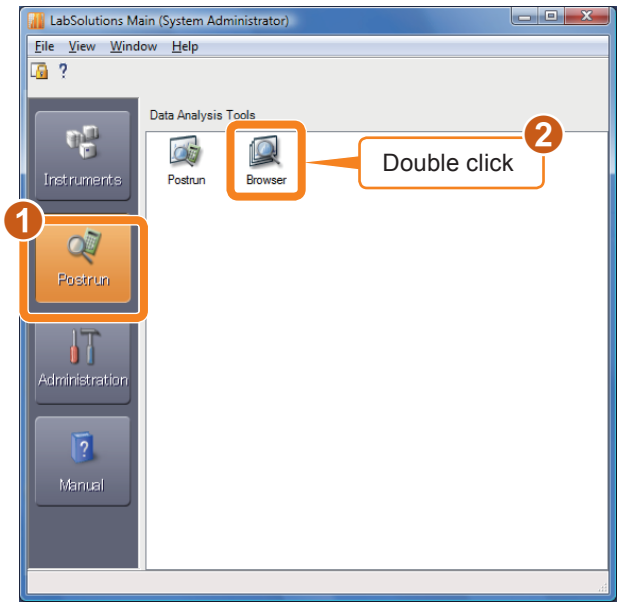
Chapter 6. Qualitative Data Analysis

6.1 Display Data Files in the [Data Browser] Window

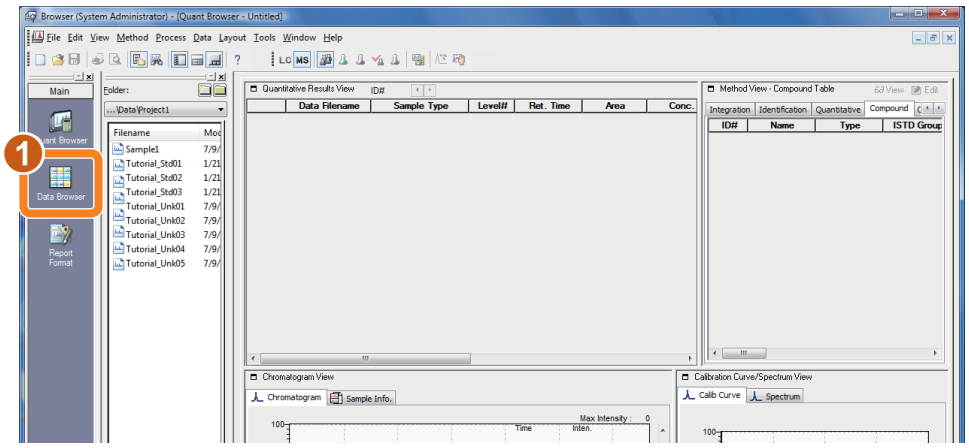
The Data Browser can be used to display chromatograms, spectra, and multiple data file information from different detectors such as MS or PDA in various formats.

Reference "12.4 Compare Data" in *Operators Guide*.

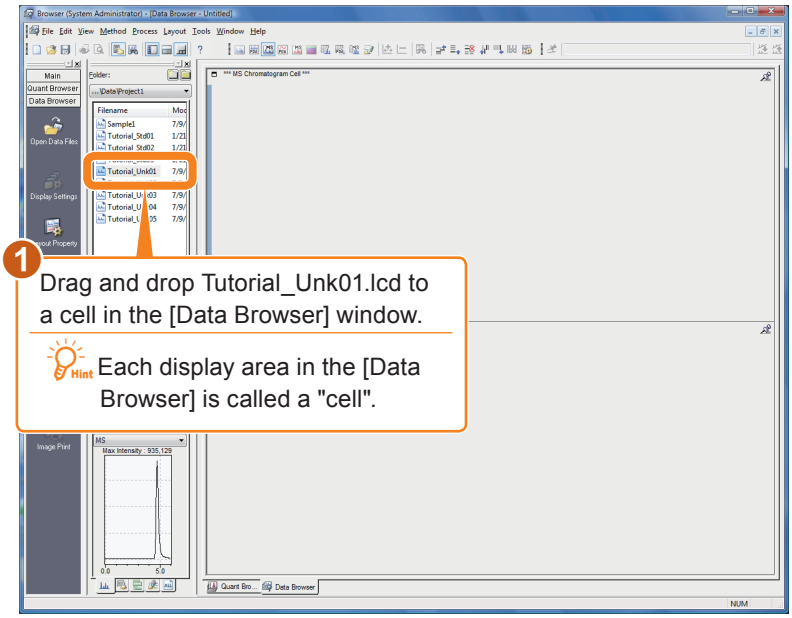
1 Open the [Browser] program.

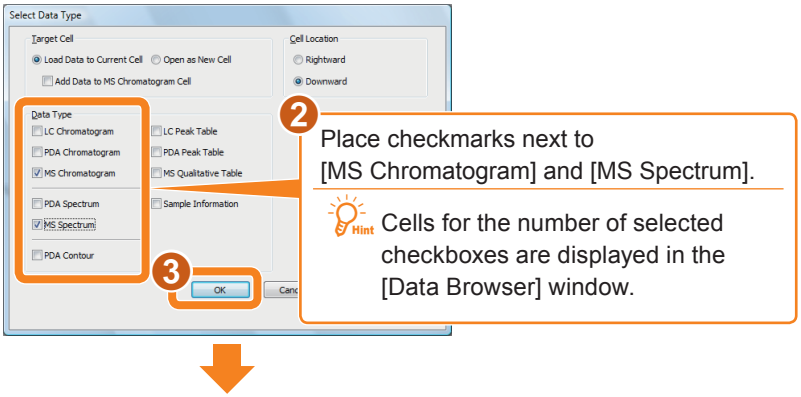


2 Open the [Data Browser] window.

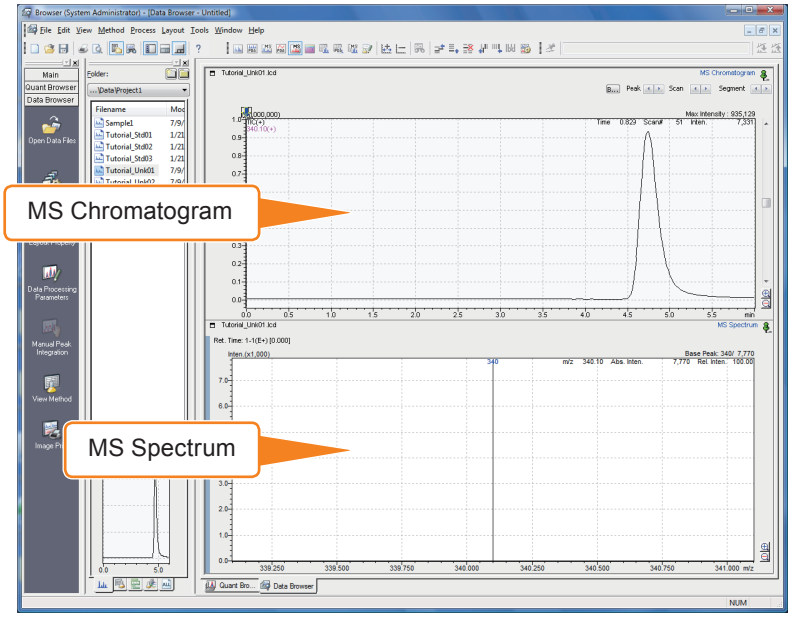


3 Select a data file.





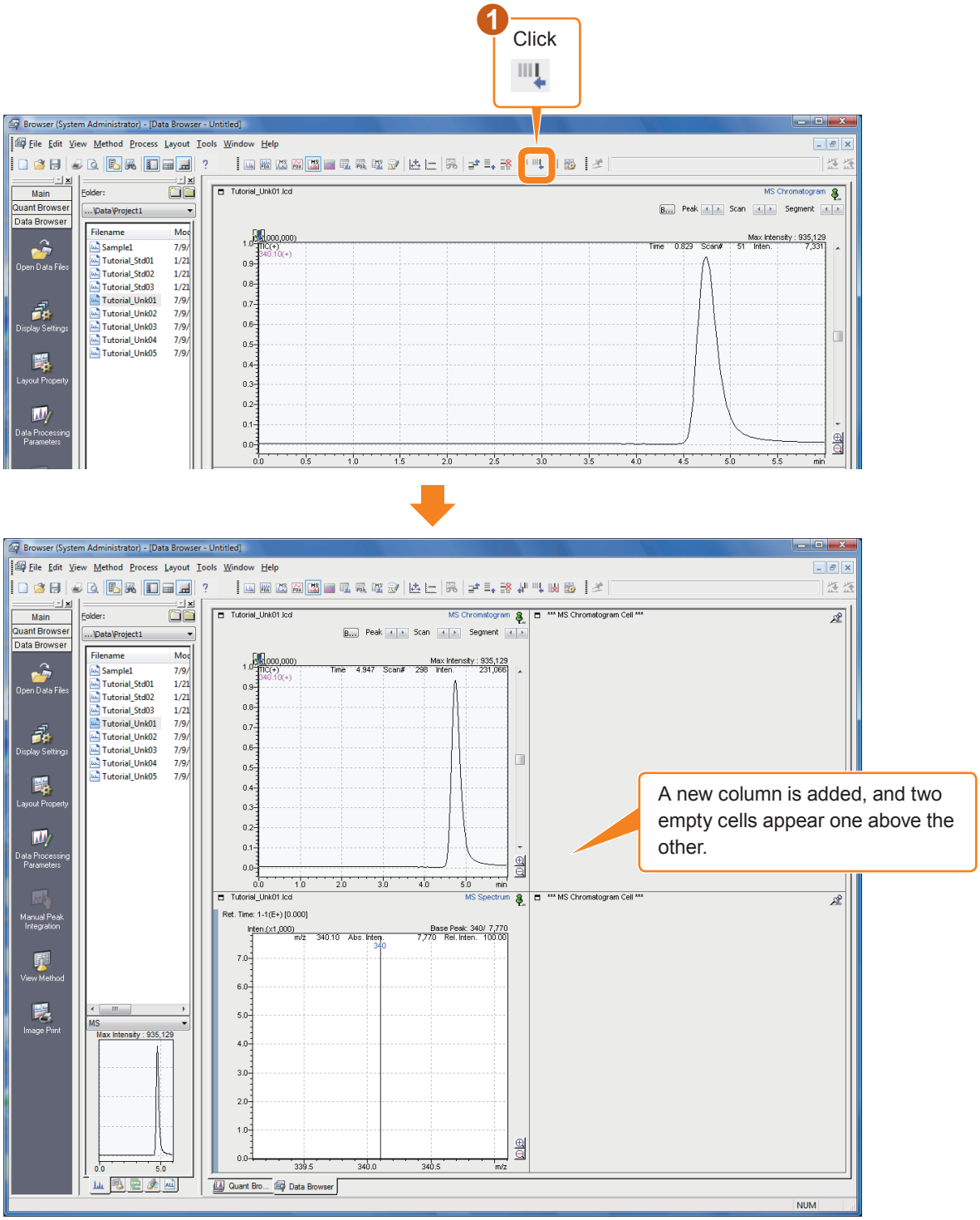
The MS chromatogram and MS spectrum are displayed.
Double click a point on the MS chromatogram to display the MS spectrum at that point.



6.2 Change the Display Layout Settings

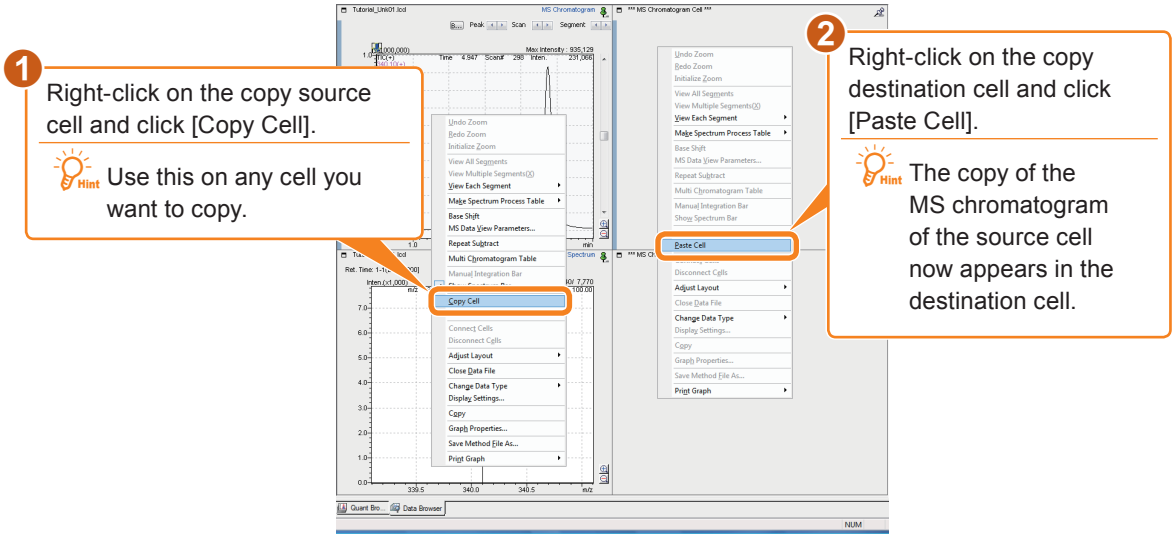
1 Add a column

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.

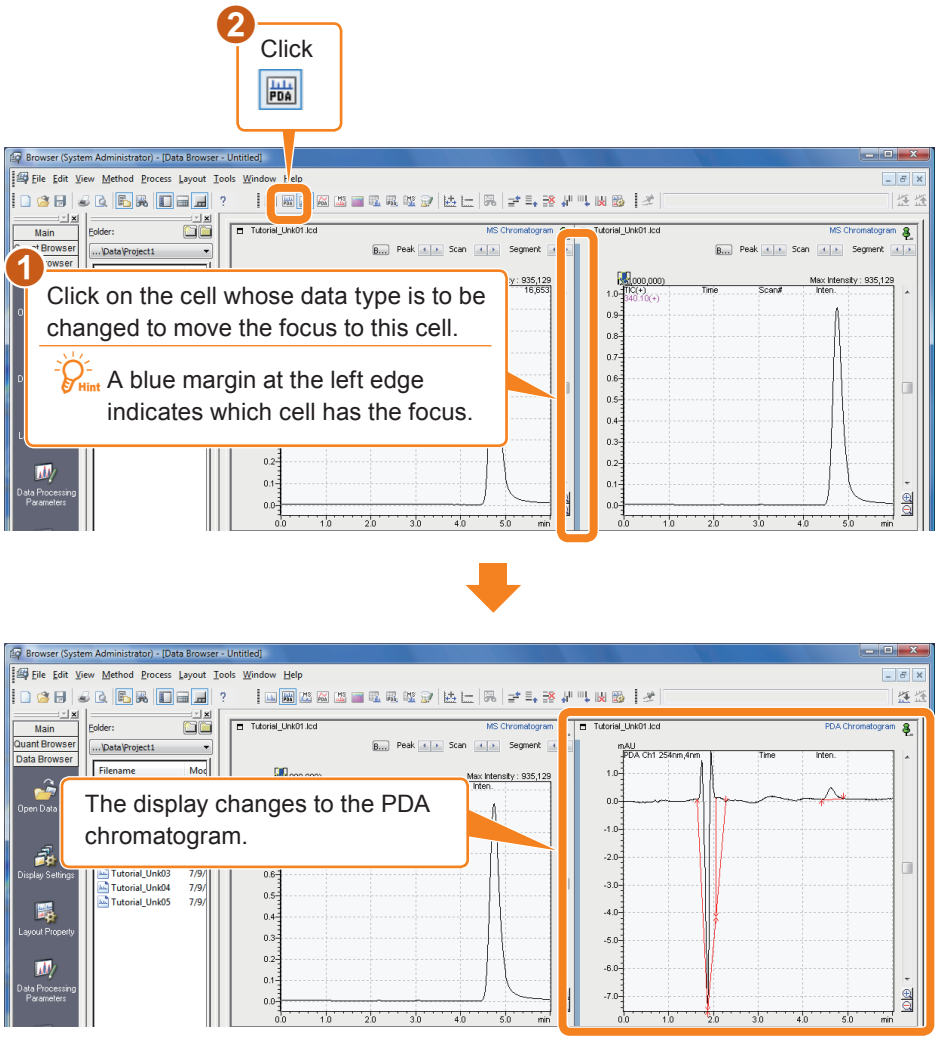


2 Copy and paste cell contents

You can copy information from one cell to another.



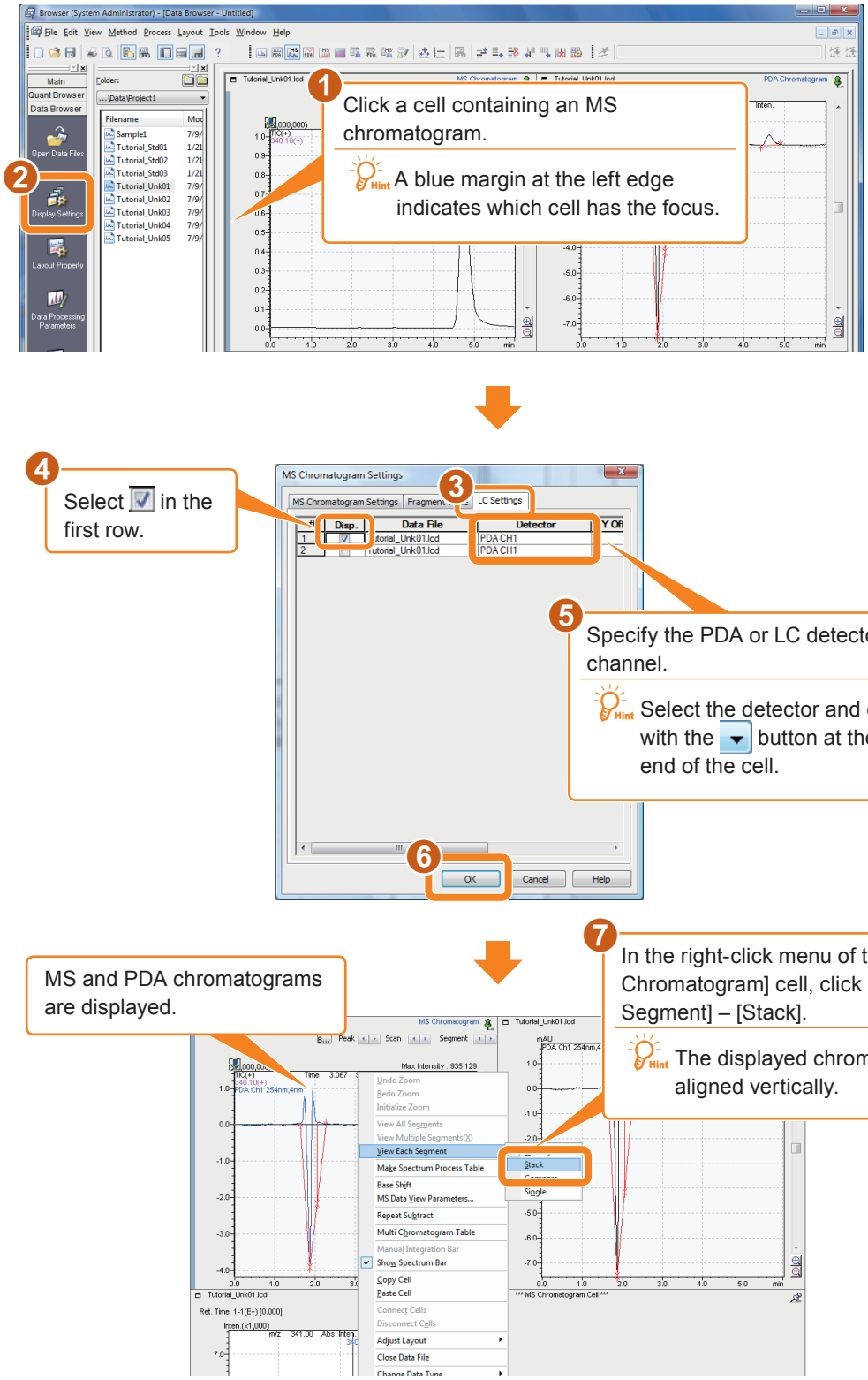
3 Change the data type.



6.3 Compare Different Types of Chromatograms

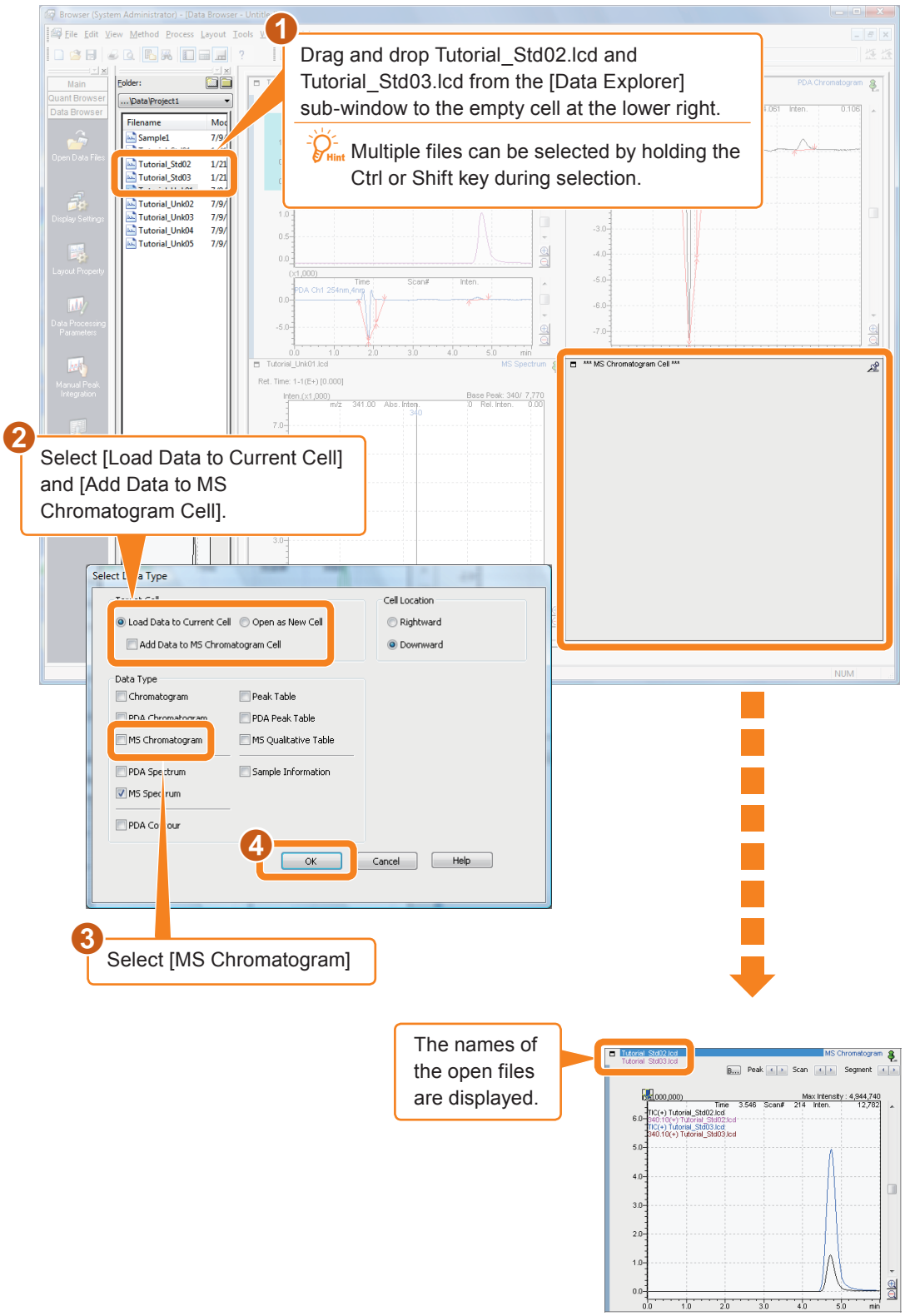
1 Compare MS and PDA chromatograms.

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



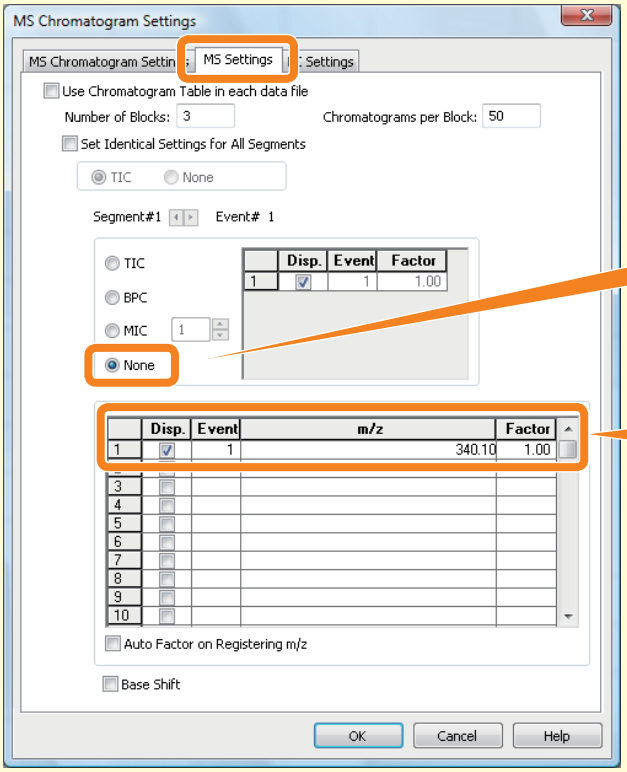
2 Compare the data for different chromatograms.

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 For SIM analysis, select m/z from the pull-down list opened by clicking the [m/z] column.

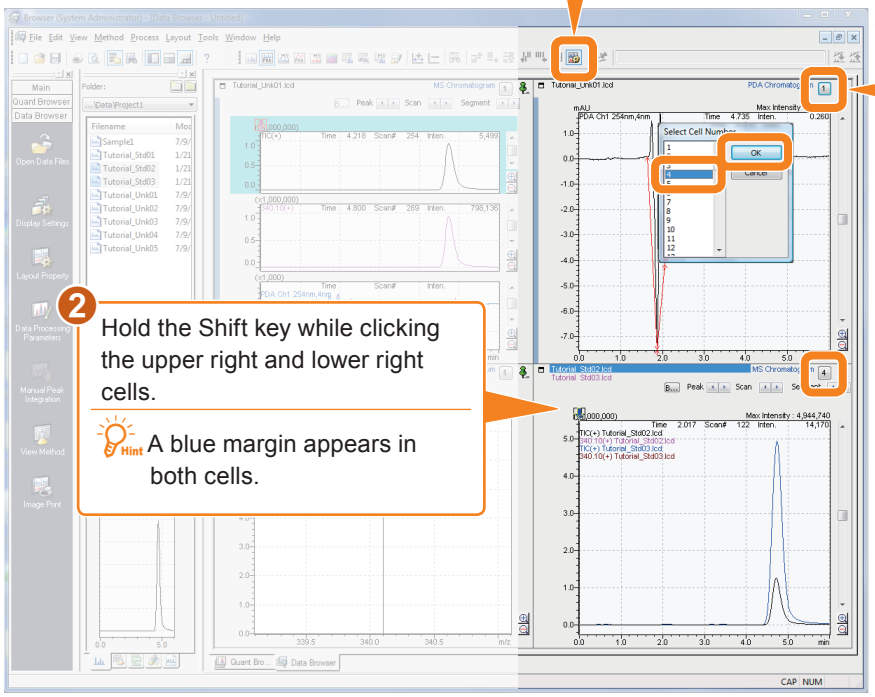
6.4 Use the Cell Fixed Function

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 

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



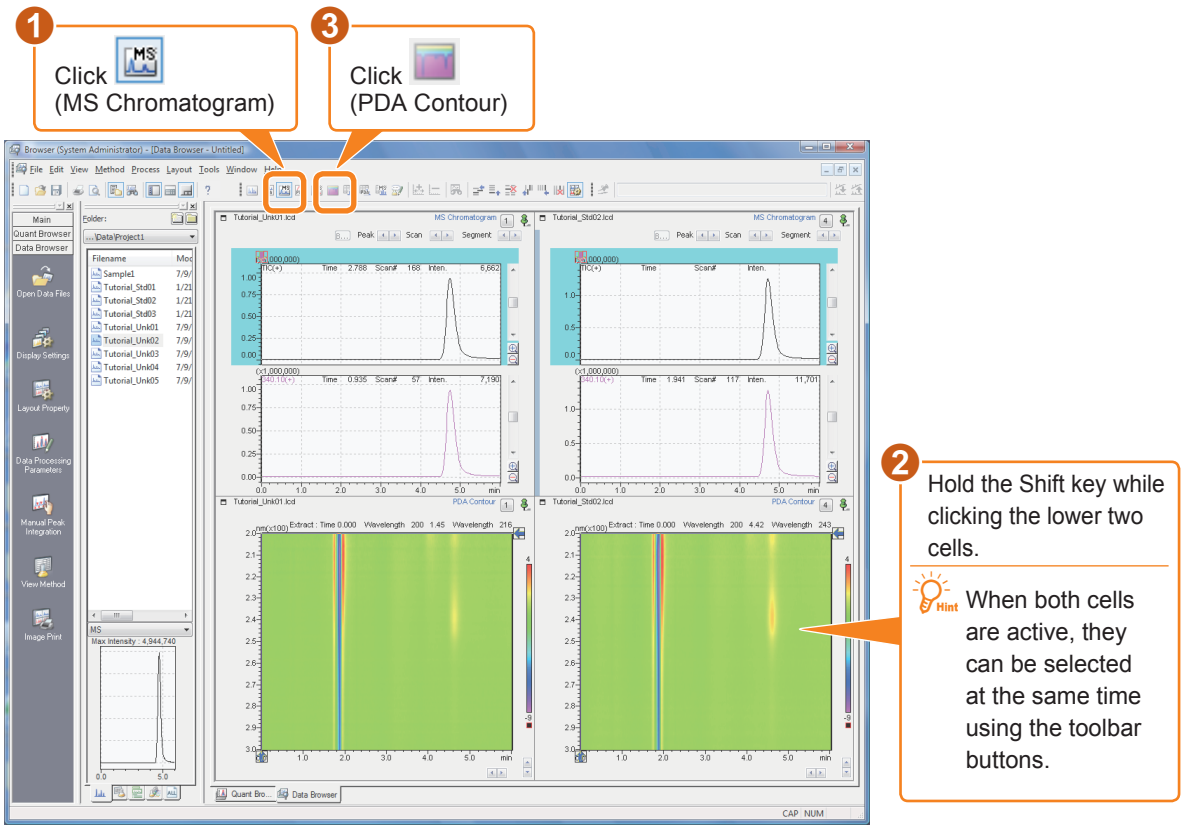
2 Hold the Shift key while clicking the upper right and lower right cells.

Hint A blue margin appears in both cells.

3 Hold the Shift key and click the [Cell Number] button.
Select cell 4, and click [OK].

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

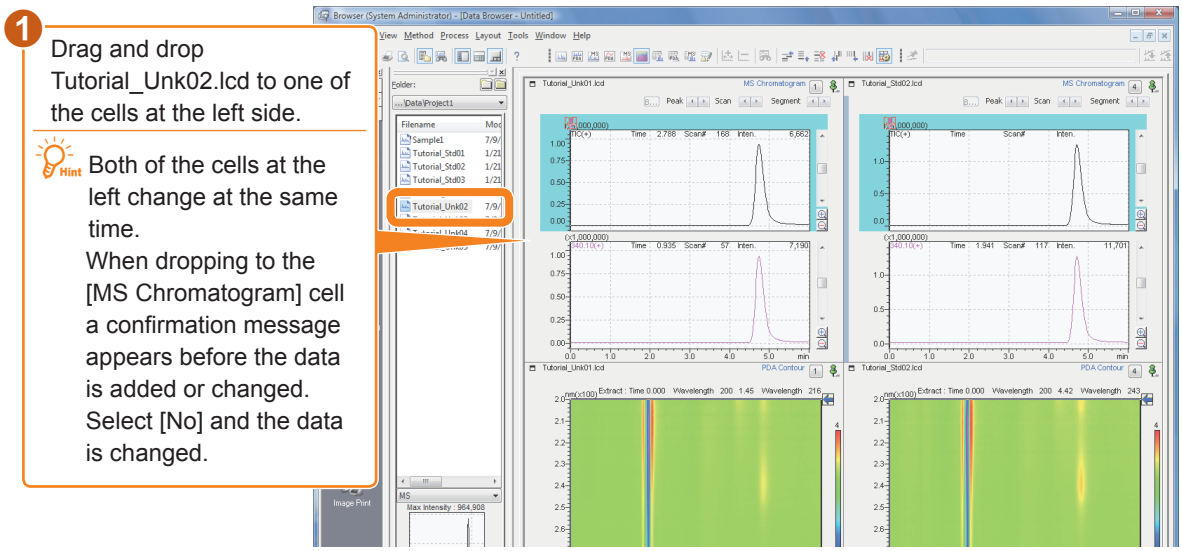
2 Display an MS chromatogram and PDA contour.



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.

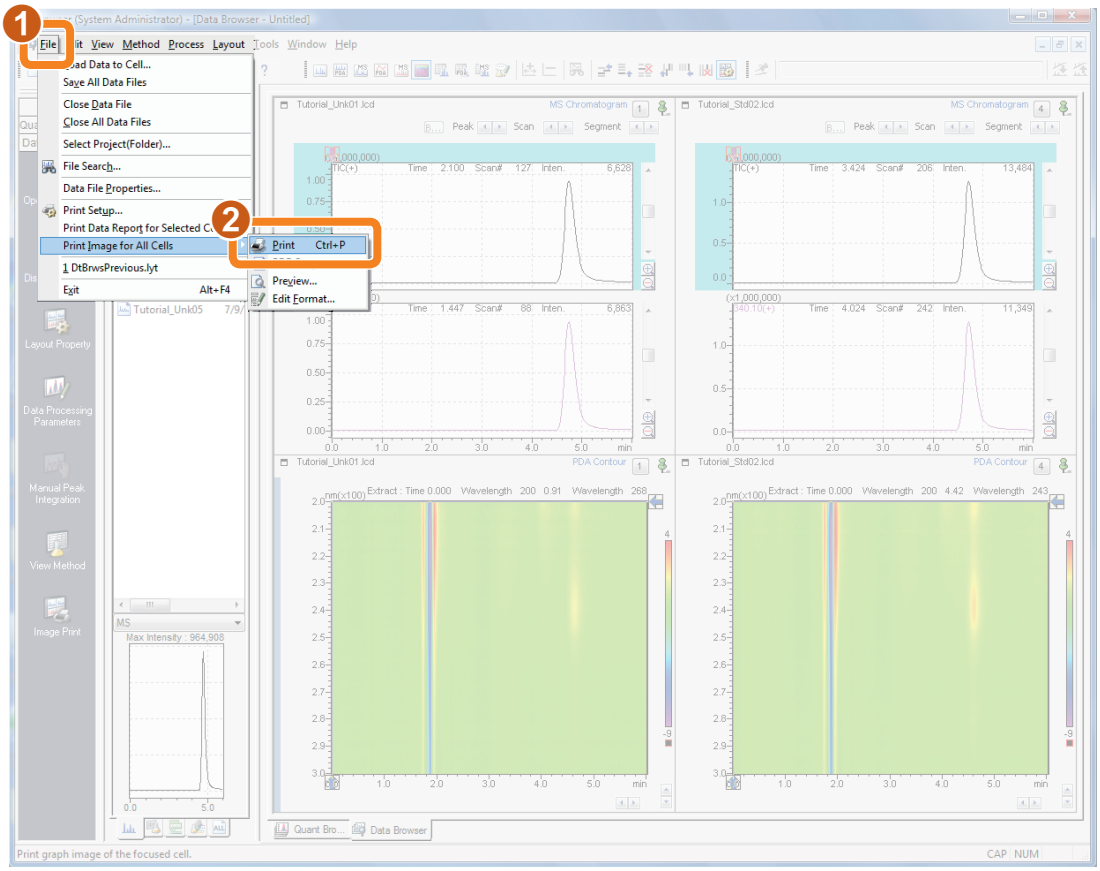
In this state, data files can be switched for easy data comparison.



6.5 Print from the [Data Browser] Window

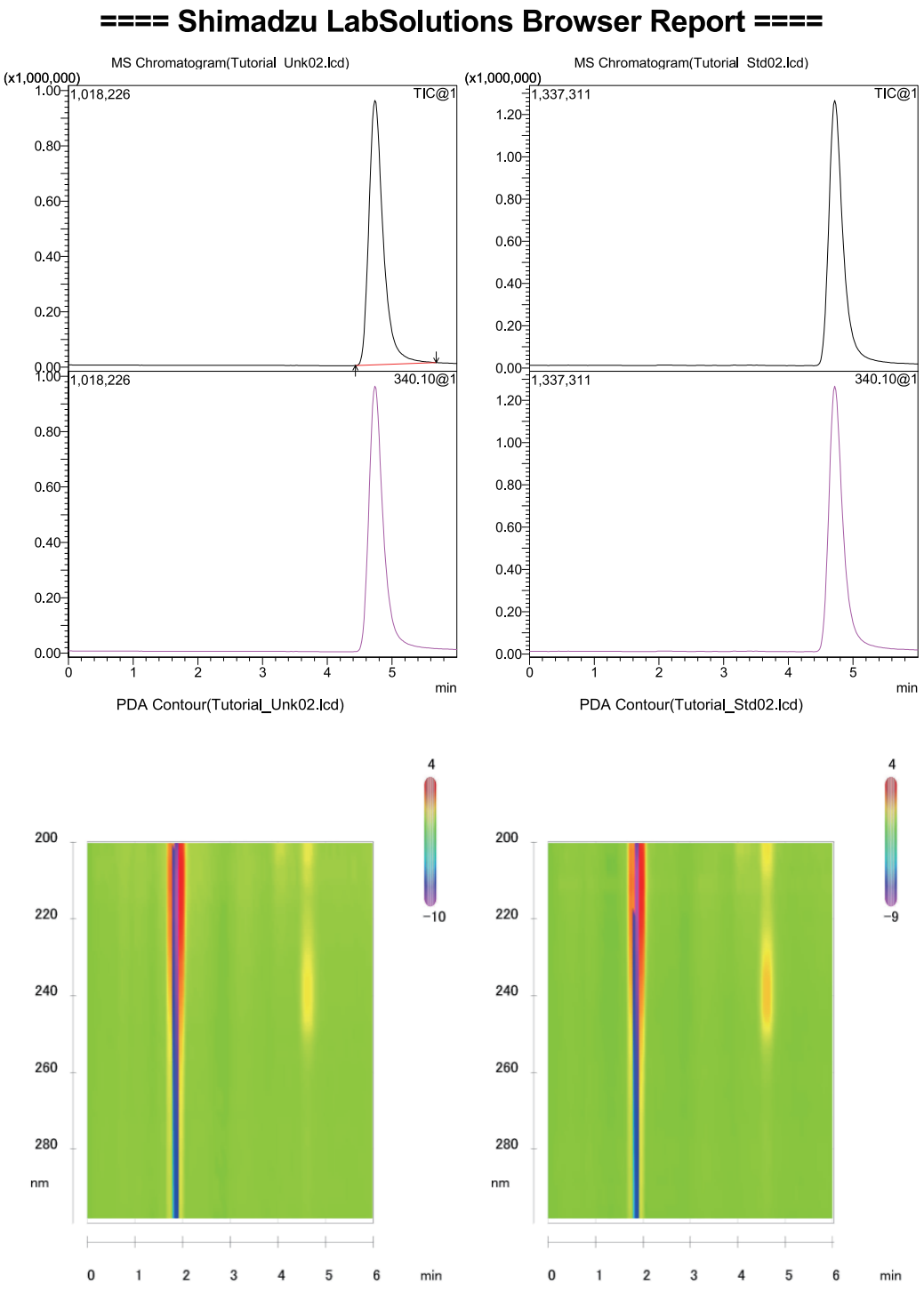
1 Print an image of the display.

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



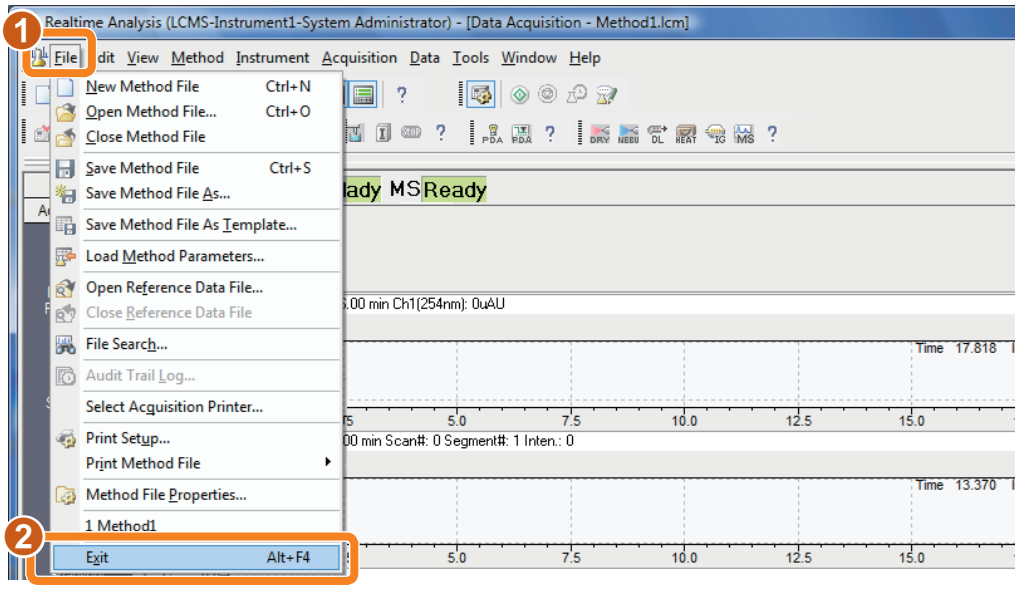
Hint Select [Print Data Report for Selected Cell] from the [File] menu to print using the report format saved in the data file.

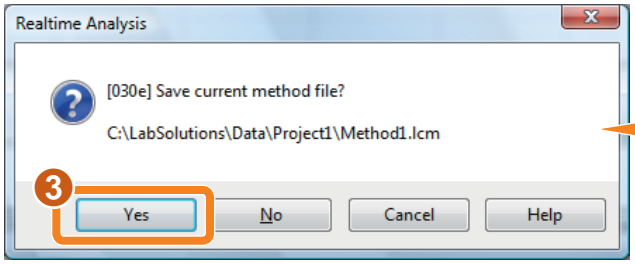
Data Browser Image Printout Example



Chapter 7. ShutDown

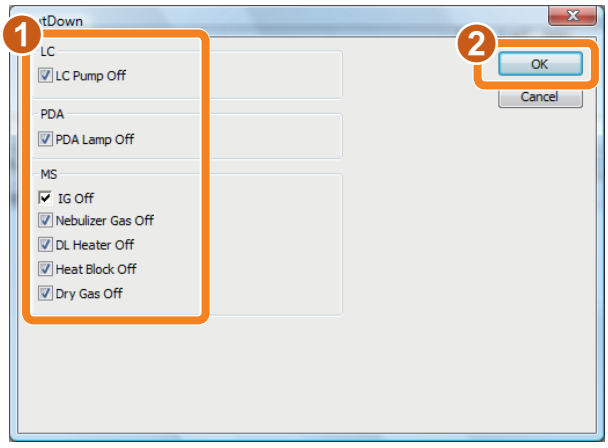
1 Close any open windows.



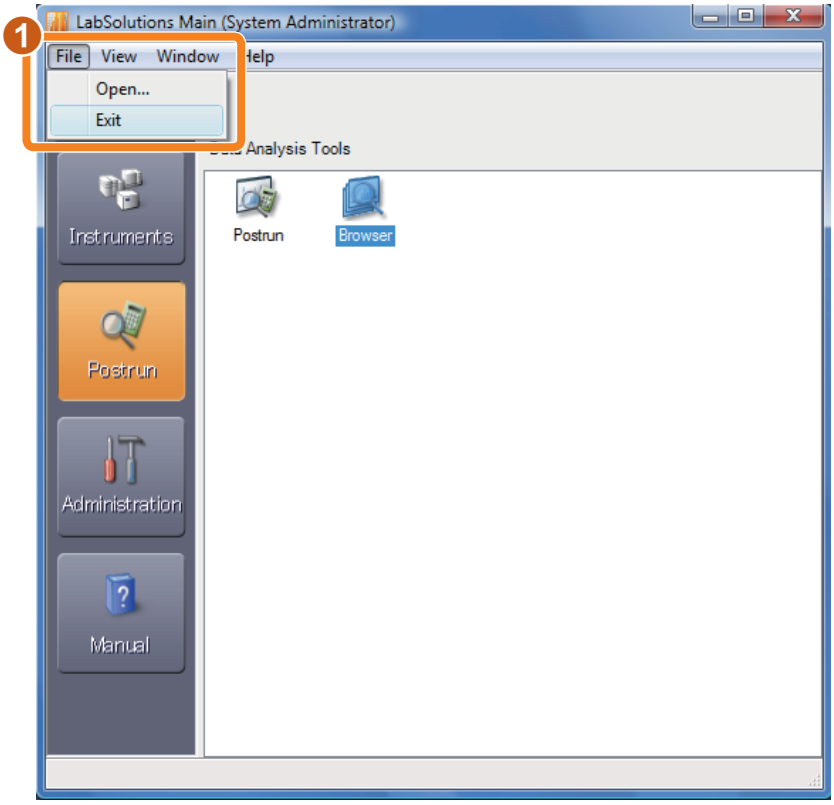


Hint This sub-window appears if there are any unsaved files.

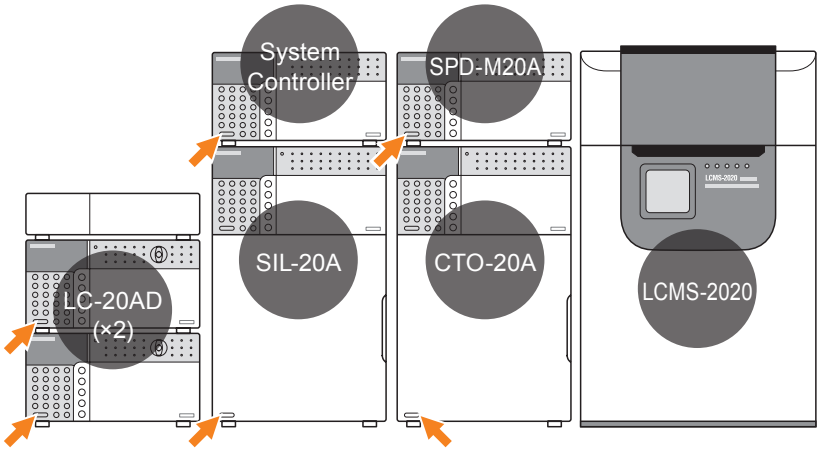
2 Stop the pump and heater from the [ShutDown] sub-window.



3 Exit LabSolutions.



4 Turn off the power to the LC modules.



Hint During routine operation, the LCMS-2020 is not turned off.

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