

Shimadzu LCMSsolution

for
LCMS-2010 / LCMS-QP8000 α

Operation Guide

Read the instruction manual thoroughly before you use the product. Keep this instruction manual for future reference.



Shimadzu Corporation

Analytical & Measuring Instruments Division

Kyoto, Japan

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Introduction

Thank you very much for purchasing the LCMSsolution software for Shimadzu liquid chromatography / mass spectrometry workstations (hereafter called "LCMSsolution").

LCMSsolution allows you to control the liquid chromatograph (hereafter called "LC") and the Mass Spectrometer (hereafter called "MS") from your personal computer, acquire chromatograms and other different kinds of data, and reanalyze the acquired data under different parameters on your personal computer.

This manual is the tutorial in the most simplified analysis procedure using LCMSsolution which helps you to catch more knowledge in other volumes or further actual operations.

The "Operation manual" and "Administration manual" are attached as separate volumes.

The Operation manual has been put together in order to familiarize you with the basic knowledge required to operate LCMSsolution. Be sure to read it thoroughly before using this software. After reading the manual, keep it in a safe place so that it can be accessed whenever necessary.

The Administration manual covers the information useful for system administration such as the support features for GLP/GMP or FDA 21CFR Part11, a set of regulations for electronic records and electronic signature. For more information on the functions of LCMSsolution, refer to this on-line manual.

This manual assumes that the reader is knowledgeable of basic operations of Windows®2000. For the operation of Windows®2000, refer to the instruction manual that comes with that product.

This manual sometimes explains commonly for LabSolutions series. And some explanations may use the drawings come from sister products like LCsolution, if it does not cause misunderstanding in the range of explanations.

Using the instruction manual




Kinds of instruction manuals

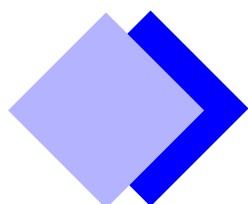
The LCMSsolution package contains the following information that describes the operational procedures and functions.

Name	Media	Description
Operation guide for LCMSsolution	Printed Document	Provides tutorial on mostly basic analysis procedure using LCMSsolution.
Operation manual for LCMSsolution	Printed Document	Explains the operational procedures for data acquisition and analysis using LCMSsolution.
Administration manual for LCMSsolution	Printed Document	Explains the operational procedures and basic idea of system administration and data management using LCMSsolution.
On-line help	LCMSsolution program	Provides detailed information on parameters and setting ranges. This is accessible from the Help menu in LCMSsolution. (For using the on-line help, refer to section “14.1.1 Using Help” in the Operation manual.)
Operation guide for LCMSsolution (PDF version)	CD-ROM disk for installation	Provides the operation guide volume of the instruction manual as a PDF file so that it can be viewed on your personal computer. The general table of contents is available, including other instruction manuals (PDF versions). It allows you to use each instruction manual via the hyperlink.
Operation manual for LCMSsolution (PDF version)	CD-ROM disk for installation	Provides the operation volume of the instruction manual as a PDF file so that it can be viewed on your personal computer. It is accessible from the Help menu in LCMSsolution. (For using this PDF, refer to section “14.1.2 Using the Online Manual” in the Operation manual.)
Administration manual for LCMSsolution (PDF version)	CD-ROM disk for installation	Provides the administration volume of the instruction manual as a PDF file so that it can be referred to on-line whenever operations related to system administration are needed. The general table of contents is available, including all the instruction manuals (PDF versions). It allows you to use each instruction manual via the hyperlink.

Legends for instruction manual

This manual uses the following legends:

Legend	Meaning
	Shows additional informations around the topic.
	Points the reference informations.
	Gives you tips.
< >	Shows a window or view name; e.g., <Data Acquisition> window or <Method> view.
[]	Shows a parameter, tab, column, cell, bar name, menu command, that can be selected from the menu bar.
[]-[] command	Shows a sequence of selecting the menu in the first [] and then selecting the command in the second []. For example, [File]-[Print] command means that you should click on the File menu and then select the Print command from the displayed list of commands.



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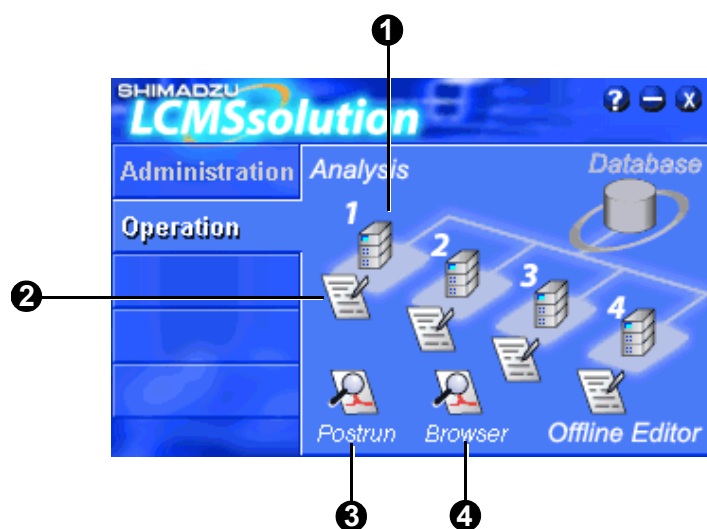
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1

Making Preparations for Analysis

1.1 Basics of LCMSsolution

■ <LCMSsolution Launcher> - [Operation] menu icon



No.	Icon	Name	Description
1		Analysis	Starts the application for configuring and controlling the system and making a single-run or batch analysis. (Starts <LCMS Analysis> in the Online mode)
2		Offline Editor	Starts the application for editing any method file or batch file not in use during the analysis. (Starts <LCMS Analysis> in the Offline mode)
3		Postrun	Starts the application for loading the acquired analysis data to create a calibration curve or perform data processing.
4		Browser	Starts the application for browsing multiple analysis data together or analyzing data together.

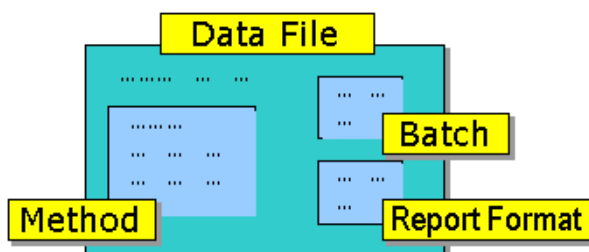
Files used in LCMSsolution

Extension	Name	Description
.lcm	Method File	Analysis condition, Data processing conditions, QA/QC settings, calibration curve information, and system configuration
.lcr	Report Format File	Report formats
.lcb	Batch File	Batch tables and batch settings
.lcd	Data File	Chromatograms, mass spectrums, peak tables, identification/quantitation results, report format, tuning results, methods, and batch table

 [Admin Manual]: [“4.1 Important File Concepts for Operation”](#)

Data structure in LCMSsolution

The data in the LCMSsolution is retained in data files, consisting various types of records and parameters such as the system configuration, fine-tuning result, system conditions, and analysis conditions that have been used to acquire and analyze data. This structure enables you to browse each data file for monitoring conditions and analysis parameters, thereby ensuring the traceability of data. This means that if a single data file is available, an analysis can be made again.



The method contained in the data file is a copy of the method file that was used to acquire and analyze data. Therefore, when any method parameter in the data file opened via <Data Analysis> is modified, the method contained in the data file is modified rather than the method file.

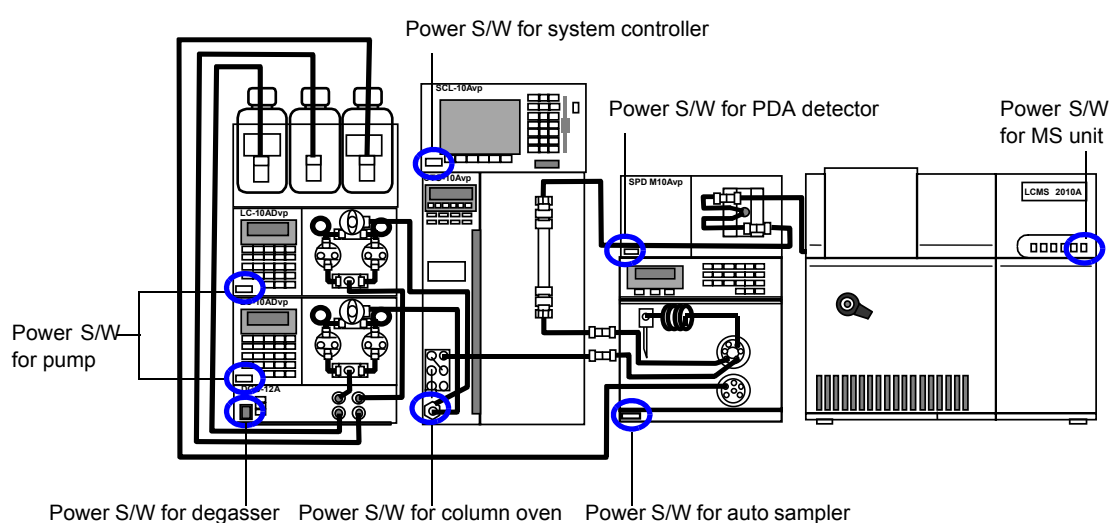
 [Admin Manual]: [“4.1 Important File Concepts for Operation”](#)

1.2 Starting the LCMSsolution

This document assumes the following system configuration as an example to describe the procedure for an analysis:
High-pressure Gradient LCMS plus PDA (= Photo Diode Array) Detectors System

Pump	LC-10ADvp = 2 units
Auto sampler	SIL-10ADvp
Column oven	CTO-10A(C)vp
PDA detector	SPD-M10Avp
Mass spectrometer	LCMS-2010A

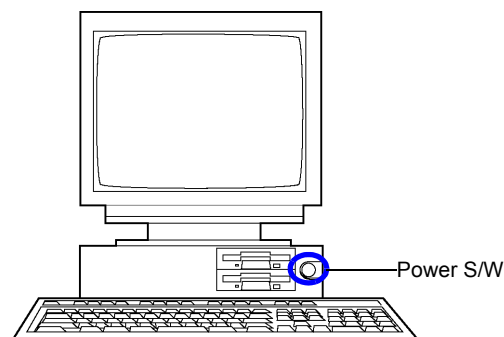
- 1 Check that the LC and MS units are On.



- 2 Check that nitrogen gas is sent to the MS unit.

- 3 Turn On the personal computer and peripheral devices to start Windows.

- 4 Enter your user ID to log on.




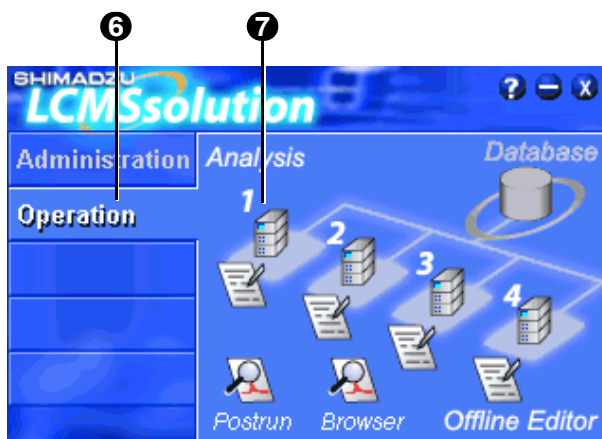
- 5 Double-click the [LCMSsolution] icon displayed on the Windows desktop.
<LCMSsolution Launcher> will be started.



1.2 Starting the LCMSsolution

6 Select [Operation] menu.

7 Click the [Analysis] icon .
The <Login> screen will appear.

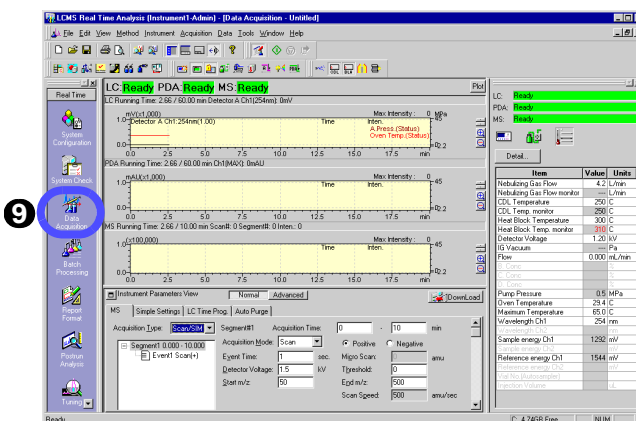


8 Select “Admin” and click the [OK] button.
The LCMS analysis program will be started with the <LCMS Analysis> main window displayed.

 [Admin Manual]: “2.4 Registering (Changing/Deleting) Users”, “2.5.2 Changing Passwords”




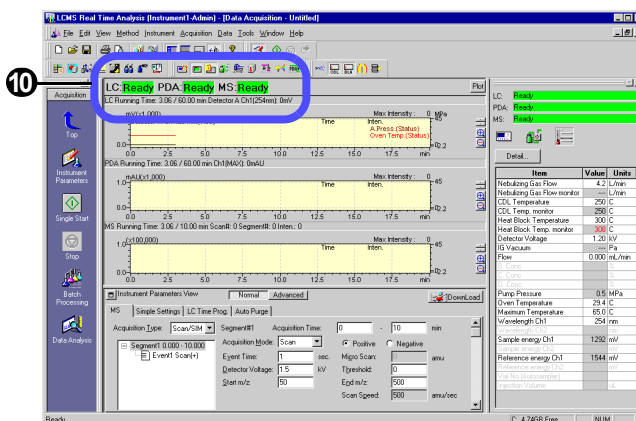
9 Click the [Data Acquisition] icon .



10 Check that “Ready” is displayed.

If “Not Connected” is displayed, properly complete <System Configuration>.

 [Operation Manual]: “14.5 Configuring System”



Description of <Data Acquisition> window

- **Toolbar**

Among the functions available on the Menu bar, the frequently used ones and the functions to directly control the analyzer are assigned to this bar.

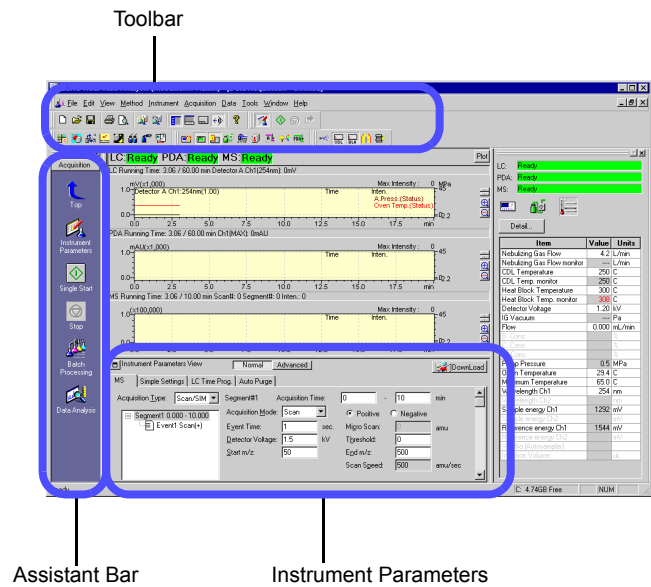
- **Assistant Bar**

The icons to operate the application in accordance with the general analysis flow are assigned to this bar.

- **Instrument Parameters**

A pane is displayed showing the parameters for the system set up on <System Configuration>.

Set those parameters for data acquisition.




2

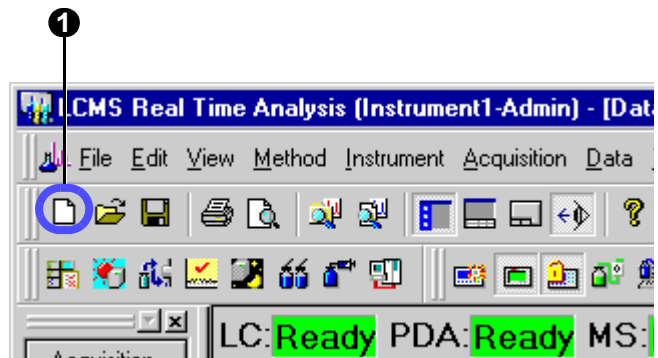
Qualitative Processing (Single-run Analysis)

Set the parameters for the LC and MS units on the <Data Acquisition> window and then make an analysis. This document assumes an example of analysis under the following analytical conditions to specifically describe the procedure for the analysis.

Column	Shim-pack VP-ODS 150mm x 2.0mm i.d. 5µm (Equivalent to Shimadzu P/N 228-34937-94)
Mobile phase	Binary Gradient mode Pump A = Water, Pump B = Acetonitrile
Sample	Papaverine 0.5, 1, 5, 25, 50 ng/µL (Shimadzu P/N 225-06613-05)

2.1 Creating a new method file

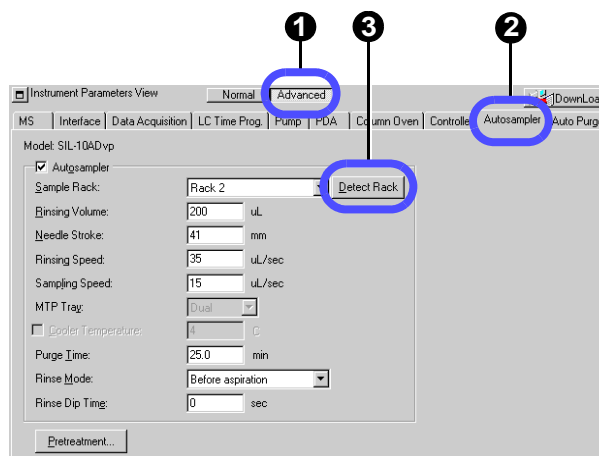
- 1 Click the [New] button .
A new method file will be opened.



2.2 Setting the LC parameters

2.2.1 Detecting the auto sampler rack


- 1 Click [Advanced] button.
- 2 Select the [Autosampler] tab.
- 3 Click [Detect Rack] button.



2.2.2 Setting the LC parameters

 [Operation Manual]: “4.2.1 Setting the LC Parameters”

- 1 Click [Normal] button
- 2 Select the [Simple Settings] tab.
- 3 Enter “6” min in [LC Stop Time].

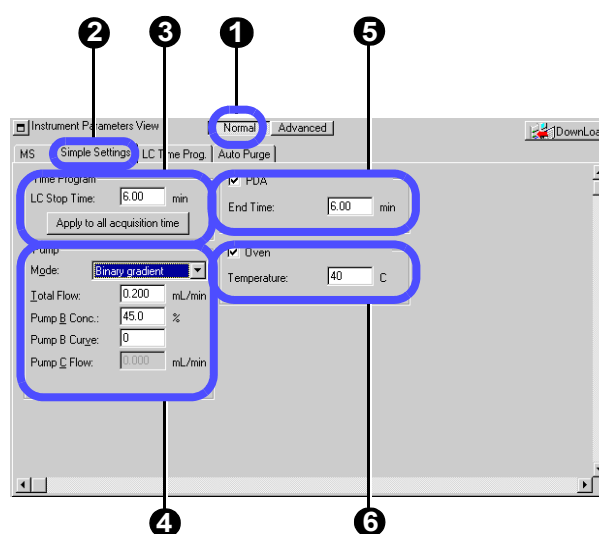
 If you click [Apply to all acquisition time] button after entering [LC Stop Time], [End Time] of all the detectors become the same.

- 4 Enter values for the pump parameters.

Mode	Binary gradient
T.Flow	0.2mL/min
B.Conc	45%

- 5 Enter “6” min in [End Time] of PDA.
- 6 Enter “40” °C for the oven temperature.

 Be sure to enter a value in [Stop/End Time] (measurement end time) in steps 3 and 5.



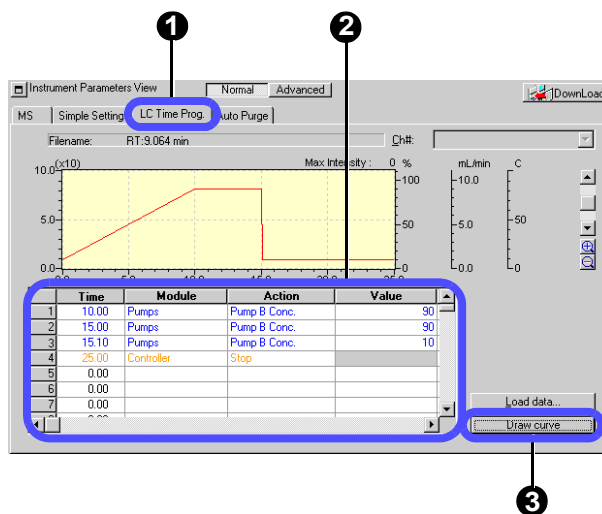
2.2 Setting the LC parameters

■ Entering the gradient mode conditions

This document describes the procedure for setting up the pumps by assuming that liquid is sent in the gradient mode at a constant mixture ratio of the mobile phase.

To change the gradient mode conditions, perform the following steps:


- 1 Select the [LC Time Prog.] tab.
- 2 Enter values in [Time], [Module], [Action], and [Value] for the time program as shown on the right side.
- 3 Click [Draw curve] button.
The entered time program will be displayed as a graph.

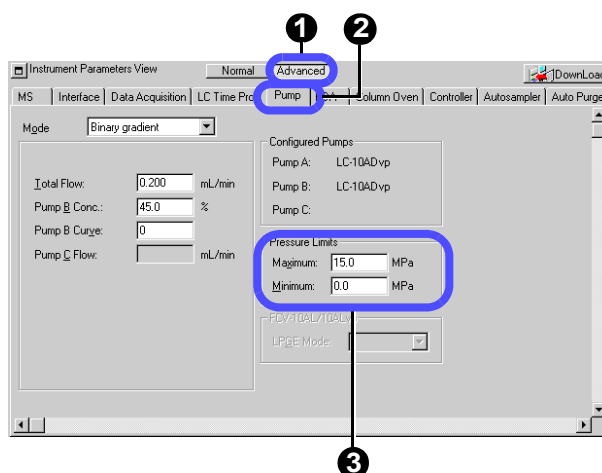


■ Setting the pressure limit of a pump

If the column or the like is in an improper state, an error may occur because of exceeding pump's upper pressure limit. In this case, change the upper pressure limit by performing the following steps:

- 1 Click [Advanced] button.
- 2 Select [Pump] tab.
- 3 Enter "15" MPa in [P.Max].

 The default value for [P.Max] is 10 MPa.



2.3 Setting the MS parameters

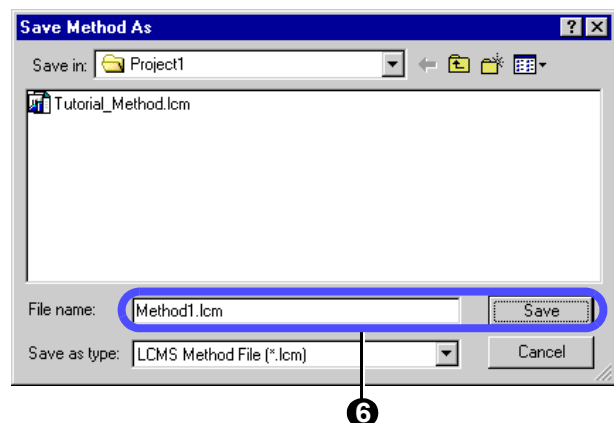
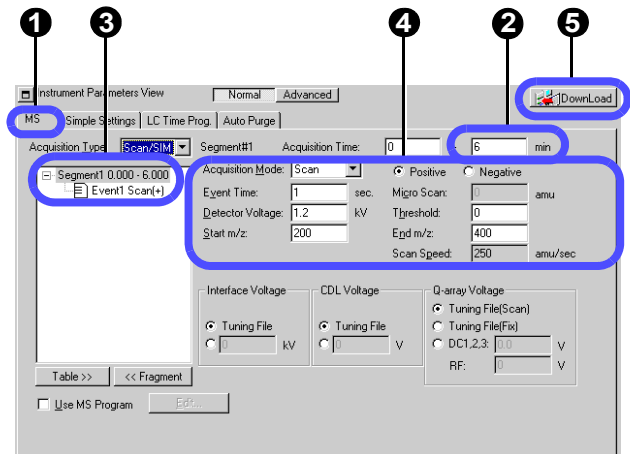
To set the MS (mass spectrometer) parameters, perform the following steps:

 [Operation Manual]: “4.2.2 Setting the MS Parameters”

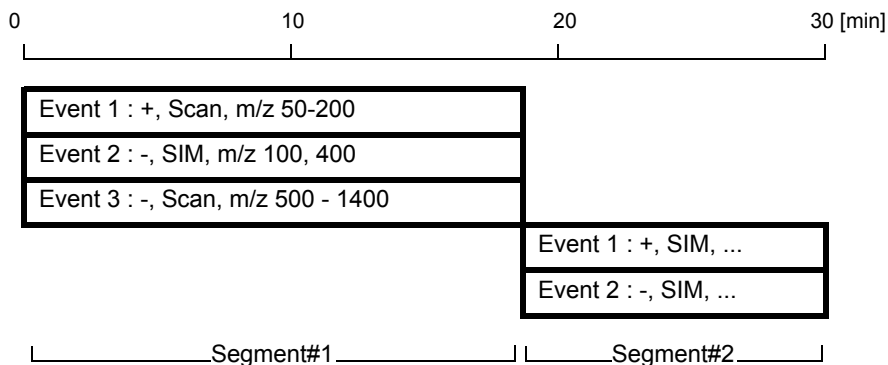
- 1 Select the [MS] tab.
- 2 Enter “6” min in [Acquisition Time].
- 3 Select an event.
- 4 Set the parameters for the selected event.

Detector voltage	1.2kV
Measurement start m/z	200
Measurement end m/z	400

- 5 Click [DownLoad] button.
The instrument parameters will be transferred to the unit.
The dialog box will be opened allowing you to save the settings (method).
- 6 Enter “Method1.lcm” for the file name and click [Save].
The method file will be saved and the set parameters will be transferred to the unit.




Segment and Event




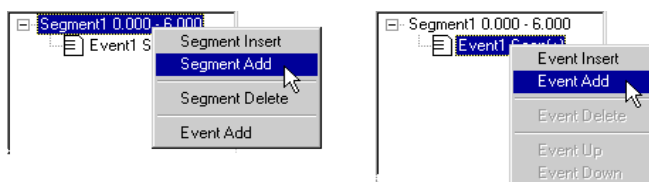
The LCMS-2010A provides the capability to allow you to change the analysis conditions in each specified time range during an analysis. The analysis conditions (a set of analysis conditions) in the specified time range are called a “Segment”. Multiple MS conditions may be specified for each segment and each of those conditions is called an “Event”. Additions of segments and events allow you to specify more complicated MS analysis conditions. This document assumes that an analysis is made under a single MS condition.

If multiple events are specified within the same segment, an analysis will be made under the condition specified for the event time and then the next event will occur. When the final event specified in the segment is finished, the first event will be resumed again. Thus, the cycle (Event#1 → Event#2 → Event#3 → Event#1... for Segment#1 in the above example) will be repeated for the time specified for the segment.

After the time specified for the segment has elapsed, similar operations will be performed for the next specified segment.

 If the “Polarity” (“Positive” or “Negative”) is changed, 400 msec is required for this change. This means that the time of the event after the polarity has been changed becomes shorter practically by 400 msec. Therefore, increase or decrease the event time as necessary.

 To add/delete any segment/event, right-click the appropriate segment/event in the event tree and select the desired option from the pop-up menu displayed.




2.4 Starting the operation of the instrument

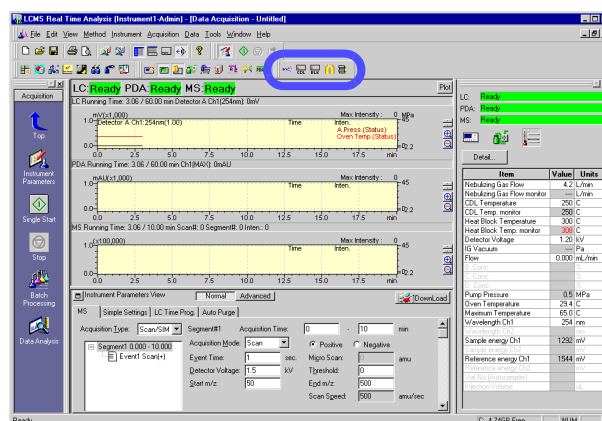
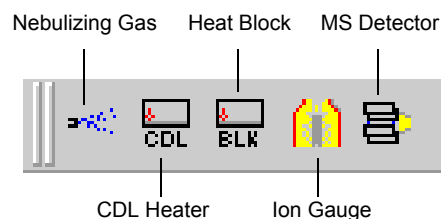
Before starting an analysis, click the “Instrument Control bar” button at the top of the screen to start the operation of the analyzer. It will take about 20 minutes until the operation becomes stable enough.

2.4.1 Starting the control of the MS unit

- 1 Click the following five buttons: [Open/Close Nebulizing Gas], [CDL On/Off], [Heat Block On/Off], [IG On/Off] (= Ion Gauge On/Off), and [MS Detector On/Off].

The MS unit will start operating.

When an analysis is made using the APCI for the interface, the [APCI On/Off] button  is added.

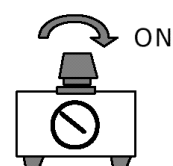


- 2 For the LCMS-2010A, turn clockwise the knob for the drying gas controller to set the pressure.

For the LCMS-2010A-ESI: 0.1 MPa

For the LCMS-2010A-APCI: 0.02 MPa

Turn the knob clockwise.



2.4 Starting the operation of the instrument

2.4.2 Starting the operation of the LC unit

- 1 Click [Instrument On/Off] button.
The LC unit will start operating under the conditions specified in the method file.

HPLC Instrument




The screenshot displays the 'LCMS Real Time Analysis' software interface. The main window shows three chromatograms for LC, PDA, and MS. The 'Instrument Parameters View' is open, showing settings for Acquisition Type (ScanVSM), Acquisition Mode (Scan), Acquisition Time (0 to 10 min), and various detector and scan parameters. The status bar at the bottom indicates 'Ready' and 'C: 47468 Free NUM'.

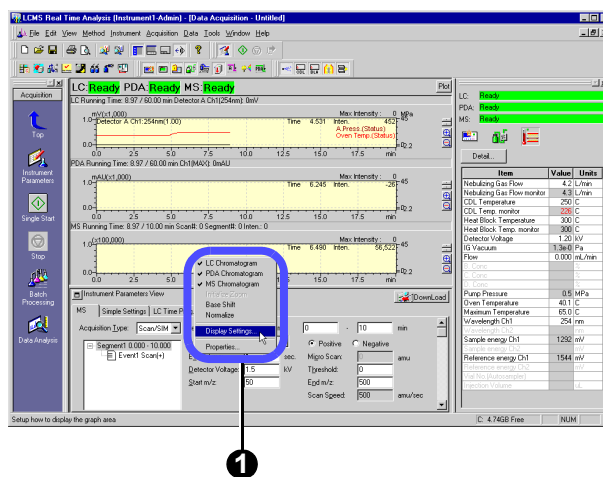
Item	Value	Units
Nebulizing Gas Flow	4.2	L/min
Nebulizing Gas Flow Monitor	45.1	L/min
CDI Temperature	250	C
CDI Temp. monitor	300	C
Heat Block Temperature	300	C
Heat Block Temp. monitor	300	C
Detector Voltage	1.20	kV
EG Vacuum	0.560	Pa
Flow	0.000	µL/min
Flow		
Pump Pressure	85	MPa
Oven Temperature	25	C
Maximum Temperature	650	C
Wavelength CDI	254	nm
Sample energy CDI	1200	eV
Reference energy CDI	1544	eV
CDI Max (Maximum)		
Detector Voltage		

2.4.3 Selecting a graph to be displayed in the <Chromatogram> view

The <Chromatogram> view allows you to specify the types and ranges of axes for the graph to be displayed.

 [Operation Manual]: “11.2 Customizing Windows”

- 1 Right-click anywhere on the graph and select the [Display Settings] menu.




- 2 Select the [MS] tab.
Enter values for m/z and other parameters for the mass chromatogram to be displayed.

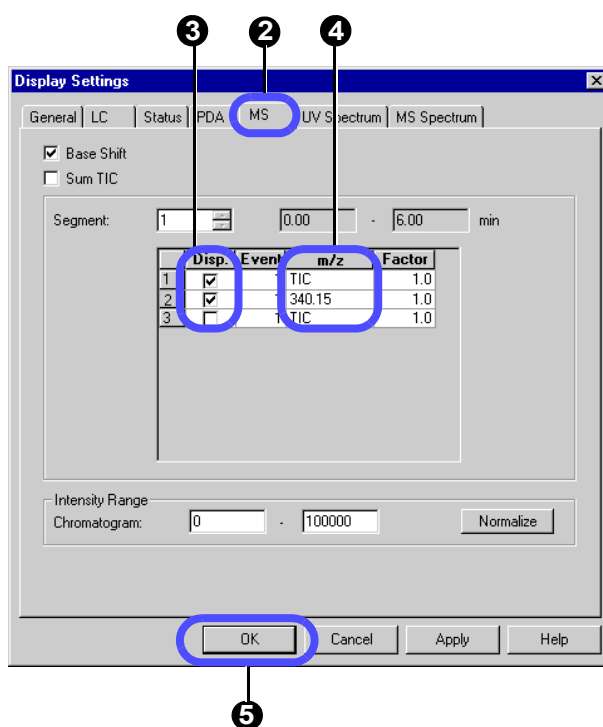
- 3 Tick the check boxes on the 1st and 2nd rows.

- 4 Enter 340.15 on the 2nd row of the m/z column.

In this example, the mass chromatogram will be displayed according to TIC and $m/z = 340.15$.


- 5 Click [OK] button.


 To leave the <Display Settings> window open, click [Apply] button.

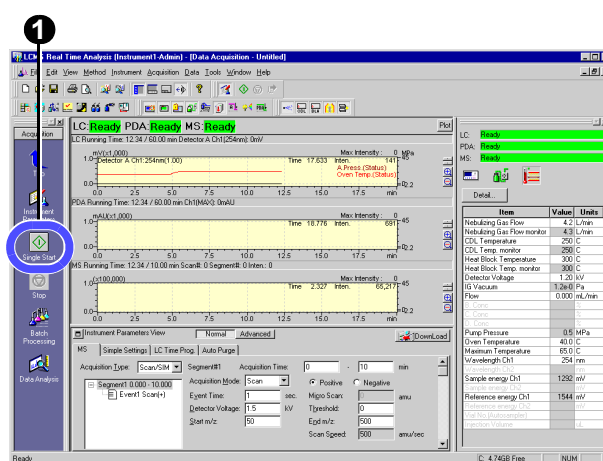


2.5 Acquiring data through a single-run analysis

To make a single-run analysis under the conditions specified in “2.2 Setting the LC parameters” and “2.3 Setting the MS parameters”, perform the following steps:

- 1 Click the [Single Start] icon . The <Single Run> window will be displayed.

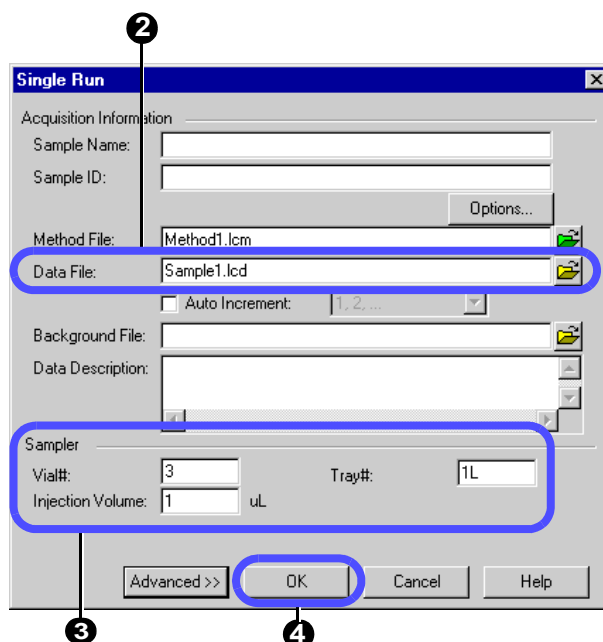
 [Operation Manual]: “4.3 Starting a Single-run Analysis”



- 2 Enter “Sample1.lcd” for the data file name to be created.

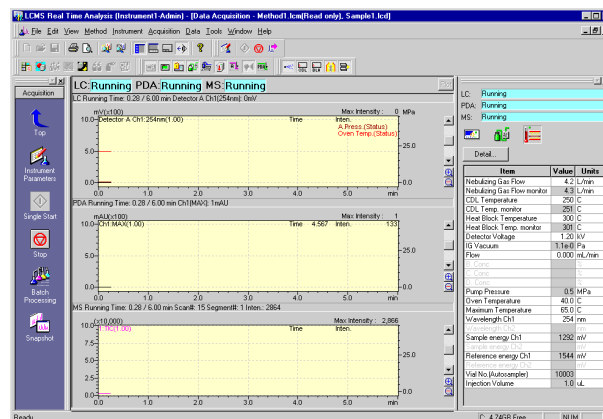
- 3 Enter vial number “3” and injection amount “1”.

In this example, previously fill 5 ng/μL of papaverine into vial No. 3 of the auto sampler, and inject 1 μL from that vial.



- 4 Click [OK] button.


The single-run analysis will be started. After the [Acquisition Time] specified in the method file has elapsed, the analysis is finished automatically.




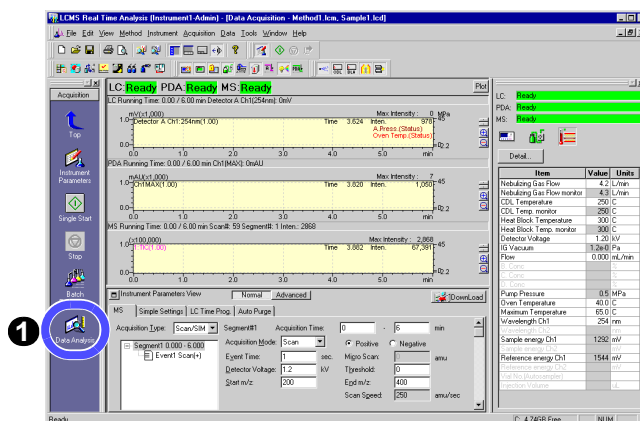
2.6 Performing qualitative processing on <MS Data Analysis>

2.6.1 Starting the <MS Data Analysis>

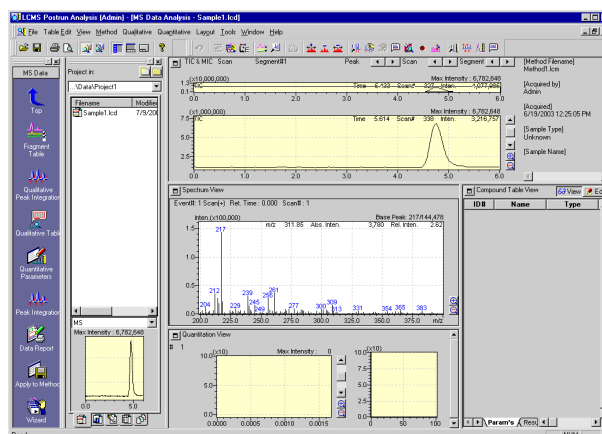
After the single-run analysis has been finished, perform data analysis as follows:

- 1 Click the [Data Analysis] icon . <MS Data Analysis> will be started. The last acquired data will be loaded and then displayed.

 [Operation Manual]: “5.1 Operation in the <MS Data Analysis> Window”



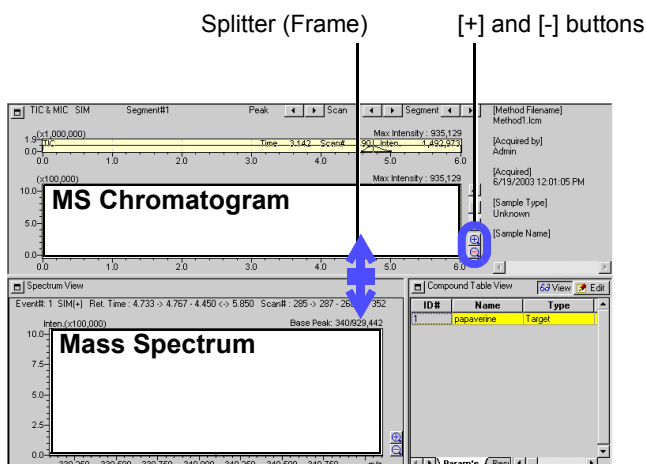
- 2 When the data file is first opened, only TIC is displayed in the <Chromatogram> View.



- 3 Dragging the cursor on each graph will allow you to enlarge that area. Right-clicking anywhere on each graph will allow you to select the [Initialize Zoom] or [Undo Zoom] option.

- 4 Clicking the [+] or [-] button will allow you to increase or decrease the level of the intensity axis.

- 5 Dragging the cursor on the splitter (frame) will allow you to change the aspect ratio of each view.

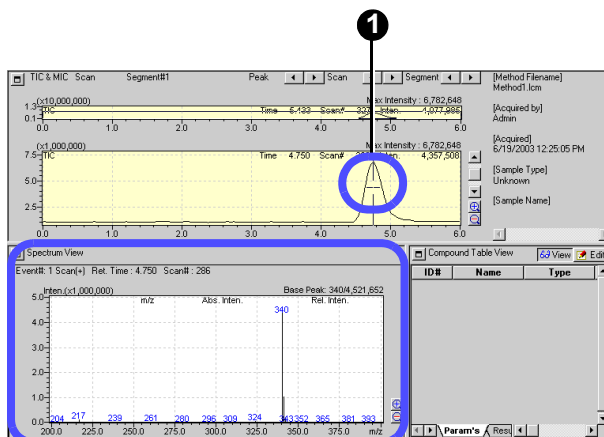


2.6.2 Displaying a mass spectrum

1 Double-click anywhere on the chromatogram.

The cut-out cursor will be moved to that time.

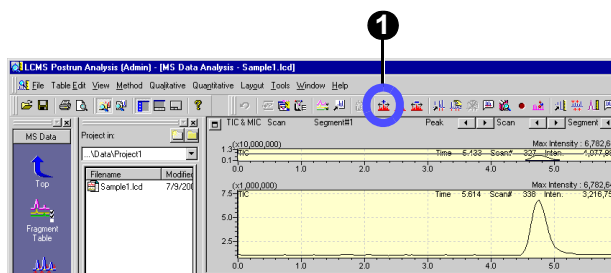
The mass spectrum for the cut-out cursor position in the <Chromatogram> View will be displayed in the <Spectrum> View.



Averaging the mass spectrum

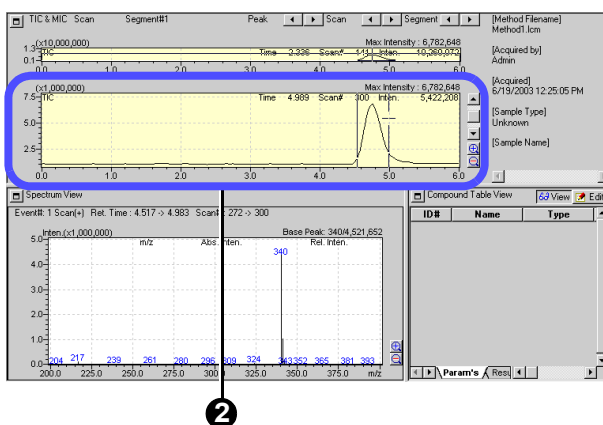
Averaging the mass spectrum will allow you to obtain a clearer spectrum.

1 Click the [Average Spectrum] button  on the Toolbar.




2 Drag the cursor on the chromatogram to define the area you want to average.

The averaged spectrum in the defined time range (between 4.517 and 4.983 min in this example) will be displayed.



■ Performing subtractive processing of a mass spectrum

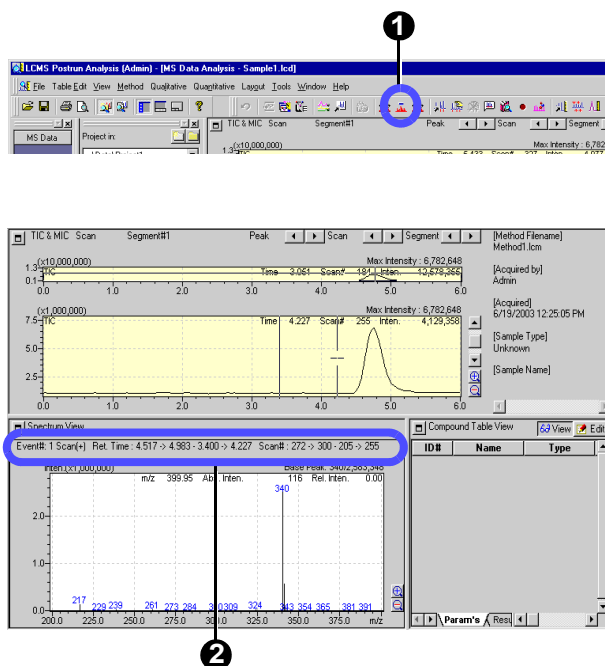
If the background mass spectrum is subtracted from the averaged spectrum, an even clearer spectrum can be obtained.

1 With the averaged spectrum displayed, click the [Average & Subtract Spectrum] button  on the Toolbar.

2 Drag the cursor on the chromatogram to define the area you want to subtract.

The spectrum obtained by subtracting the background will be displayed.

The information displayed above the spectrum graph indicates that the averaged spectrum for retention time between 3.400 and 4.227 min has been subtracted from that for retention time between 4.517 and 4.983 min.




■ Registering the averaged/subtracted spectrum in the “Spectrum Process Table”

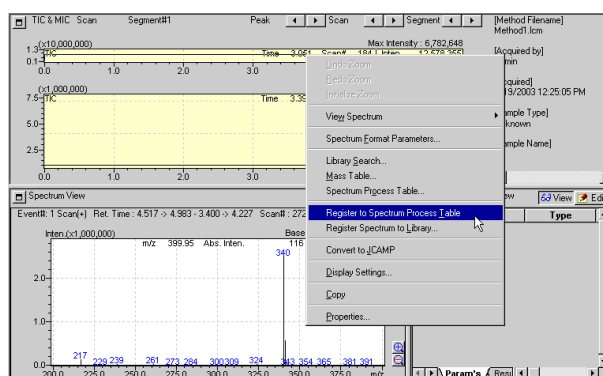
If you register the averaged/subtracted spectrum in the spectrum processing table, you will be able to reproduce that spectrum easily on a later day.

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

The averaged/subtracted mass spectrum will be registered.

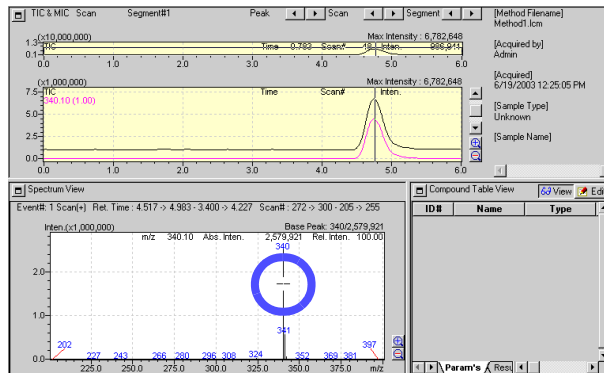


Alternatively, it can also be registered by clicking the  button on the Toolbar.




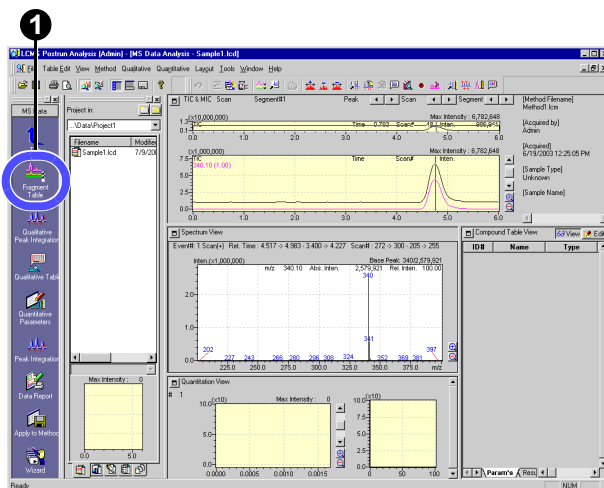
2.6.3 Displaying a mass chromatogram

- 1 Double-click a mass spectrum peak.
A mass chromatogram will be additionally displayed in the <Chromatogram> View.
The settings for the mass chromatogram are registered in the <Fragment Table> window.



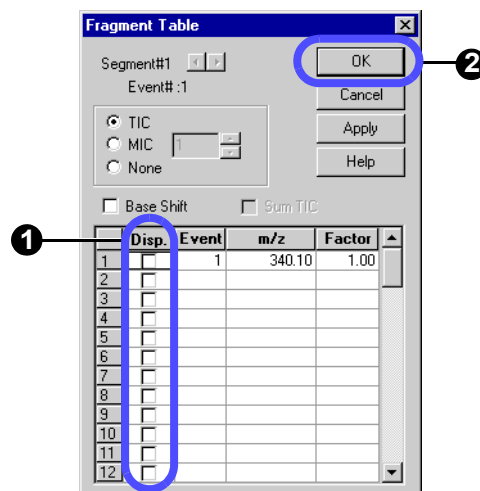
Opening the <Fragment Table> window

- 1 Click the [Fragment Table] icon .
The <Fragment Table> window will be displayed.




Deleting the erroneously registered chromatogram

- 1 Remove a tick mark from the check box in the [Disp.] column on <Fragment Table> window.
- 2 Click [OK] button.
The window will be closed and the chromatogram will be hidden.



2.7 Performing peak integration (peak detection)

In this example, change the integration conditions in a single-run analysis and then perform peak integration again as follows:

- 1 Click the [Qualitative Peak Integration] icon .

The <Qualitative Peak Integration> window will be displayed.

- 2 Select the [Integration] tab.

- 3 Select "Detail" for the integration method.

If you select Auto (Area) or Auto (Height), peaks in the number close to the entered maximum number of peaks will be detected.

- 4 Enter "10" sec in Width.

If you specify the minimum width of peaks to be detected, the noise peak will be eliminated. Peaks will be detected to the extent that the half-width value is one fourth the Width value.

- 5 Enter "1000" /min for the Slope value.

This is the parameter that determines the start and end points of the peak. When the absolute value of the gradient of the chromatogram becomes this value, the start and end points of the peak are determined there.

- 6 Click [OK] button.

The post-run will be carried out using the qualitative integration parameters you have set.

- 7 Click the [Qualitative Table] icon .

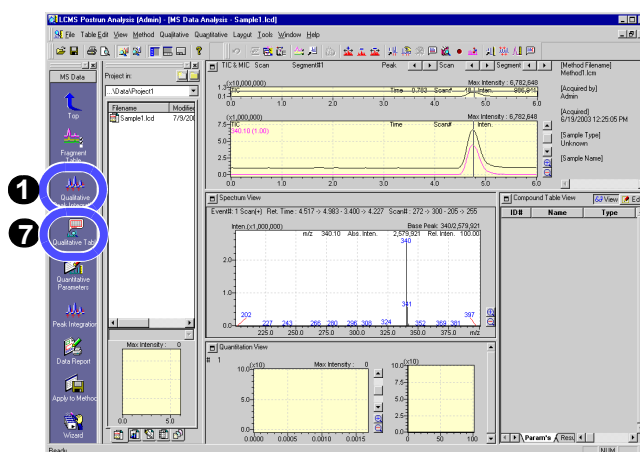
The <Qualitative Table> window will be displayed.

- 8 Select the [TIC] tab.

The integration result will be displayed.



The [Spectrum Process] tab allows you to check the registered averaged spectrum.



Peak	Ret. Time	Peak Start	Peak End	m/z	Area	Area%
1	4.759	4.433	5.467	TIC	104584013	100

2.7 Performing peak integration (peak detection)

Simple procedure for setting the integration parameters

Temporarily enter a little smaller values for Width and Slope and then double them, and see how peaks are detected*. In the example given in this document, first enter Width 10 and Slope 1000 and then Width 20 and Slope 2000.

* If the Width value is excessively increased, no minute noises will be detected as peaks.

If the Slope value is excessively increased, no moderate changes in the baseline will be detected as peaks.

Repeat the above steps and when the unnecessary peaks become undetectable, adopt the integration parameter at that point.


Checking data with <Data Explorer>

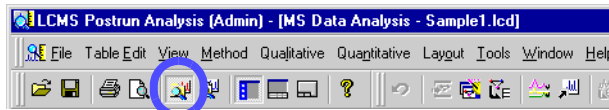
The LCMSsolution manages the data files, method files, batch files, and other related files in “Project Folders”.

<Data Explorer> allows you to manage the project of the LCMSsolution more effectively.

Project folders may be freely created, copied, or handled with <Data Explorer> of the LCMSsolution and the standard Explorer of Windows.

[Operation Manual]: “13.2 Managing Files Effectively”
[Admin Manual]: “6.1.1 Customizing Data Explorer Display Data”

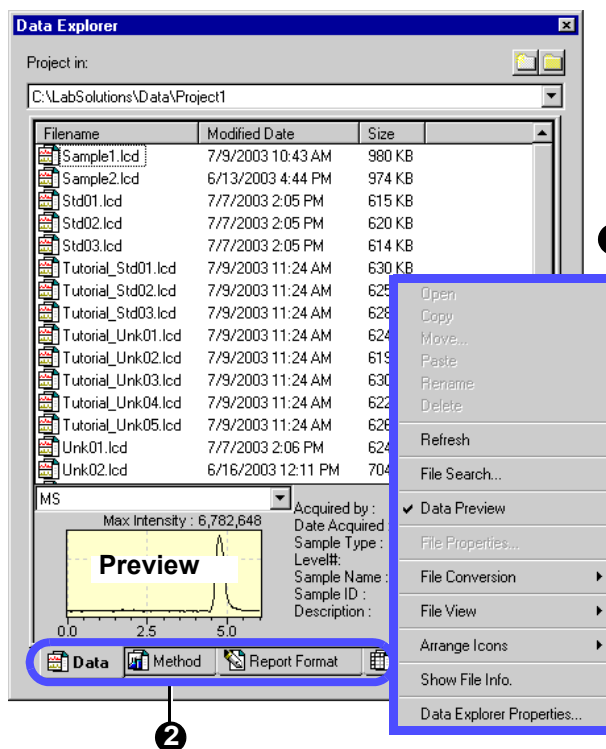
1 Click the [Data Explorer] button .
This will toggle between displaying and hiding <Data Explorer>.



2 Change the display for each file type.

Double-clicking the file or dragging and dropping it to the window will allow you to load the file.

3 Right-click anywhere on the file icon.
A popup menu will appear.



Data Preview
The highlighted data file can be previewed.
Part of the sample information can also be checked.


Show File Info.
When “Detail” for [File View] is selected, the sample name and other additional information will also be displayed as the file information.

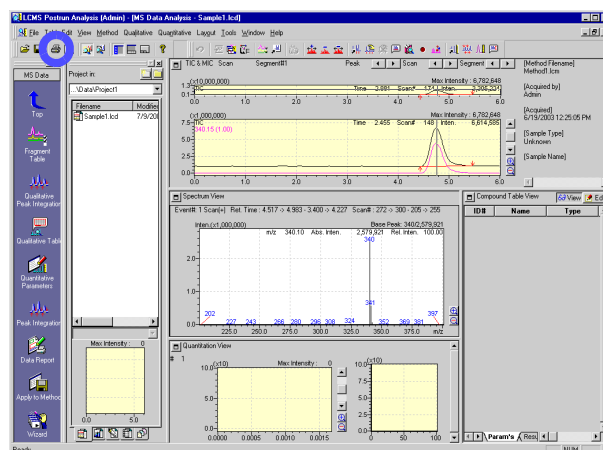
2.8 Printing out the analysis result

To print out the result of qualitative processing, perform the following steps.

2.8.1 Printing out a “Graph Image”

Print out the chromatogram and MS spectrum displayed on the screen as follows:

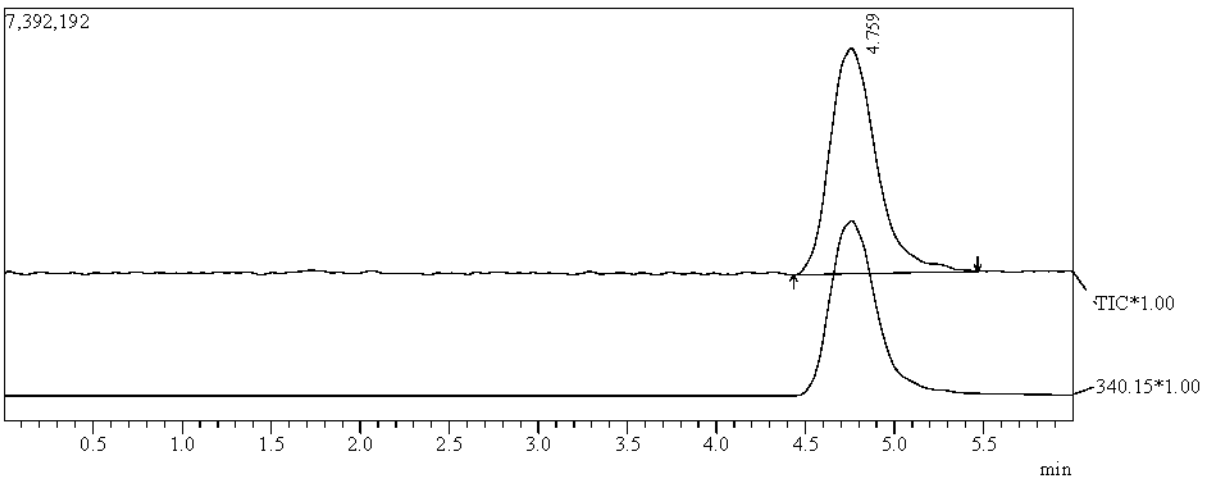
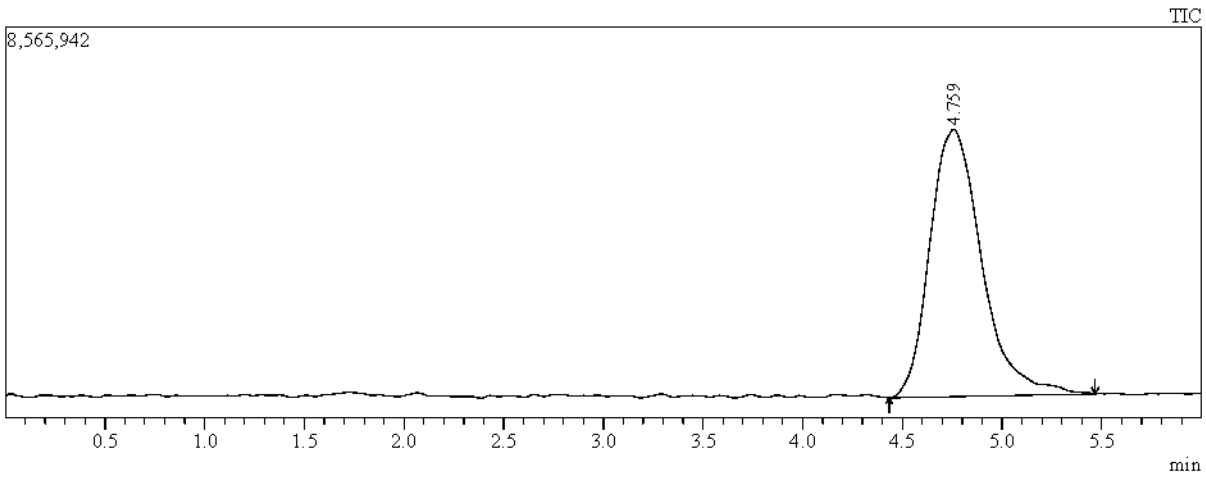
- 1 Click the [Print] button .
[Print Image] will be carried out.



■ Example of printing out a graph image

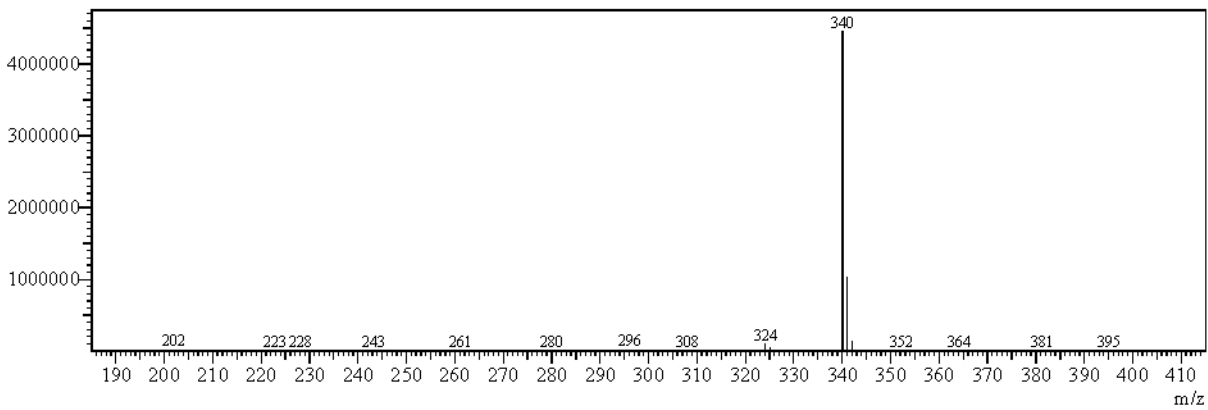
==== Shimadzu LCMSsolution Data Report ====

<Chromatogram>



<Spectrum>


Retention Time: 4.767(Scan#: 287)
Max Peak: 106 Base Peak: 340.10(4457918)
Spectrum: Averaged 4.750-4.783(286-288)
Background: Calc Polarity: Pos Segment: 1 - Event: 1

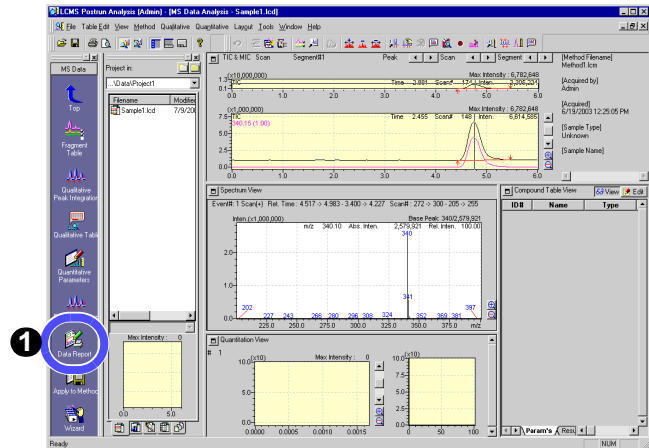


2.8.2 Selecting a layout for printing

<Data Report> allows you to print out a report image in the report format edited in the layout edit pane. In this example, load the preinstalled report format file “Sample1.lcr” to print out a graph image.


 [Operation Manual]: “10.2 Reprinting Data Processing Results”

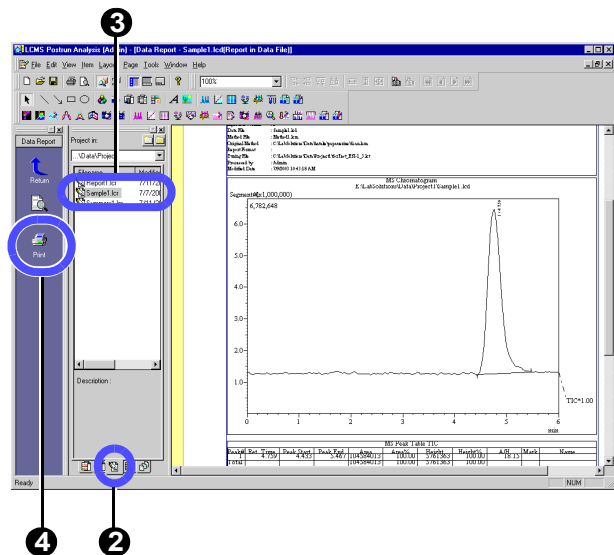
- 1 Click the [Data Report] icon .
The data report will be displayed.



- 2 Select the [Report Format] tab with <Data Explorer>.

- 3 Drag and drop the file icon to the layout edit pane located on the right side.
The “Sample1.lcr” report format will be displayed.

- 4 Click the [Print] icon .
The report in the layout edit pane will be printed out.



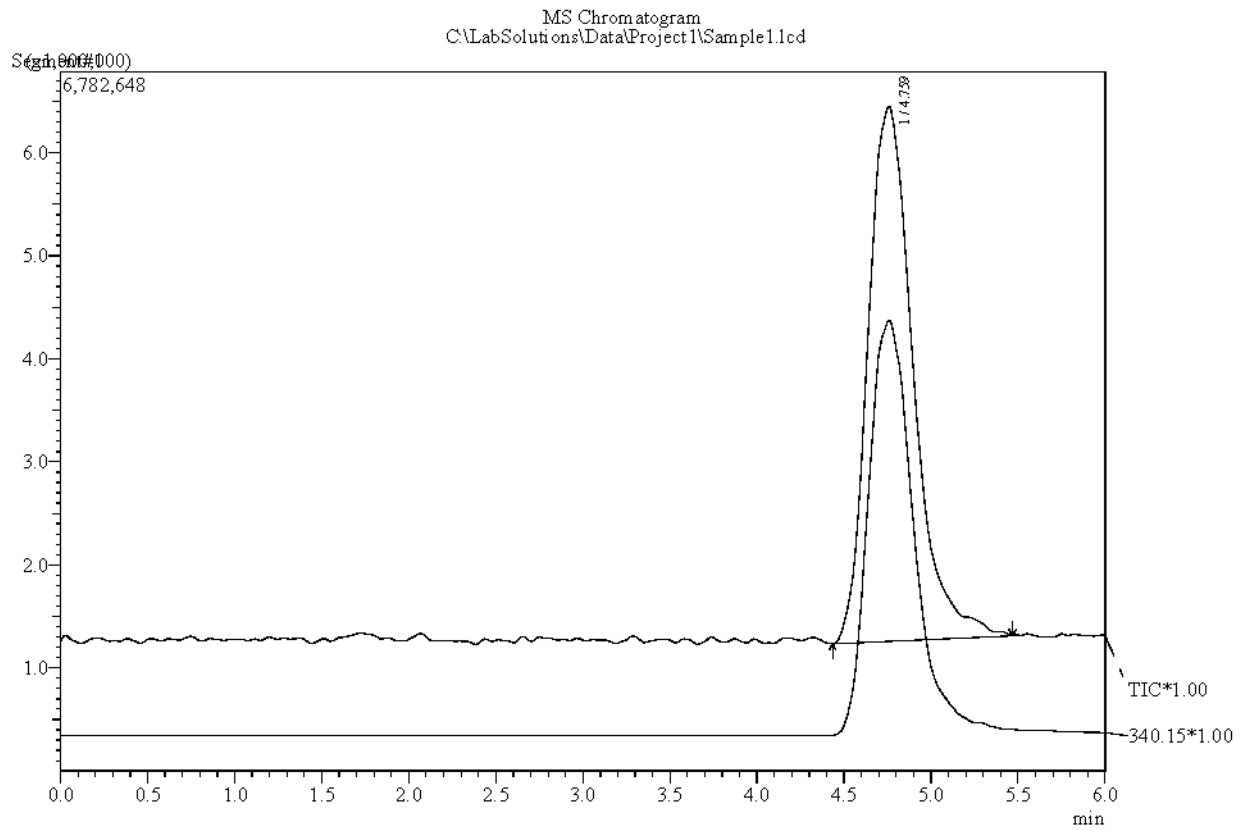
2.8 Printing out the analysis result

Example of using the report format file for printing

Sample Information

```

Acquired by      : Admin
Date Acquired   : 6/19/2003 12:25:05 PM
Sample Type     : Unknown
Level#         : 0
Sample Name     :
Sample ID      :
ISTD Amount    : [1]=1 [2]=1 [3]=1 [4]=1 [5]=1
Sample Amount   : 1
Dilution Factor : 1
Vial#         : 2
Injection Volume : 1
Data File      : Sample1.lcd
Method File    : Method1.lcm
Original Method : C:\LabSolutions\Data\Project1\Method1.lcm
Report Format   :
Tuning File    : C:\LabSolutions\Data\Project1\ESI-1_5.lct
Processed by   : Admin
Modified Date  : 7/9/2003 10:43:18 AM
    
```



MS Peak Table TIC

Peak#	Ret. Time	Peak Start	Peak End	Area	Area%	Height	Height%	A/H	Mark	Name	ID#	Event
1	4.759	4.433	5.467	104584013	100.00	5761363	100.00	18.15		Papaverine	1	1-1
Total				104584013	100.00	5761363	100.00					

3

Quantitative Processing (Batch Analysis)

3.1 Creating a “Compound Table”


In the quantitative processing, the concentration of the compound contained in an “Unknown Sample” is calculated by creating a “Calibration Curve” with a “Standard Sample” of a known concentration, which contains the same compound as that being quantitatively analyzed.

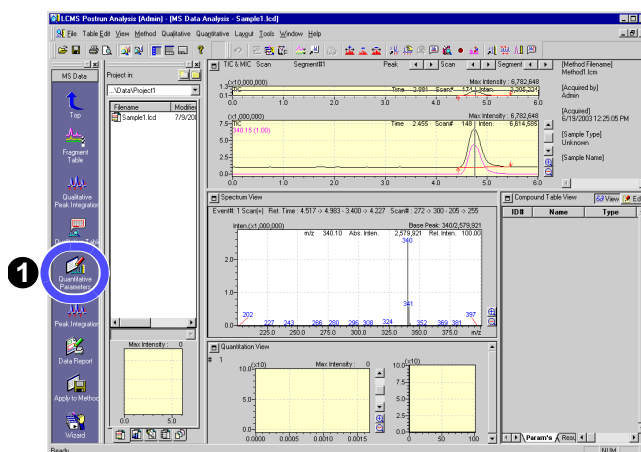
In this example, inject 1 μL of a standard sample containing 0.5, 1, and 5 $\text{ng}/\mu\text{L}$ of papaverine to create a calibration curve. Simulate the quantitative processing to analyze 0.75 $\text{ng}/\mu\text{L}$ of papaverine as an unknown sample.

 [Operation Manual]: “5.5.2 Editing a “Compound Table””, “5.5.4 Using <Compound Table Wizard>”

3.1.1 Setting the quantitative parameters in <MS Data Analysis>

Set the quantitative parameters in the following steps using the papaverine data (Sample1.lcd) that has been loaded to <MS Data Analysis> in the previous chapter.

- 1 Click the  [Quantitative Parameters] icon.

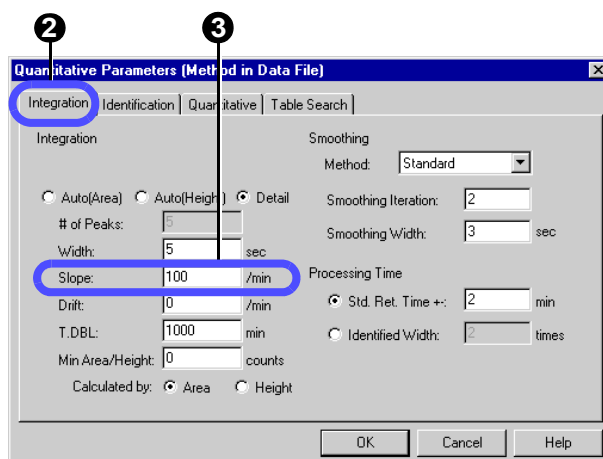


- 2 Select the [Integration] tab.

- 3 Enter “100” /min for Slope.

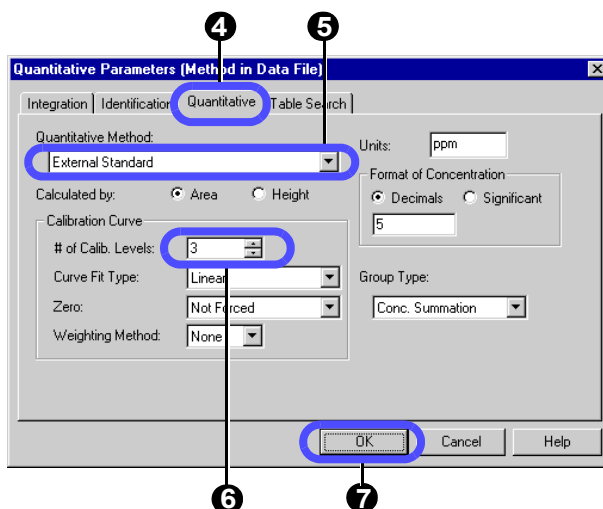
In principle, enter a value equivalent to 1/2000 the targeted peak height.

If no peak is detected, reduce the Slope value by half.




3.1 Creating a “Compound Table”

- 4 Select the [Quantitative] tab.
- 5 Select “External Standard” for [Quantitative Method].
- 6 Enter “3” for [# of Calib. Levels].
- 7 Click [OK] button.





3.1.2 Creating a “Compound Table”


To complete the quantitative settings for each compound, set “Compound Table” to [Edit Mode].

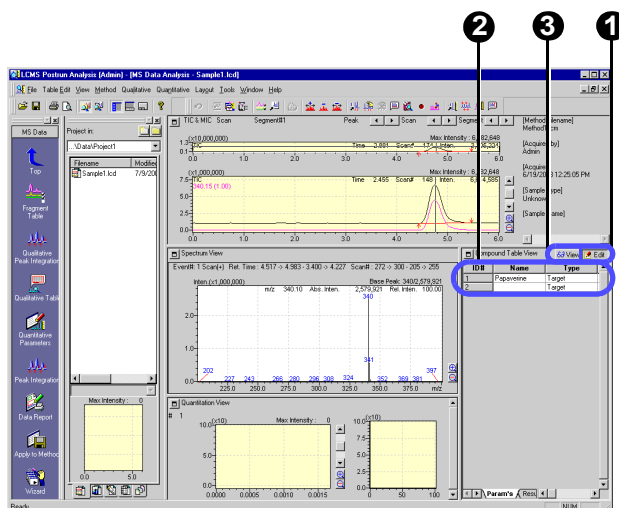
- 1 Click [Edit] button  in the <Compound Table> View.
- 2 Enter values in the “Compound Table”.

Name	Type	m/z	Ret. Time	Conc. 1	Conc. 2	Conc. 3
Papaverine	Target	340.15	4.800	0.5	1	5


 If you click a peak in the <Chromatogram> View with the [Ret. Time] cell highlighted, the retention time for that chromatogram peak will be entered automatically.

 If you click a peak in the <Spectrum> view with the [m/z] cell highlighted, the m/z value for that spectrum peak will be entered automatically.

- 3 Click [View] button  .
The edited settings will be established.



■ Checking and saving the quantitative parameters/compound table


1 Click the [Peak Integration] icon .

2 Check for the identification mark (▼) on the chromatogram peak.

The identification mark is given to the identified peak.

The peak has the (↑) and (↓) marks at the starting and end points, respectively.

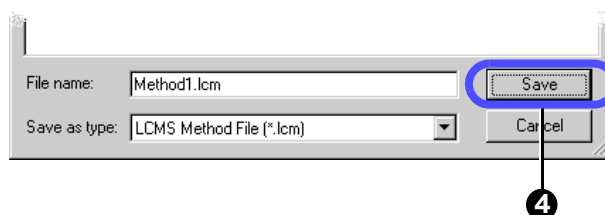
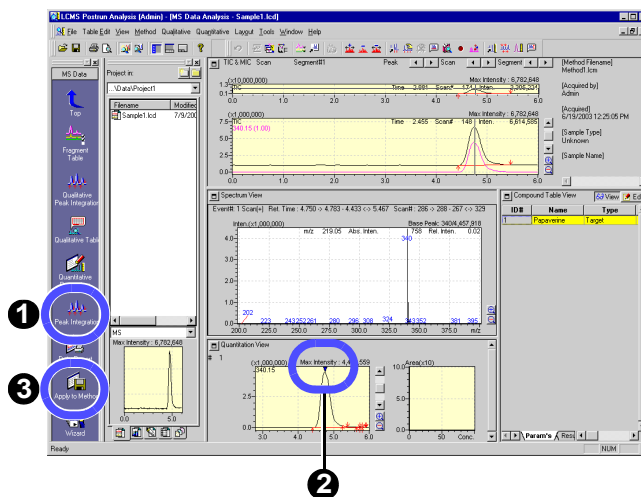
If the peak integration fails, adjust the Slope value among the integration parameters.

3 Check that the peak has been identified properly, and then click the [Apply to Method] icon .

The Save dialog box will be opened.

4 Check that “Method1.lcm” is selected for the file name, and then click [Save] button.

The method file will be overwritten.



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