Shimadzu LCMSsolution

for LCMS-2010 / LCMS-QP8000 $\!\alpha$

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 tutrial 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 thouroughly 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 tutrial 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 administra- tion 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 installa- tion	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 installa- tion	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 installa- tion	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.
1 B	Points the reference informations.
Ŷ	Gives you tips.
< >	Shows a window or view name; e.g., <data acquisition=""> window or <method> view.</method></data>
[]	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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Making Preparations for Analysis

1.1 Basics of LCMSsolution

<LCMSsolution Launcher> - [Operation] menu icon



No.	lcon	Name	Description
1	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)</lcms>
2	R	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)</lcms>
3	Postrun	Postrun	Starts the application for loading the acquired analysis data to create a calibration curve or perform data processing.
4	Browser	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 sys- tem configuration
.lcr	Report Format File	Report formats
.lcb	Batch File	Batch tables and batch settings
.lcd	Data File	Chromatograms, mass spectrums, peak tables, iden- tification/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

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.



Enter your user ID to log on.



CMSsolution disp

displayed on the Windows desktop.



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



LabSolIIIIOIIS Lemseolution

8

User ID

Password

Admin

×

ΠK

Cancel

Help

•

- 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"



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10 Check that "Ready" is displayed.

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

[Operation Manual]: "14.5 Configuring System"

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2dam mv2 130 Ega mv2 300 injection Volume 14. Scan Sgredt 500 amu/rec		2	Vial No.(Autosampler)	
Scan Sgeed: 500 anw/sec		gomme job Eganze job	Injection Volume	uL.
		Scan Sgeed 500 amu/sec		

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.

, u 🛩 🖬			
🔚 🖲 A.			
	LLC:Ready PDA:Ready MS:Ready Plat		
Acquisition	LC Buoring Time: 3 06 / 80 00 min Detector & Ch1(254cm): BmV	LC: Ready	
	start 2000 Merchander - 0.10	PDA: Ready	
	1.0 Detector A Ch1:254nm(1.00) Time Inten.	MS: Ready	
Im	A Press (Status)	- at 1-	
		🔤 🔐 🚛 -	
	0.0 2.5 5.0 7.5 10.0 12.5 15.0 17.5 min	Dated	
	PDA Running Time: 3.06 / 60.00 min Ch1(MAX): 0mAU		
Instrument	mAU/x1.000) Max Intensity: 0	Item	Value Uni
Parameters	1.0-Time Inten. F45	Nebulizing Gas Flow	4.2 L/min
	E 1 E	Nebulizing Gas Flow monitor	L/min
	0.0-	COL Temperature	250 C
Single Start	0.0 2.5 5.0 7.5 10.0 12.5 15.0 17.5 min	Heat Block Temperature	200 C
	MS Running Time: 3.06 / 10.00 min Scan#: 0 Segment#: 0 Inten.: 0	Heat Block Temp, monitor	308 C
		Detector Voltage	1.20 kV
	1.0 Time Inten. 45	IG Vacuum	Pa
Stop		Flow	0.000 mL/m
2015	- co-	B. Conc	2
		Conc	
Batch	Ellista meri Parametero Viesa	P. o Pressure	0.5 MPa
Processing	Numa Availad	0 D Temperature	29.4 C
	MS Simple Settings LC Time Prog. Auto Purge	M mum Temperature	65.0 C
		W velength Ch1	254 nm
	Acquisition Type: Scan/SIM Segment#1 Acquisition Time: 0 III min	V elength Ch2	nm
Data Analysis	Reserver 10000-10000 Acquisition Mode: Scan C Positive C Negative	S ple energy Lh1	1292 mV
	Event Scarit Event Time 1 one Minor Scar	R manage amount Chil	1544 with
	Detectory/above 15 IV Threaded	B cence energy Chi	1344 111
	gelecia voldge. 115 kV Tgjesiola. 10	V No.(Autosampler)	
	Start m/z 50 Egd m/z 500	In tion Volume	
	Scan Speed 500 anw/sec		



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 **1**. A new method file will be opened.



2.2 Setting the LC parameters

2.2.1 Detecting the auto sampler rack

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



2.2.2 Setting the LC parameters

[Operation Manual]: "4.2.1 Setting the LC Parameters"



Enter "6" min in [End Time] of PDA.



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.

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:

- 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.
- 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:

Click [Advanced] button.

Select [Pump] tab.

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"

Enter "6" min in [Acquisition Time].



2

Select an event.

Set the parameters for the selected event.

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



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.

Astronometers	Normal Advanced	9 9	5
MS Simple Settings LC Time P	rog. Auto Purge		
Acquisition Type Scan/SIM	Segment#1 Acquisition Time:	0 6	min
	Acquisition Mode: Scan Eyent Time: 1 Detector Voltage: 1.2 KV Start m/z:	Positive C Negative Migro Scan: 0 Threshold: 0 End m/z: 400 Scan Speed: 250	amu amu/sec
Table >>	Tuning File Vitage CDL Voltage Tuning File KV O	le C Tuning File(Scar C Tuning File(Scar C Tuning File(Fix) C DC1,2,3: 0 RF: 0	i) V V
Use MS Program			

Save Method As	? ×
Save in: 🔄 Project1 💽 🔶 🗈	💣 🎟 -
Tutorial_Method.lcm	
File name: Method1.lcm	Save
Save as type: LCMS Method File (*.lcm)	Cancel
	111
6	

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 \rightarrow Event#2 \rightarrow Event#3 \rightarrow 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.

Segment1 0.000	• 6 000 Segment Insert	⊡-Segment1	0.000 - 6.000	
	Segment Add		Event Inse	ert
	Segment Delete		Event Add	
	Segment Delete		Event Dele	
	Event Add		Eventille	
			Event Dov	

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] (= lon <u>G</u>auge On\Off), and [MS Detector On/ Off].

The MS unit will start operating.







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.



2.4.2 Starting the operation of the LC unit

Click [Instrument On/Off] button.

The LC unit will start operating under the conditions specified in the method file.

HPLC	Instrument		
	📴 💼 🔝 🕼 📩	I ?	īĿ,
LCMS Real LCMS Real LCMS Real LCMS Real LCMS Real LCMS Real LCMS Real LCMS Real	ana Analysis (Instances I Adam) = (D-24 Angustanos Unidad) Ter Mahod Johannes Assistato (Des Lots Mader Mo D. J. M. (1977) = (1977) = (1977) = (1977) = 21 dist = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) = (1977) =		-@>
Acquisition	LC Ready PDA-schady MS. Ready PM LC Ready PDA-schady MS. Ready PM 10 2010 00 m0 betters A 511/54m (511) 10 2	LC: Ready PDA: Ready MS: Ready Emil: All Signal Sig	±x
Instrument Parameters Single Start	Concretely (in the star) solution intervence under 10 ^{-44,161,000} 10 ^{-44,161,000} 10 ^{-44,161,000} 10 ^{-45,151,151,151,151,151,151,151,151,151,1}	Item Nebulizing Gas Flow Nebulizing Gas Flow monitor CDL Temperature CDL Temperature Heat Block Temperature Heat Block Temperature Heat Block Temperature Detector Voltage 15 January	Value Units 4.2 Umin 4.3 Umin 250 C 234 C 300 C 300 C 301 C 1.20 KV 1.50 Rp
Stop Batch Processing	0 1000 125 150 125 120 125 120 125 120 125 120 125 120 125 120 125 120 125 120 125 120 125 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120 120	Bow Bit Status Bow Bit Status Di Conc Dump Pressure Dwin Temperature Maximum Temperature Wavelength Ch1	0.000 mL/min 0.05 MPa 29.2 C 65.0 C 254 nm
Data Analysis	Programming (jee [i_con/km]) generating (som ⊥ 0 = 0 Parlies C Parlies	Wavelength Ch2 Sample energy Ch1 Sample energy Ch2 Reference energy Ch2 Reference energy Ch2 Vial No (Autocample) Trijecton Volume	1292 mV mV 1544 mV mV

$2.4.3 \hspace{0.1in} \text{Selecting a graph to be displayed in the <Chromatogram> view}$

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"

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

Check PDA Ready MS Ready For Accord MS Ready	1월 1월 1월 2월 1월	
Displayed Book Display	Bit Ready Poll Common Section 100 (Section 100 (Sect	1
Open Activity Accentration Liper EconvSH © Power State Power State <td>Mini Hendrigi, Ogi Mini He</td> <td>Value Units 4.2 Units monitot 4.3 Units 250 C 226 C use 300 C 1.20 kV 1.3e0 Pa 0.000 mL/min 0.000 mL/min 4.0.1 C 8.50 C</td>	Mini Hendrigi, Ogi Mini He	Value Units 4.2 Units monitot 4.3 Units 250 C 226 C use 300 C 1.20 kV 1.3e0 Pa 0.000 mL/min 0.000 mL/min 4.0.1 C 8.50 C
Scan Speed 500 amu/rec	Densities D I0 mn M Properties P Notative Notative Service strenge Properties M Notative Notative Notative Notative Properties Service strenge Service strenge Notative Notative Notative Notative Properties Service strenge Service strenge Notative	254 rm 1232 rW 1132 rW 11 1544 rW 12 rW

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.
- 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.



Click [OK] button.

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

ieneral LC ! I Base Shift □ Sum TIC	Status PDA	MS UV S x	ectrum MS Sp	pectrum	
Segment:	1 Disp. E	0.00 vent m/z TIC 340.15 TIC TIC	• 6.00 Factor 1.0 1.0	min	
Intensity Range Chromatogram:	0	- 10000	0	Normaliz	:e

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.</single>
Ĩ	Coperation Manual]: "4.3 Starting a Single-run Anal- ysis"

- 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/ μ L of papaverine into vial No. 3 of the auto sampler, and inject 1 μ L from that vial.

CC i Real Time Analyzis (Instrument ▲) E Edit View Method Instrument A □ (F ■ ④ Q → Q ■ E	I-Admin) - [Data Acquisition - United] cquistion [248] Cob Window Heb 5 ⊊ → ♥ ♥ 1 ⊈ � ⊕ 1 ≠	X
Acce bin Acce bin	Im 20 (20 (20 (20 (20 (20 (20 (20 (20 (20 (
Data Reverse 1000000000000000000000000000000000000	55 75 125 120 175 m2 Dotal 00.00 00.00 00.00 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100 100<	em Value Units as Flow 4.2 Unin as Flow 4.3 Unin stre 250 C comitor 250 C
MS Running Time 12.34 /7 Stop Batch Refer	0.00 m/scalt 0 Seguent 0 Inn. 0 100 m/scalt 0 Seguent 0 Inn. 1 100 m/scalt 0 Seguent 0 Segue	rep. monitor 300 C age 1.20 kV 1.2e0 Pa 0.000 mL/min
Processing Data Analysis Data Analysis Data Analysis	The Toron Data Starting S	Auto 40.0 C opprehre 65.0 C Lh2 254 rm Lh2 1230 m/ y Lh1 1243 m/ y Lh2 104 105 serger Lh1 1544 m/ serger Jh2 sm/ sm/
Ready		B Free NUM
Single Run		×
Acquisition Informat	ion	
Acquisition Informat Sample Name: Sample ID:	ion	
Acquisition Informat Sample Name: Sample ID: Method File:	ion	ins
Acquisition Informat Sample Name: Sample ID: Method File: Data File:	ion	ins
Acquisition Inform at Sample Name: Sample ID: Method File: Data File:	Optio Method1.lcm Sample1.lcd Auto Increment: 1, 2,	ins
Acquisition Informat Sample Name: Sample ID: Method File: Data File: Background File:	Optio Optio Method1.lcm Sample1.lcd Auto Increment: 1, 2,	ns
Acquisition Informat Sample Name: Sample ID: Method File: Data File: Background File: Data Description:	ionOptio	
Acquisition Informat Sample Name: Sample ID: Method File: Data File: Background File: Data Description: Sampler Vial#: Injection Volume:	ion	ns
Acquisition Informat Sample Name: Sample ID: Method File: Data File: Background File: Data Description: Sampler Vial#: Injection Volume:	Option Option Method1.lcm Sample1.lcd Auto Increment: 1, 2, Auto Increment: 1, 2, Tray#: 1L	
Acquisition Informat Sample Name: Sample ID: Method File: Data File: Background File: Data Description: Sampler Vialt#: Injection Volume: Ad	ionOptio Method1.lcm Sample1.lcd Auto Increment: 1, 2,	ns
Acquisition Informat Sample Name: Sample ID: Method File: Data File: Background File: Data Description: Sampler Vial#: Injection Volume: Ad	ion	ns





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:



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"



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



- 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.

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

- 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

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.

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.

- With the averaged spectrum displayed, click the [Average & Subtract Spectrum] button **m** 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.

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

The averaged/subtracted mass spectrum will be registered.





2.6.3 Displaying a mass chromatogram

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

Click the [Fragment Table] icon

The <Fragment Table> window will be displayed.



Deleting the erroneously registered chromatogram

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

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:

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.
- 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 halfwidth value is one forth the Width value.

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.

Click [OK] button.

The postrun will be carried out using the qualitative integration parameters you have set.

7

6

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.







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"

Click the [Data Explorer] button 🙀

This will toggle between displaying and hiding <Data Explorer>.

🔯 LCMS Postrun A	nalysi	is (Admir	n) - (MS Da	ta Analysis	- Sampl	e1.lcd		
<u>ℜ</u> Eile Table <u>E</u> dit	⊻iew	<u>M</u> ethod	Qualitative	Qua <u>n</u> titative	Lay <u>o</u> ut	<u>T</u> ools	<u>W</u> indow	<u>H</u> elp
🖻 🖬 🎒 🖪		2		8 0	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.

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.

roject in:			
:\LabSolutions\Data\Pro	ject1		<u> </u>
Filename	Modified Date	Size	▲
Sample1.lcd	7/9/2003 10:43 AM	980 KB	
Sample2.lcd	6/13/2003 4:44 PM	974 KB	
🗄 Std01.lcd	7/7/2003 2:05 PM	615 KB	
針 Std02.lcd	7/7/2003 2:05 PM	620 KB	
🔄 Std03.lcd	7/7/2003 2:05 PM	614 KB	
Tutorial_Std01.lcd	7/9/2003 11:24 AM	630 KB	
Tutorial_Std02.lcd	7/9/2003 11:24 AM	625	Open
Tutorial_Std03.lcd	7/9/2003 11:24 AM	628	
Tutorial_Unk01.lcd	7/9/2003 11:24 AM	624	Move
Tutorial_Unk02.lcd	7/9/2003 11:24 AM	619	
Tutorial_Unk03.lcd	7/9/2003 11:24 AM	630	Rename
Tutorial_Unk04.lcd	7/9/2003 11:24 AM	622	
Tutorial_Unk05.lcd	7/9/2003 11:24 AM	626	Defeat
Unk01.lcd	7/7/2003 2:06 PM	624	herresh
Unk02.lcd	6/16/2003 12:11 PM	704	File Search
MS Max Intensity :	Acquired	by: 🔽	Data Preview
Build interiority :	A Sample T	ype:	
Preview	Sample II	ame: I	File Conversion 🔹 🕨
++++++++++++++++++++++++++++++++++++++	-/	n:	File View 🕨
Blata Methor	5.0 1 St Beport Format		Arrange Icons 🔹 🕨
			Show File Info.
			Data Explorer Properties

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:



[Print Image] will be carried out.



Example of printing out a graph image

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

<Chromatogram>



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.



Click the [Print] icon 🎒

The report in the layout edit pane will be printed out.



Example of using the report format file for printing

104584013





576

Total

3.1 Creating a "Compound Table"

ysis)

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.

Quantitative Processing (Batch Anal-

In this example, inject 1 μ L of a standard sample containing 0.5, 1, and 5 ng/ μ L of papaverine to create a calibration curve. Simulate the quantitative processing to analyze 0.75 ng/ μ 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.



Select the [Quantitative] tab.

5 Select "External Standard" for [Quantitative Method].

Enter "3" for [# of Calib. Levels].

7 Click [OK] button.

Attemporation Indentification Quantitative Method: External Standard Calculated by: Calibration Curve # of Calib. Levels: Curve Fit Type: Zero: Weighting Method:	Quantitativ Quantitativ Area J Linear Not Frice None	C Height	Units: Format © Dec Group Ty Conc.	ppm of Concentration imals C Signifi pe: Summation <u>v</u>	cant

3.1.2 Creating a "Compound Table"

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

Click [Edit] button 📝 Edit in the <Compound Table> View.

Enter values in the "Compound Table".

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

F 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.



The edited settings will be established.



Checking and saving the quantitative parameters/compound table

- 1 2
- Click the [Peak Integration] icon Mu
- Check for the identification mark (▼) on
 the chromatogram peak.
 - The identification mark is given to the identified peak.
 - The peak has the (\uparrow) and (\downarrow) 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.



<u> </u>			
File name:	Method1.lcm		Save
Save as type:	LCMS Method File (*.lcm)	•	Carcel

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