Gas Chromatograph Mass Spectrometer GCMS-QP2010 Series Operation Guide For GCMSsolution Ver. 2.6

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

SHIMADZU CORPORATION

ΚΥΟΤΟ JAPAN

ANALYTICAL & MEASURING INSTRUMENTS DIVISION

This page is intentionally left blank.

In order to ensure the safe use of this product, observe the following points.

- Follow the procedures described in the instruction manual.
- Observe precautionary information.
- Do not disassemble or modify this product without permission.
- ♦ If repairs are required, contact your Shimadzu representative.

Microsoft and Windows are registered trademarks of Microsoft Corporation in the United States and other countries. Other product and company names mentioned herein are trademarks or registered trademarks of their respective companies.

"Microsoft[®] Windows[®]" is abbreviated to "Windows".

<< Notices >>

- All rights are reserved, including those to reproduce this document or parts there of in any form without permission in writing from Shimadzu Corporation.
- Information in this document is subject to change without notice and does not represent a commitment on the part of the vendor.
- Any errors or omissions which may have occurred in this document despite the utmost care taken in its production will be corrected as soon as possible, but not necessarily immediately upon detection. We appreciate notification of any errors or omissions.
- Shimadzu Corporation is not responsible for errors or injuries resulting from following the instructions in this document.
- Shimadzu Corporation is not responsible for errors or injuries resulting from the use of equipment by the customer.
- Replacement parts for this product will be available for a period of seven (7) years after discontinuation of the product. Thereafter, such parts may cease to be available. Note, however, that the availability of parts not manufactured by Shimadzu Corporation is determined by the manufacturer of those parts.
- The contents of PC hard drives may be lost due to unforeseen circumstances. In order to protect important data, be sure to make backup copies on a regular basis.

© 2010 Shimadzu Corporation. All rights reserved.



Introduction

Thank you for purchasing the GCMS-QP2010-series gas chromatograph mass spectrometer. This document is intended to explain basic operations to first-time users. Refer to the instruction manual or the appendix of this document for more details, including information related to maintenance and inspection.

This document assumes that the user has a working knowledge of Windows. There are references to functions and terminology specific to Windows; refer to a Windows user manual as necessary. Users who have never worked with Windows should read a Windows user manual before using this document.

Product Warranty

Shimadzu Corporation provides the following warranty for this product.

Details

1. Period:	Please contact your Shimadzu representative for information concerning the extent of your product's warranty.
2. Terms:	If a fault attributable to Shimadzu Corporation occurs within the warranty period, we will perform the necessary repairs or part replacement free of charge. Note, however, that it may not be possible to replace products that have short life cycles, such as PCs and their peripheral devices and parts, with the same models.
3. Limitation of Liability	 In no event will Shimadzu be liable for any lost revenue, profit or data, or for special, indirect, consequential, incidental or punitive damages, however caused regardless of the theory of liability, arising out of or related to the use of or inability to use the product, even if Shimadzu has been advised of the possibility of such damage.
	2) In no event will Shimadzu's liability to you, whether in contract, tort (including negligence), or otherwise, exceed the amount you paid for the product.
4. Items Not Covered:	The following items are not covered by this warranty, even if they occur during the warranty period.
	1) Faults resulting from incorrect use
	2) Faults resulting from repairs or modifications implemented by parties other than Shimadzu Corporation or companies designated by Shimadzu Corporation
	 Faults occurring after use in combination with hardware or software other than that designated by Shimadzu Corporation
	4) Faults in equipment and damage to data and software, including the OS, resulting from computer viruses
	5) Faults in equipment and damage to data and software, including the OS, resulting from power failures, including power interruptions and momentary voltage drops
	6) Faults in equipment and damage to data and software, including the OS, resulting from turning OFF the power switch on the equipment without following the proper shutdown procedures
	7) Faults not originating in the equipment itself
	8) Faults occurring after use in severe environmental conditions, such as those subject to high temperatures, high humidity levels, corrosive gases, or vibrations
	 Faults resulting from fires, earthquakes and other natural disasters, contamination by radioactive or toxic substances, wars, riots, criminal activities, and other types of force majeure
	10) Faults occurring after the product is moved or transported following initial installation
	 11) Faults occurring in consumable parts or parts dependent on them Note: Recording media, such as floppy disks and CD-ROMs, are also regarded as consumable parts.

* If a warranty certificate or a similar form of document is provided with the product, or if a contract specifying warranty terms has been signed, then the regulations specified in such a document take precedence.

The warranty period for products with special specifications or for system products is specified separately.

About This Operation Guide

Notation

This operation guide uses the notation described below.

Notation	Meaning
	Indicates a potentially hazardous situation which, if not avoided, could result in serious injury or possibly death.
	Indicates a potentially hazardous situation which, if not avoided, may result in minor to moderate injury or equipment damage.
MOTE	Indicates additional information that is provided to ensure the proper use of this product.
Reference	Indicates the location of related information. "Items indicated by this notation mean that this (new) feature/function is downward compatible with version 2.5. The new features are designed to make the software easier to use and/or increase productivity. However, the user still has the option to either use the same method used in version 2.5 or use the new features by following the steps provided in this manual."
[]	Indicates items displayed on the screen, such as buttons, menu selections, settings, windows, and icons. Example: Click [OK].

Safety Precautions

These safety precautions contain important safety-related information. Be sure to read them before using the product and observe them during use.

- Making internal repairs to the product is potentially dangerous. Such repairs must be performed by specially trained Shimadzu personnel.
- Do not disassemble or modify the product without authorization. Doing so may compromise safety.
- Read the instruction manual thoroughly before handling or operating the equipment, and be sure to following the procedures described.
 Not handling the equipment as described is potentially dangerous.

Installation Site Precautions

WARNING

- The solvents used with the gas chromatograph mass spectrometer may be flammable or toxic. Install the product in a well-ventilated room.
 Otherwise, solvent vapors may cause poisoning, or ignite and cause a fire.
- Do not use this product in an environment containing combustible gases. Doing so may cause a fire.
- Do not place flammable materials near the column oven exhaust at the back of the gas chromatograph.
 Doing so may cause a fire.
- Install the product on a surface that is level, stable, and strong enough to support the product's weight.

Otherwise, the product may tip over or fall off the surface.

Do not install the product in locations subject to large amounts of corrosive gas or dust. Otherwise, performance may be adversely affected and the product's service life may be shortened.

High-Pressure Gas Precautions

WARNING

• High-pressure gas cylinders are used to supply the carrier gas. Follow the instructions received from the cylinder suppliers and handle the cylinders carefully.

Not doing so may cause poisoning or a fire.

- Keep the cylinders in a well-ventilated outdoor location that is not directly exposed to sunlight, and use pipes to convey the gas indoors. For liquefied gases, this is required by law.
- Ensure that the temperature of gas cylinders never exceeds 40 °C and that there are no naked flames within 2 m of the cylinders.
- Ensure that the installation site is well ventilated and, as part of the daily inspection procedure, check for gas leaks using soapy water. Do not smoke or use open flames within 5 m of equipment using highly combustible gases, such as acetylene, hydrogen, and propane, or potentially combustible gases, such as oxygen and nitrous oxide. Keep a suitable fire extinguisher nearby at all times.
- Secure the cylinders with ropes or by some other method to prevent them from falling over.
- Be sure to use oil-free pressure reducing valves. Also, do not use pipes in which oil is present on the inner surfaces that make contact with the gas.
- After using the gas, close the main valve immediately.
- · Check that the pressure gauges are functional at least once every three months.
- Warning signs (adhesive aluminum plates) that indicate hydrogen gas use are provided free of charge. Contact your Shimadzu representative in cases of particular necessity.

Legal authorization is required to use cylinders with a capacity of 300 m³ or greater. Refer to high-pressure gas control laws, liquid petroleum gas safety regulations, general high-pressure gas safety regulations, and fire safety laws for more information.

Operation Precautions

WARNING

- Wear safety glasses when handling solvents or when injecting samples into the gas chromatograph. If solvent gets into the eyes, it may cause blindness. If solvent does get into the eyes, immediately flush with large amounts of water and seek medical attention.
- Do not place solvents near PCs, printers, or other types of office equipment. Doing so may cause a fire or equipment failure.
- Do not use flammable sprays (e.g., hair sprays and insecticide sprays) near the product. They may ignite and cause a fire.

Handling Emergencies

Take the measures described below in the event of an emergency, such as a malfunction of the gas chromatograph mass spectrometer.

Before resuming operation, take appropriate precautions and, if necessary, contact your Shimadzu representative.

Emergency Shutdown Procedure

- 1 Turn OFF the gas chromatograph mass spectrometer.
- 2 Turn OFF all accessories.
- 3 Close the main valves for the pipes supplying carrier gas, hydrogen, and air.
- 4 Disconnect the power supply.
 - If the power cable is attached to a switchboard, turn OFF the switchboard.
 - ◆ If the power cable is plugged into an outlet, unplug the cable.

This page is intentionally left blank.

Contents

1 Overall Configuration of GCMSsolution

1.1	Programs	.1
1.2	Flowchart of Operating Procedure	.2

2 Starting GC/MS

2.1	Turning ON the Power	3
2.2	Layout of Operating Areas	4
2.3	Inspecting Consumable Items and Maintenance Parts	5
2.4	System Configuration2.4.1Setting the Modules Used for Analysis2.4.2Checking Column Information2.4.3Enabling the Modules Used for Analysis	6 7
2.5	Vacuum System Startup	10
2.6	Checking for Vacuum Leakage	11
2.7	Autotuning	13 14

3 Creating a Folder

	3.1	Creating a Folder with Data Explorer	1	8
--	-----	--------------------------------------	---	---

4 Qualitative Analysis

4.1	Creating a	a Method File	20
		Setting Autosampler Parameters	
	4.1.2	Setting GC Parameters	21
	4.1.3	Setting MS Parameters	22
	4.1.4	Setting Similarity Search Parameters	23
	4.1.5	Saving the Method File	25

Contents

Repeating	g Autotuning	25
Sequentia	al Analysis	26
4.3.1	Creating a Batch File	26
4.3.2	Editing a Batch File 🅼 Ver. 2.5	29
4.3.3	Saving Batch Files	32
4.3.4	Executing Sequential Analysis	33
Analyzing	g Data	34
4.4.1	Loading Data Files	34
4.4.2	Zoom in on a Peak in the Chromatogram and Displaying Mass Spectra	35
4.4.3	Removing the Background	37
4.4.4	Searching for Similarity 🎼 Ver. 2.5	38
4.4.5	Displaying Mass Chromatograms	39
4.4.6	Registering Spectra Displayed for Target Compounds	
	<i>I G P</i> Ver. 2.5	40
4.4.7	Editing the Spectrum Process Table	40
4.4.8	Saving Data Files	42
Printing C	Qualitative Analysis Reports	43
4.5.1	Loading Report Formats	43
4.5.2	Editing Report Formats	44
4.5.3	Outputting Reports	47
	Sequentia 4.3.1 4.3.2 4.3.3 4.3.4 Analyzing 4.4.1 4.4.2 4.4.3 4.4.3 4.4.4 4.4.5 4.4.6 4.4.7 4.4.8 Printing O 4.5.1 4.5.2	 4.3.2 Editing a Batch File Ver. 2.5

5 Quantitative Analysis

5.1	Creating a	Method File	
	5.1.1 (Creating a Compound Table	
	5.1.2 (Creating a SIM Table	53
5.2	Sequential	Analysis	
		Creating a Batch File	
	5.2.2	Editing a Batch File 🎜 Ver. 2.5	58
		Saving Batch Files	
	5.2.4	Executing Sequential Analysis	59
5.3	Analyzing [Data	60
	5.3.1 (Checking and Correcting Calibration Curves	60
	5.3.2	Re-quantifying after Correcting a Calibration Curve	67
	5.3.3 (Checking and Correcting Quantitation Results	69
5.4	Printing Qu	antitative Analysis Reports	73
	-	Creating and Outputting Quantitative Analysis Reports	

6 Shutting Down GC/MS

6.1	Vacuum System Shutdown7	6
6.2	Turning OFF the Power7	7

Appendix A File Format

Appendix B Viewing Help

B.1	Viewing H	lelp	.79
	B.1.1	Displaying Help from the Assistant Bar	.79
	B.1.2	Displaying Help from the Menu Bar	.79
	B.1.3	Displaying Help with the F1 Key	. 80

Appendix C Using Data Explorer

Appendix D Maintenance

Maintenance	.83
Easy sTop (Applicable to QP2010 Ultra and QP2010 SE models)	.85
Reset Procedure for Usage Frequencies and Usage Times	.87
Changing Replacement Guidelines for septa and Glass Inserts	.89
	Easy sTop (Applicable to QP2010 Ultra and QP2010 SE models) Reset Procedure for Usage Frequencies and Usage Times I Ver.2.5

Appendix E Single Analysis (Manual Injection)

Appendix F Index Searches

Appendix G Displaying Chromatograms

G.1	Displaying Chromatograms from Fragment Tables	.96
G.2	Displaying Chromatograms from Mass Spectra	.98

Contents

Appendix H Editing and Adding Batch Files During Sequential Analysis

H.1	Editing Batch Files	
H.2	Adding Batch Files (Batch Queue)	
	H.2.1 Creating Batch Files to Add	
	H.2.2 Adding Batch Files	

Appendix I Reducing the Carrier Gas Flow Rate After Sequential Analysis and Using the Ecology Mode

I.1	Reducing	the Carrier Gas Flow Rate After Sequential Analysis	105
	I.1.1	Creating a Method File That Reduces the Carrier Gas Flow Rate	105
	I.1.2	Creating Batch Files	
I.2	Ecology I	Mode	
	(This feat	ture applies to QP2010 Ultra and QP2010 SE models.)	109
	I.2.1	Setting the Mode Manually	109
	1.2.2	Setting the Mode Using Batch Processing	

Appendix J Printing Reports

J.1	Printing Ir (Printing \$	mages Spectra and Chromatograms Displayed in Windows)	112
J.2	Creating	Reports	
	J.2.1	Using Templates	
	J.2.2	Using Previously Created Report Files	
	J.2.3	Manually Setting Report Content	

Overall Configuration of GCMSsolution

1.1 Programs

GCMSsolution is made up of the programs described below.

Select the program that is appropriate for the purpose (e.g., analysis or data processing).

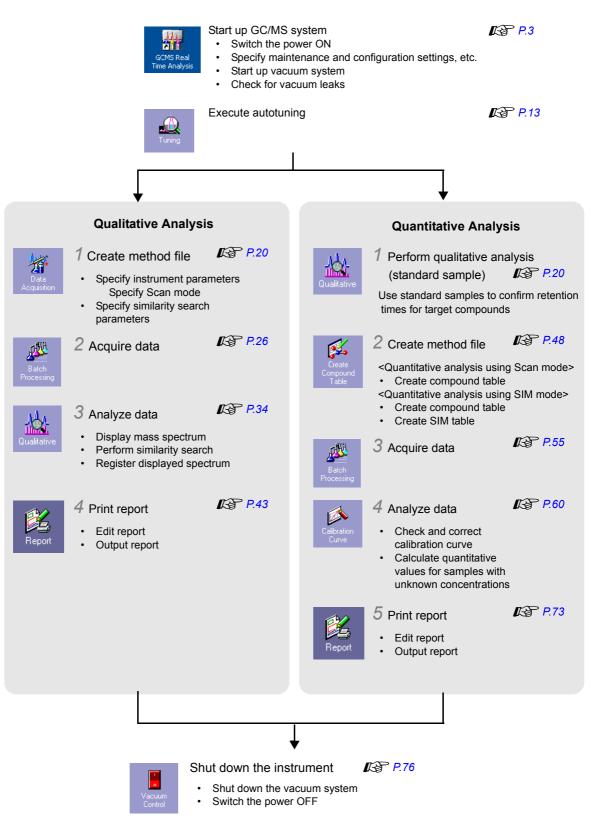
Icon	Name	Description
GCMS Real Time Analysis	GCMS Real Time Analysis	Used to start up and shut down the instrument, make configuration settings, and perform analysis.
GCMS Analysis Editor	GCMS Analysis Editor	Used to create and edit method files and batch files during analysis.
GCMS Postrun Analysis	GCMS Postrun Analysis	Used to perform qualitative and quantitative processing, print reports, and perform other tasks involving data processing.
GCMS Browser	GCMS Browser	Used to perform qualitative and quantitative processing, print reports, and perform other data processing tasks for multiple data files.

K Ver. 2.5

This manual describes operating instructions primarily for new features added in GCMSsolution Version 2.6. However, items indicated with "

Icons and windows for functions that can only be used on QP2010 Ultra or QP2010 SE model will not be displayed on the software if the GCMS model used is QP2010, QP2010 Plus or QP2010S.

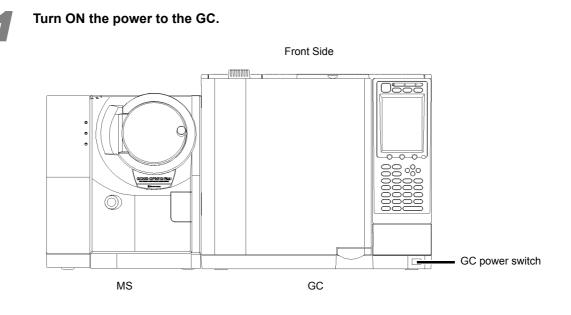
1.2 Flowchart of Operating Procedure





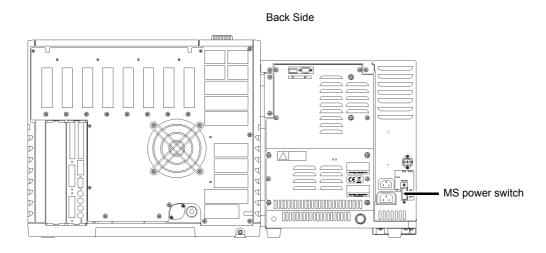
2.1 Turning ON the Power

Switch ON any peripheral or accessory equipment connected to the system, before switching ON the main GC/MS system.





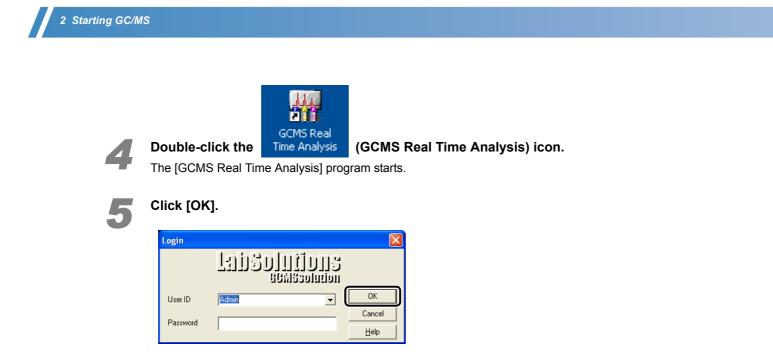
Turn ON the power to the MS.



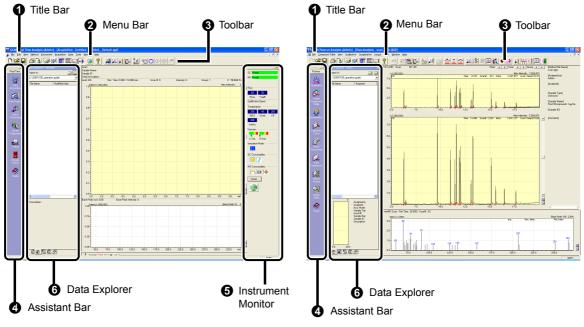


Turn ON the power to the PC, printer, and display.

2



2.2 Layout of Operating Areas



GCMS Real Time Analysis

GCMS Postrun Analysis

No.	Name	GCMS Program	Explanation
0	Title Bar	Real Time Analysis, Analysis Editor, Postrun Analysis, and Browser	Displays the name of the program, process, and file currently running or being processed.
0	Menu Bar	Real Time Analysis, Analysis Editor, Postrun Analysis, and Browser	Displays command menus corresponding to the window currently open.
8	Toolbar	Real Time Analysis, Analysis Editor, Postrun Analysis, and Browser	Displays command tool buttons corresponding to the window currently open.

2.3 Inspecting Consumable Items and Maintenance Parts

No.	Name	GCMS Program	Explanation
0	Assistant Bar	Real Time Analysis, Analysis Editor, Postrun Analysis, and Browser	Command icons are arranged in order of typical operation sequence. The assistant bar is named according to the window that is currently open. For example, when the [Batch] window is open, the assistant bar is named the [Batch] assistant bar.
6	Instrument Monitor	Real Time Analysis	Displays analytical instrument parameter values in real time.
6	Data Explorer	Real Time Analysis, Analysis Editor, Postrun Analysis, and Browser	Used to easily load analytical data or method files. It lists files in the selected folder, according to file type.

The assistant bar, instrument monitor, and Data Explorer can be shown or hidden by selecting [Show/Hide] on the [View] menu.

2.3 Inspecting Consumable Items and Maintenance Parts

Check the state of the GC/MS consumable items using the procedure described below.



Move the mouse pointer over the icon for a consumable item in the instrument monitor to display the current state and the recommended replacement point for the corresponding item.

When a consumable item approaches its recommended maximum usage frequency, the background of the corresponding icon turns black to alert the user.



This note is shown when mouse pointer is moved over the septum icon. This means that the septum has been used 13 times out of a maximum 100 times.

When replacing the analysis column, or when a consumable item has passed its recommended replacement point, perform maintenance with reference to *"Appendix D Maintenance" P.83*.

Depending on the analysis content, the appropriate replacement frequency may be greater than the recommended frequency.

2.4 System Configuration

Check and set the modules used for analysis using the procedures described below.

2.4.1 Setting the Modules Used for Analysis



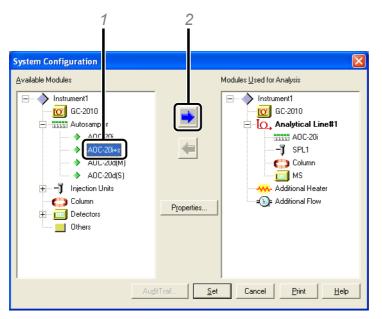
Click the [System Configuration] icon on the [Real Time] assistant bar.

The [System Configuration] window opens.





Check that the components shown in the [Modules Used for Analysis] area correspond to the actual modules in the GC/MS system that are to be used for the analysis.



If the modules to be used for current analysis do not correspond to the modules shown in this window, set as shown in the following example:

- 1 Select [AOC-20i+s] in the [Available Modules] area if for example, AOC-20i with AOC-20s are to be used for analysis.
- 2 Click it register the module in [Modules Used for Analysis].

2.4.2 Checking Column Information

Information for the column attached to the instrument must be specified correctly. Check or change the column information settings after installing a column.

Double-click the (Column) icon in [Modules Used for Analysis]. The [Modules of Analytical Line#] window opens.

System Configuration		
Available Modules Instrument1 GC 2010 Trim Autosampler Column Column Decorators		Modules Used for Analysis
	P <u>r</u> operties	Additional Heater

If the column to be used is not displayed under [Selected Column] area:

1 Click the name of the column to be used in the [Registered Columns] table.

dules of Analytical Line	¥1			
AOC-20i SPL1 Column M	5			
Please input the column informa	tion on the [Re	egistered Columns] tab	ole, and click th	ne [Select] button.
Selected Column Name : Rtx-624 Serial # : 657772 Length : 60 m Max. Usable Temp. : 24 Registered Columns	0 °C	Thickness : 1.8 Diameter : 0.3; Installation Date :	2 mm	3
Column Name	Serial #	Thickness (um)	Length (m)	Diameter (mr
1	657772	1.8	60	0.
Rtx-5MS	904661	0.25	30	0.

2 Click [Select].

The column information is displayed under [Selected Column].

SPL1 Column M					
	5				
put the column inform	ation on the [Re	egistered Columns] tab	ole, and click th	ne [Select] button	
: Rtx-5MS #: 904661 h: 30 m Usable Temp. : 35	i0 °C	Diameter : 0.2	5 mm	19	
Column Name	Serial #	Thickness (um)	Length (m)	Diameter (mr	
Rtx-624	657772	1.8	60	0.	
Rtx-5MS	904661	0.25	30	0.	
		Select	Add	> Delete	
	ed Column :: Rtx-5MS #: 904661 h: 30 m Usable Temp.: 35 sred Columns	ed Column :: Rtx-5MS #: 904661 h: 30 m Usable Temp.: 350 °C ered Columns Column Hame Serial # Rtx-624 657772 Rtx-5MS 904661	ad Column :: Rtx-5MS #: 904661 Thickness: 0.21 h: 30 m Diameter: 0.22 Usable Temp.: 350 °C Installation Date : ared Columns Column Name Serial # Thickness (um) Rtx-624 657772 1.8 Rtx-5MS 904661 0.25	ed Column :: Rtx-5MS #: 904661 Thickness: 0.25 um h: 30 m Diameter: 0.25 mm Usable Temp.: 350 °C Installation Date: 5/11/200 ared Columns Column Name Serial # Thickness (um) Length (m) Rtx-624 657772 1.8 60 Rtx-5MS 904661 0.25 30	:: Rtx-5MS #: 904661 Thickness: 0.25 um h: 30 m Diameter: 0.25 mm Usable Temp.: 350 °C Installation Date: 5/11/2009 ered Columns Column Name Serial # Thickness (um) Length (m) Diameter (mr Rtx-624 657772 1.8 60 0. Rtx-5MS 904661 0.25 30 0

If the column to be used is not registered:

- 1 Click [Add].
 - A row is added.

dules of Analytical Lin	e#1				(
OC-20i SPL1 Column N	IS				
Please input the column inform	ation on the [Re	gistered Columns] tal	ole, and click th	ne [Select] button.	
Selected Column					
Name : Rtx-5MS					
Serial # : 904661		Thickness : 0.2	5 um		
Length: 30 m		Diameter : 0.2	5 mm		
Max. Usable Temp. : 3	50 °C	Installation Date :	5/11/200)9	
Registered Columns					
Column Name	Serial #	Thickness (um)	Length (m)	Diameter (mr	
1 Rtx-624	657772	1.8	60	0.	
2 Rtx-5MS	904661	0.25	30	0.	
		0	0		
<				>	
				/	
			·		

2 Enter the column information.

Column information is usually indicated on the packaging box of the column, on the column tag, or in the column specification sheet that is usually included inside the column box.

lules	of Anal	ytical Lir	1e#1			
0C-20i	SPL1	Column	MS			
Please i	input the d	column infor	mation on the [R	Registered Columns] t	able, and click t	he [Select] button.
	ted Colum					
Nam	ne: al#:	Rtx-5MS		Thickness: 0.	DE	
Leng	gth :	30 m	l	Diameter : 0.1	25 mm	
	. Usable T	•	350 °C	Installation Date :	5/11/20	09
	tered Colu	•		Installation Date :		
<u>R</u> egis	tered Colu	umns umn Name			Length (m)	
	tered Colu	umns umn Name 4	Serial #	Thickness (um)	Length (m)	Diameter (mr
	tered Colu Colu 1 Rtx-624	umns umn Name 4 S	Serial # 657772	Thickness (um)	Length (m)	Diameter (mr
	tered Colu Colu 1 Rtx-624	umns umn Name 4 S	Serial # 657772	Thickness (um)	Length (m)	Diameter (mr
	tered Colu Colu 1 Rtx-624	umns umn Name 4 S	Serial # 657772	Thickness (um)	Length (m)	Diameter (mr

The maximum temperature that can be specified for the column oven, interface, and sample injection unit is normally the [Max. Usable Temp] setting entered here. For the protection of columns, always enter a [Max. Usable Temp] setting.



Click [OK].

The [System Configuration] window returns.

Modules of Analytical Line#	#1				
ADC-20i SPL1 Column MS					
Please input the column informa	tion on the [Re	egistered Columns] tal	ole, and click th	ne [Select] ł	outton.
- Selected Column					
Name: Rtx-5MS					
Serial # : 904661		Thickness : 0.2	5 um		
Length: 30 m		Diameter: 0.2			
) °C	Installation Date :	5/11/200)9	
<u>R</u> egistered Columns					
Column Name	Serial #	Thickness (um)		Diameter	(mr
1 Rtx-624 2 Rtx-5MS	657772 904661	1.8 0.25	60 30		0.
2 144-0410	004001	0.20			
					>
Description :		Select	Add	<u>D</u> elete	:
Des <u>c</u> iption.					
					~
<				>	
				1	
		0	к (Cancel	Help

2.4.3 Enabling the Modules Used for Analysis



Click [Set].

The system configuration information is transferred to the instrument.

System Configuration		
System Configuration ▲vailable Modules Instrument1 GC-2010	→→	Modules Used for Analysis Instrument1 GC-2010 Analytical Line#1 SPL1 Column MS Additional Heater Additional Flow
Aud	Properties	Cancel <u>Print</u> <u>H</u> elp

2.5 Vacuum System Startup

Open the carrier gas cylinder valve to supply carrier gas.

If carrier gas is being controlled by accessory/peripheral equipment, use that equipment to supply carrier gas before starting the vacuum system.



Click the [Vacuum Control] icon on the [Real Time] assistant bar.

The [Vacuum Control] window opens.





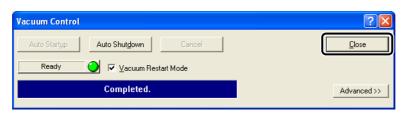
Click [Auto Startup].

The vacuum system starts.

Vacuum Control	? 🛛
Auto Startup Auto Shutdown Cancel	Close
Not Ready 🛛 🔽 Vacuum Restart Mode	
	Advanced >>



When [Completed] is displayed, click [Close].



2.6 Checking for Vacuum Leakage

Wait for 10 minutes after starting up the vacuum system.



Click the [Tuning] icon on the [Real Time] assistant bar.

The [Tuning] window opens.

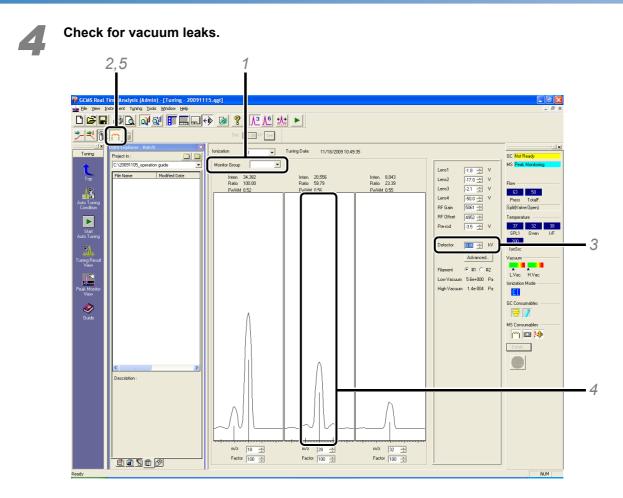




Click the [Peak Monitor View] icon on the [Tuning] assistant bar. The [Peak Monitor] window opens.







- 1 Click the arrow button in [Monitor Group] setting, and select [Water, Air] from the list.
- 2 Click (Filament ON/OFF) to turn ON the filament. Peaks will be displayed in the three windows.
- 3 Change the detector voltage gradually by clicking the up or down arrow buttons so that the peak height for m/z 18 (water) corresponds to half the height of the display window.
- Compare the peak heights for *m*/*z* 18 (water) and *m*/*z* 28 (nitrogen).
 Check that the peak height for *m*/*z* 28 (nitrogen) is not more than twice that for *m*/*z* 18 (water).

If the peak height for m/z 28 (nitrogen) is more than twice that for m/z 18 (water), it is possible that there is an air leak. Search for the location of the leak.

Reference

Refer to the System User's Guide for details on how to check for vacuum leaks.





Close the [Tuning] window.

The message [Save current tuning file?] is displayed. Click [No].

GCMS Re	eal Time Analysis		×
2	[0311] Save current ⁻ C:\GCMSsolution\Syst	-	t.qgt
<u>Y</u> e:	s <u>N</u> o	Cancel	Help

2.7 Autotuning

Wait for approximately 2 hours (before starting qualitative analysis) or 4 hours (before starting quantitative analysis) after starting up the vacuum system and then perform autotuning using the procedures described below.

2.7.1 Setting Analysis Conditions

If no analysis conditions have been created, start from "2.7.2 Executing Autotuning" P.14.

If a method file is already created, parameters can be specified in the instrument according to the following procedure.

However, parameters for an accessory or peripheral equipment, except for AOC-20 auto-injector/autosampler, cannot be specified by using the following procedure. When using an accessory/peripheral equipment, set the parameters on the equipment itself, or by using the software specific to that equipment/ device.



Click the [Data Acquisition] icon on the [Real Time] assistant bar.

The [Acquisition] window opens.





Click 🖻 (Open) on the toolbar.



2 Starting GC/MS



Select the method file to load, then click [Open].

The method file is loaded.

Open Metho	d File		? 🗙
Look jn: 隘	20091105_operation guide	• + 1	-11 📩
PAH_Scan			
File <u>n</u> ame:	PAH_Scan		<u>O</u> pen
Files of <u>type</u> :	GCMS Method File (*.qgm)	•	Cancel



Select [Download Initial Parameters] on the [Acquisition] menu.

dmin) -	Method - [Acq	uisitia	on - PAH	_Sc		
ment Ac	quisition Data	Tools	Window	Hel	GC Read	dy
ᇓᄛ	Plot			9	MS Rea	dy
<mark>الا</mark> آن	Sample Login			_{	Flow —	
etho	Download		a	me :	100	15
	Start		- 1	:	Press	TotalF.
ration	Extend		C	riptio	Split(Valv	/e:Open)
	Stop			n(×1		
	Download Initial I	Parame		1421		

If the message "The hardware configuration for this method is different from the current instrument configuration. The measurement condition in the method file is modified according to the current instrument configuration." appears, click [OK].

2.7.2 Executing Autotuning



Click the [Tuning] icon on the [Real Time] assistant bar.

The [Tuning] window opens.





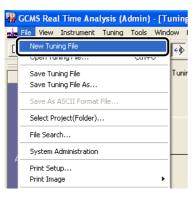
Click the [Peak Monitor View] icon on the [Tuning] assistant bar.

The [Peak Monitor] window opens.





Select [New Tuning File] on the [File] menu.





Select Tuning Mode appropriate for the application. (This feature applies to QP2010 Ultra and QP2010 SE models.)

When creating a new tuning file, choose the tuning mode appropriate for the concentration level of target compounds being measured. Since the tuning file is created with an emission current corresponding to the selected mode, it enables measuring samples with an appropriate dynamic range.

- QP2010 Ultra:High concentration (20 μA), standard (60 μA, default), or high sensitivity (150 μA)
- QP2010 SE:High concentration (20 μA) or standard (60 μA, default)





Select the filament to be used.

Detector	1.00 ÷ kV
	Advanced
Filament	⊙ #1 ⊙ #2
Low Vacuum	5.6e+000 Pa
High Vacuum	1.6e-004 Pa

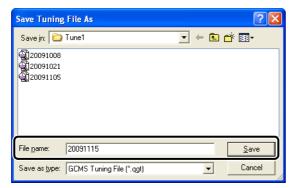
2 Starting GC/MS 6 Click the [Start Auto Tuning] icon on the [Tuning] assistant bar. If the formation of t



0

Enter a file name and click [Save] to start autotuning.

When autotuning is completed, a report is printed.





Close the [Tuning] window.

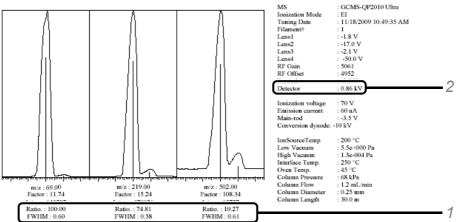
The message [Save current tuning file?] is displayed. Click [Yes].

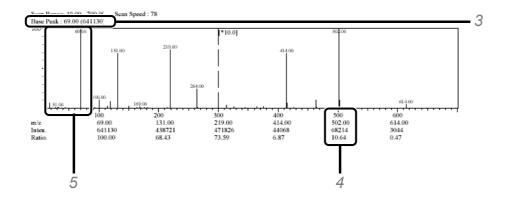
2.7.3 Checking Autotuning Results

C:\GCMSsolution\System\Tune1\20091115.qg

Check the results of autotuning.

Controlation and the rest for the rest





- 1 Check that the FWHM (full width at half maximum) values are in the range 0.5 to 0.7.
- 2 Check that the detector voltage does not exceed 2 kV.
- 3 Check that the base peak values are 18 or 69.
- 4 Check that the relative intensity ratio for m/z 502 is at least 2 % (for QP2010S and SE : 1 %).
- 5 Check that the peak intensity for m/z 69 is at least twice that for m/z 28.

If any irregularities are discovered above, possible causes could include a vacuum leak, poor column connections, or contaminated ion source.

See "Appendix D Maintenance" P.83 to implement corrective measures.

Creating a Folder

3.1 Creating a Folder with Data Explorer



Click the [Data Acquisition] icon on the [Real Time] assistant bar.

The [Acquisition] window opens.





Click 💐 (Data Explorer) on the toolbar to display Data Explorer.





Click [] (Project (Folder) Selection).

The [Project (Folder) Selection] window opens.

Data Explorer - Me	ethod 🛛 🔀
Project in :	
C:\20091105_oper	ation guide
File Name	Modified Date
PAH_Scan	11/12/2009 1:43 PM



Click the GCMSsolution folder in the C drive in Data Explorer and click [New Folder]. The [Create New Folder] window opens.

Project(Folder) Selection	
Look in : C:\GCMSsolution	 Close
	New Folder

Type a folder name and click [OK].

A folder is created in the GCMSsolution folder in the C drive and the [Project (Folder) Selection] window returns.

Create New Folder
Create New Folder under the
C:\GCMSsolution
Please input new folder name
20091115_operation guide
OK Cancel <u>H</u> elp



Click [Close].

To select an existing folder, see "Appendix C Using Data Explorer" P.81.

4 Qualitative Analysis

4.1 Creating a Method File

Set the instrument (i.e., autosampler, GC, MS) parameters and similarity search parameters using the procedure described below.

Use default values for parameters that are not covered by the following explanations.



Click the [Data Acquisition] icon on the [Real Time] assistant bar.

The [Acquisition] window opens.





Select [New Method File] on the [File] menu.

-	GCMS Real Time Analysis (Admin)	- [Ac
	File Edit View Method Instrument	Acquis
C	New Method File	
	Close Method File	
	Save Method File Save Method File As	
	Save Method As Template	et. T
	Load Method Parameters	
	Open Reference Data File Close Reference Data File	
	Select Project(Folder)	

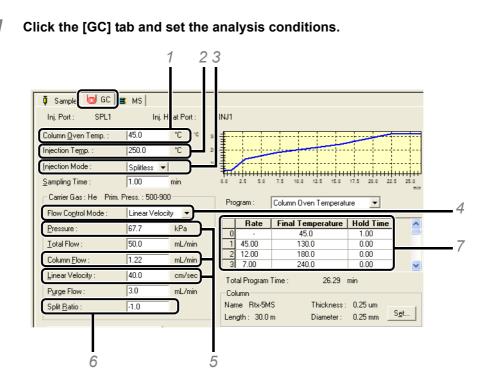
4.1.1 Setting Autosampler Parameters

1

ck the [Sampler] tab	and spec	cifv the	numbe	er of rin
🏮 Sampler 🔂 GC 🗃 MS				
A0C-20i				
# of <u>R</u> inses with Solvent (Pre-run) :	1]		
# of Rinses with Solvent (Post-run) :	3	,		
# of Rinses with <u>S</u> ample :	1	1 I		
Plunger Speed(Suction) :	High	O Middle	C Low	
⊻iscosity Comp. Time :	0.2	sec		
Plunger Speed(Injection) :	High	Middle	C Low	
Syringe Insertion Speed :	🖲 High	C Low		
Injection Mode :	0: Normal			S <u>e</u> t

4.1.2 Setting GC Parameters

Advanced...



- 1 Input an initial temperature for the column oven (40 to 100 °C).
- 2 Input an injection temperature based on consideration of the boiling point of the target compound (200 to 300 °C).
- 3 Select [Split] or [Splitless].



Selecting Injection Mode

- Split: Select this mode if the concentration of the target compound is high. As a rough guideline, select this mode when the target compound concentration is greater than 10 ng/uL.
- Splitless: Select this mode if the concentration of the target compound is low. As a rough guideline, select this mode when the target compound concentration is less than 10 ng/uL.
- 4 Select [Pressure] when the method calls for a constant pressure mode, and select [Linear Velocity] when the method calls for a constant linear velocity mode for the carrier gas. When no reference method is available, select [Linear Velocity].
- 5 When no reference method is available, refer to the table "Typical Pressure Settings for Carrier Gas" to set an initial value for the pressure. The linear velocity will be set automatically.

Typical Procedure Collarige for Califor Cal	
Middle bore capillary column	Semi-

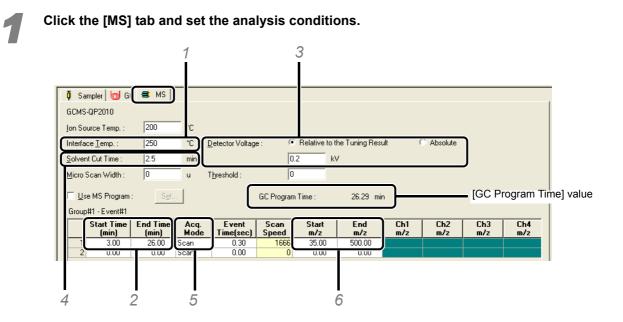
Typical Pressure Settings for Carrier Gas

Middle bore capillary column (I.D. 0.25 mm)		Semi-wide bore capillary column (I.D. 0.32 mm)	
30 m	60 m	30 m	60 m
75 to 150 kPa	100 to 250 kPa	30 to 50 kPa	50 to 100 kPa

6 If "Split" is selected as the injection mode, enter a split ratio. If "Splitless" is selected, enter "-1.0".

7 Set appropriate conditions for separating the target compound from other peaks.

4.1.3 Setting MS Parameters



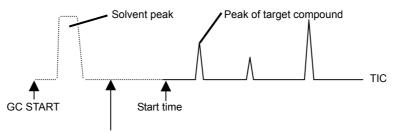
1 Input [Interface Temp.] (200 to 300 °C).

2 Input [Start Time] and [End Time] according to the note below.

In the absence of information about the elution time of the solvent peak, set [Start Time] to zero minutes, and set [End Time] to the [GC Program Time] value. After one analysis of a standard sample or the solvent, and obtaining the solvent peak profile, change the [Start Time] to a time after the end of the solvent peak (see the figure shown on page 23).

- 3 Click [Relative to the Tuning Result].
 - If peak intensity is too low, change the value within the range +0.1 to +0.3., as necessary.
- 4 Input a value that is 0.5 minutes less than the [Start Time] setting. (If the resulting value is less than zero, enter "0".)

Relationship between Start Time and Solvent Elution Time



Solvent elution time (Detector ON)

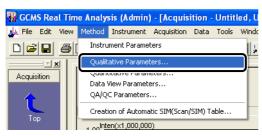
- 5 Select [Scan].
- 6 Enter the mass range to be measured, where [Start m/z] is the lower mass limit, and [End m/z] is the upper mass limit. The typical value for [Start m/z] is 35, and the typical value of [End m/z] is the highest molecular weight of the target compounds in the sample plus some margin of error (+15).

4.1.4 Setting Similarity Search Parameters



Select [Qualitative Parameters] on the [Method] menu.

The [Qualitative Parameters] window opens.





2

Click the [Similarity Search] tab and set the search conditions.

Qualitative Parameters	
Peak Integration Spectrum Proces: Similarity Search	Retention Index Column Performance
Library File Name: Min.9	
C:\GCMSsolution\Library\NIST08.LIB	1
C:\GCMSsolution\Library\NIST08s.LIB 0	Max.Hit#: 25
0	✓ Do not include duplicate hits
0	Reverse Search Ret. Index Allowance
0	- 10 + 10
Post-search: 🦵 Match <u>C</u> ase	,,
Index	Parameter
1 No Setting	
	>
	OK Cancel Help
2	4

The [Open File] window opens.

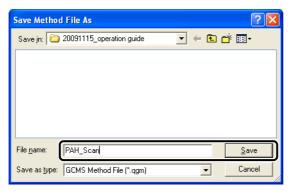
Open				? 🛛
Look in: 隘	Library	•	+ 🗈 🖻	* 📰 •
NIST08				
File <u>n</u> ame:	NIST08			<u>O</u> pen
Files of <u>type</u> :	LibraryFile (*.LIB)		•	Cancel

Open the library to be used.

- 2 To remove a library from the selection, highlight the library file name by dragging the mouse over it, then press the [Delete] key.
- 3 Select [Do not include duplicate hits].
- 4 After completing the settings, click [OK] to return to the original window.

4.1.5 Saving the Method File

	🎇 GCMS Real Time Analysis (Admin) - [Ac	
	ile Edit View Method Instrument Acqui: المالي File	
	New Method File Open Method File Ctrl+O Close Method File Save Method File Save Method File As Save Method As Template et	
2	Enter a file name and click [Save].	



4.2 Repeating Autotuning

If autotuning has not been performed under the analysis conditions, perform the procedures described under "2.7 Autotuning" P.13.

4.3 Sequential Analysis

Create a batch file necessary for qualitative analysis and perform sequential analysis using the procedures described below.

4.3.1 Creating a Batch File

To use an existing batch file, follow the procedure starting in "4.3.2 Editing a Batch File [Ver. 2.5" P.29.



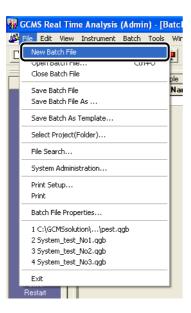
Click the [Batch Processing] icon on the [Real Time] assistant bar.

The [Batch Table] window opens.





Select [New Batch File] on the [File] menu.





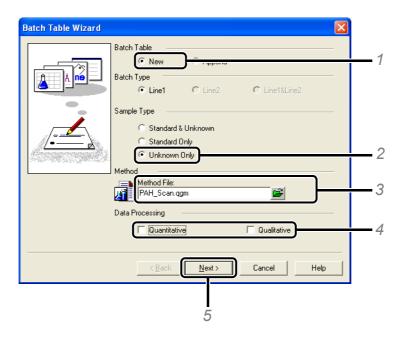
Click the [Wizard] icon on the [Batch] assistant bar.

The [Batch Table Wizard] window opens.





With the Batch Table Wizard, make the appropriate settings and create a batch table.



1 Click [New].

- 2 Click [Unknown Only].
- 3 Click 🔎 and specify the method file to be used.
- 4 Deselect both [Data Processing] items.
- 5 Click [Next].

Batch Table Wizard - Line1 Unknown Sample (1)	
Unknown Sample Vial #: 1: 1: 1: Sample Count: 10: Injection Volume: 1 uL Sample Name: Unknown Sample Auto-increment Sample ID: UNK-0001 VAuto-increment	6 7
6 Input [Vial #] and [Sample Count]. 7 Input [Injection Volume].	
8 Click [Next]. Batch Table Wizard - Line1 Unknown Sample (2) Data Create Filenames Automatically Data File Name: Sample01 Mato-increment Report Format File: Data Description	9
< Back Finish Cancel Help	

9 Enter [Data File Name]. If the file name ends with a number, the files are named sequentially.

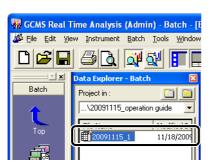
10

10 Click [Finish]. The batch table is displayed.

4.3.2 Editing a Batch File

For routine analyses, it may be more convenient to partially edit and execute existing batch files. The following procedures describe how to edit information in specified row(s) collectively.

Double-click the batch file to be edited.





Add or delete rows depending on the number of samples being analyzed.

Folder: C:\GCMSsolution\20091115_operation guide								
	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	
1	1	Methylene Chloride		0:Unknown	IT QT	PAH_SIM.qgm	20091115_blank.qgd	
2	2	PAH 0.005ppm	STD-0001	1:Standard:(I)	ITQT	PAH_SIM.qgm	20091115_STD1.qgd	
3	3	PAH 0.01ppm	STD-0002	1:Standard	IT QT	PAH_SIM.qgm	20091115_STD2.qgd	
4	4	PAH 0.05ppm	STD-0003	1:Standard	IT QT	PAH_SIM.qgm	20091115_STD3.qgd	
5	5	PAH 0.1ppm	STD-0004	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD4.qgd	
6	1	Blank	UNK-0001	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample01.qgd	
7	6	river water 1	UNK-0002	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample02.ggd	
8	7	river water 2	UNK-0003	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample03.ggd	

1 Click on the row number to be edited to highlight the whole row. Multiple rows can be selected by dragging the mouse over multiple row numbers.

Folder: C	Folder: C:\GCMSsolution\20091115_operation guide						
	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File
1	1	Methylene Chloride		0:Unknown	ITQT	PAH_SIM.qgm	20091115_blank.qgd
2	2	PAH 0.005ppm	STD-0001	1:Standard:(I)	ITQT	PAH_SIM.qgm	20091115_STD1.qgd
3	3	PAH 0.01ppm	STD-0002	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD2.qgd
4	4	PAH 0.05ppm	STD-0003	1:Standard	IT QT	PAH_SIM.qgm	20091115_STD3.qgd
5	5	PAH 0.1ppm	STD-0004	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD4.qgd
6	1	Blank	UNK-0001	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample01.qgd
7	6	river water 1	UNK-0002	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample02.qgd
8	57	river water 2	UNK-0003	0:Unknown	IT QT	PAH <u>SIM.qqm</u>	20091115 sample03.gqd

2 Right-click on the selected row, and select the appropriate editing command from the menu that is displayed.

Copy Row
Add Row
Insert Row
Paste Row
Delete Row

Menus	Explanation			
Copy Row	Copies the selected row.			
Add Row	Adds a row to the end.			
Insert Row	Inserts a new row above the selected row.			
Paste Row	Pastes the copied row.			
Delete Row	Deletes the selected row.			

In addition, rows can be added easily by repeatedly entering "1" as the vial number and pressing the down arrow key on the keyboard.

¹

The following steps can be performed to quickly copy the contents of one row onto several rows, or to fill in the contents of several rows quickly. Serial numbers will be added to the end of the sample name and data file name, for examples, in the edited rows.

3

Edit the vial number, sample name and data file name in an existing row, which is to be the first of several rows to be edited.

Folder: C:\GCMSsolution\20091115_operation guide							
	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File
1	1	Methylene Chloride		0:Unknown	ITQT	PAH_SIM.qgm	20091115_blank.qgd
2	2	PAH 0.005ppm	STD-0001	1:Standard:(I)	ITQT	PAH_SIM.qgm	20091115_STD1.qgd
3	3	PAH 0.01ppm	STD-0002	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD2.qgd
4	4	PAH 0.05ppm	STD-0003	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD3.qgd
5	5	PAH 0.1ppm	STD-0004	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD4.qgd
6	1	Blank	UNK-0001	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample01.qgd
7	6	river water 1	UNK-0002	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample02.qgd
8	7	river water 2	UNK-0003	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample03.qgd
9	1			0:Unknown	ITQT		

- 1 Directly enter the vial number and sample name. Add a number at the end of sample name.
- 2 To set the data file name, click within the cell, then click the arrow buttons that appear. The [Select Data File] window opens.

Directly enter the data file name in the [Select Data File] window, then click [Open].

Select Data File	? 🛛
Look jn: 🛅 20091115_operation guide 💽 🗲	🗈 💣 🎟 -
File name: 20091115_sample01.qgd	<u>O</u> pen
Files of type: GCMS Data File (*.qgd)	Cancel

MOTE

It is not necessary to type file extensions when entering data file names.

3 To set the method file, click within the cell, then click the arrow buttons that appear. The [Select Method File] window opens. Select the method file to use.

Select Meth	od File 🔹 💽 🔀
Look jn: ଢ	20091115_operation guide 💽 👉 🛅 🖝
PAH_Scan	
PAH_SIM	
M VOCSIM	
File <u>n</u> ame:	PAH_Scan.qgm
Files of type:	GCMS Method File (*.ggm)
The of gpc.	



Drag the mouse from the edited row to the row specified with serial numbers.

Folder: C:	older: C:\GCMSsolution\20091115_operation guide							
	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	
1	1	Methylene Chloride		0:Unknown	ITQT	PAH_SIM.qgm	20091115_blank.qgd	
2	2	PAH 0.005ppm	STD-0001	1:Standard:(I)	ITQT	PAH_SIM.qgm	20091115_STD1.qgd	
3	3	PAH 0.01ppm	STD-0002	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD2.qgd	
4	4	PAH 0.05ppm	STD-0003	1:Standard	IT QT	PAH_SIM.qgm	20091115_STD3.qgd	
5	5	PAH 0.1ppm	STD-0004	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD4.qgd	
6	1	Blank	UNK-0001	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample01.qgd	
7	6	river water 1	UNK-0002	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample02.ggd	
8	7	river water 2	UNK-0003	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample03.ggd	
9	1			0:Unknown	IT QT			
10	1			0:Unknown	IT QT			
11	1			0:Unknown	IT QT			
12	1			0:Unknown	IT QT			
13	1			0:Unknown	ΤΩΤΙ			

To collectively edit specified cells, without changing other settings, drag the mouse across the cells to edit and perform the operation described in step 6.

For example, this can be used to edit the vial numbers and data file names for standard samples used to create calibration curves (for quantitative analysis).

Folder: C:\GCMSsolution\20091115_operation guide								
	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File		
1	Methylene Chloride		0:Unknown	ITQT	PAH_SIM.qgm	20091115_blank.qgd		
2	PAH 0.005ppm	STD-0001	1:Standard:(I)	ITQT	PAH_SIM.qgm	20091115 STD1.gqd 🗣		
3	PAH 0.01ppm	STD-0002	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD2.qgd		
4	PAH 0.05ppm	STD-0003	1:Standard	IT QT	PAH_SIM.qgm	20091115_STD3.qgd		
5	PAH 0.1ppm	STD-0004	1:Standard	ITQT	PAH_SIM.qgm	20091115 STD4.gqd		
6	Blank	UNK-0001	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample01.qgd		



Select [Fill Down] on the [Edit] menu.

The entire content of the first row is copied.

🚻 GCM	S Rea	al Tim	e Analysis	(Admi	n) -
🖉 File	Edit	View	Instrument	Batch	Too
	Ei	l Cariac			_
	Fi	l Down			
	a	ut		Ctrl+X	0:
Bate	Co	ру		Ctrl+C	- H
	Pa	aste		Ctrl+V	2



Select [Fill Series] on the [Edit] menu.

Edited parameters will be appended with serial numbers.

🚻 GCM	S Rea	al Tim	e Analysis	(Admi	n) - [
🖉 File	Edit	View	Instrument	Batch	Tool
	Fil	l Series			
		DOMU			_Ľ
	0	ut		Ctrl+X	09
Bate	Co	ру		Ctrl+C	24
	Pa	iste		Ctrl+V	he

4.3.3 Saving Batch Files

1	
	-

Select [Save Batch File As] on the [File] menu.

-	GCM	S Rea	al Tim	e Analysis	(Admi	n) - [E	
<u>w</u>	File	Edit	View	Instrument	Batch	Tools	
	0	pen Ba	ch File atch File atch File		Ctrl+0		
	Sava Ratch File						
	Sa	ave Ba	itch File	As		n S	
	Sa	ave Ba	itch As	Template		Vn S	



Open the folder where the method file is saved, enter a name, and save the file.

Save Batch I	File As	×
Save jn: 🗀	20091115_operation guide 💽 🔶 🖻 📸 📰 🗸	
File <u>n</u> ame:	20091115_1 Save	ก
		IJ
Save as <u>t</u> ype:	GCMS Batch File (*.qgb) Cancel	

4

4.3.4 Executing Sequential Analysis

Set the syringe rinse solvent and samples in the autosampler.



Click the [Start] icon on the [Batch] assistant bar.

Analysis starts.



• To abort batch processing, click the



(Stop) icon on the [Batch] assistant bar.

- To modify or add batch files while analysis is in progress, see "Appendix H Editing and Adding Batch Files During Sequential Analysis" P.99.
- To execute only specified rows, select the rows by clicking or dragging the mouse, then start the analysis.

Select Batch Execution Range				
Execution Range	Start			
C All Rows	Cancel			
• Selected Row[s] 3-6,9-10	Help			

4.4 Analyzing Data

Use the procedure described below to perform basic qualitative data processing for data measured in Scan mode, for examples, to display mass spectra, perform background subtraction, and perform similarity search.



(GCMS Postrun Analysis) icon.

The [GCMS Postrun Analysis] program starts.



Click the [Qualitative] icon on the [Postrun] assistant bar.



Double-click the

4.4.1 Loading Data Files



With reference to "*Appendix C Using Data Explorer*" *P.81*, double-click the data file to be analyzed.

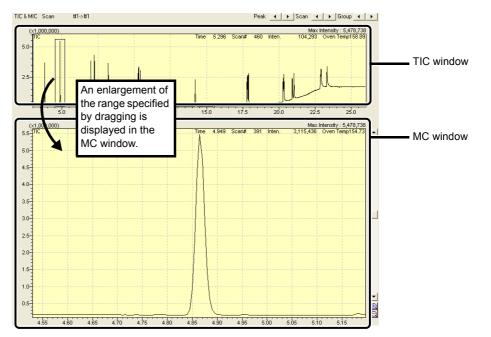
The data file to be analyzed opens.

Data Explorer - Data	×					
Project in :						
\20091115_operation guide						
Eile Manne	1					
C	Annuined					
20091115_Sample1						
6						

4.4.2 Zoom in on a Peak in the Chromatogram and Displaying Mass Spectra

Specify a range in the TIC window by dragging the mouse so that both the peak top and baseline are highlighted.

Drag the mouse so that both the peak top and baseline are displayed.



The top window displays the full chromatogram, and the second window displays any enlarged portion of the same chromatogram.

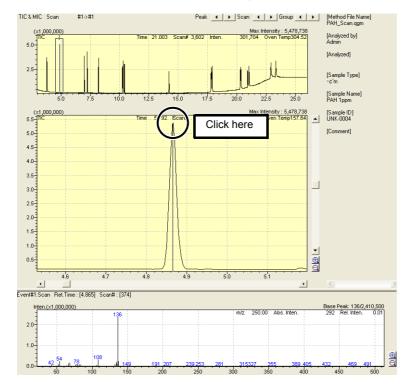
To undo the zoom, right-click in the MC window and select [Undo Zoom] on the pop-up menu.

4 Qualitative Analysis

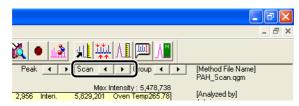


Move the mouse pointer to the peak top and double-click.

The mass spectrum for the peak top is displayed.



If a mass spectrum location other than the peak top is displayed, align the bar position with the peak top by clicking Scan .



If a red peak appears in the mass spectrum, it indicates that the signal intensity for this m/z has exceeded the scale. To display the proper mass spectrum for target compounds, click the left or right

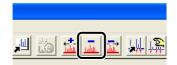
arrow buttons Scan **()** to select a mass spectrum that shows no red peaks.

4.4.3 Removing the Background

The mass spectrum corresponding to a peak in the chromatogram has a contribution from the background. This background mass spectrum may interfere with the subsequent qualitative analysis, hence it needs to be subtracted from the compound's mass spectrum. The steps shown in this section describe the procedure for removing the background mass spectrum from a compound's mass spectrum.

Click 📠 (Spectrum Subtraction) on the toolbar and position the mouse pointer in the MC window.

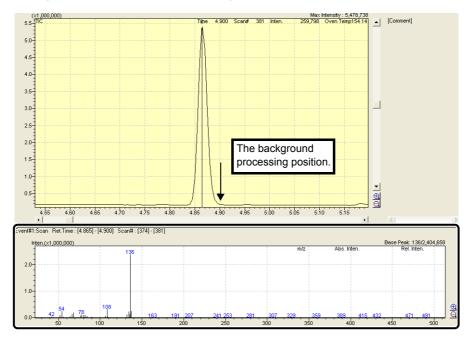
A bar is displayed.



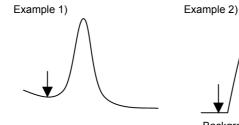


Double-click at the background processing position (see NOTE below).

The target spectrum, from which the background spectrum has been subtracted, is displayed.



With the following types of peaks, process the parts indicated by arrows as background.



Example 3)

Background spectrum can be subtracted from one of positions.

4

4 Qualitative Analysis

4.4.4 Searching for Similarity K Ver. 2.5

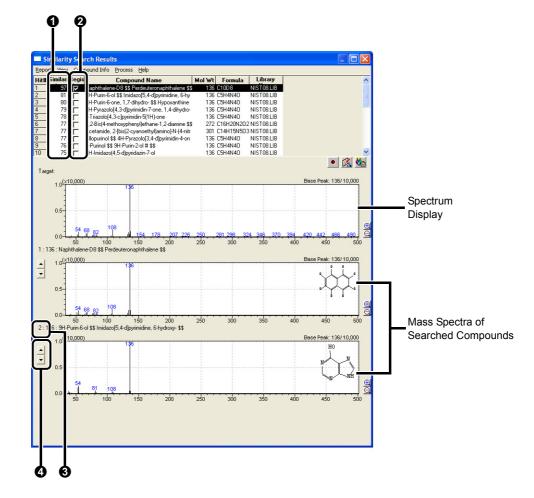


Click the [Similarity Search] icon on the [Qualitative] assistant bar. The [Similarity Search Results] window opens.





Click the **v** buttons on the left of the mass spectra as appropriate and check the mass spectra for the compounds found.



No.	Explanation
0	Similarity: The closer this value is to 100, the greater the similarity in mass spectra.
0	To enter a compound name in the spectrum table, select the box for the applicable compound.
0	Hit numbers for the compounds found.
4	Use to switch between the mass spectra for the compounds found.



After checking the mass spectra, click **e** (Register Target Spectrum to Spectrum Process Table).

The mass spectrum is registered.

Registering identification results in the spectrum process table allows referencing those results at a later time or outputting them as a report.



Close the [Similarity Search Results] window.

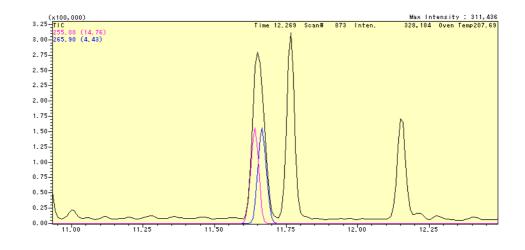
4.4.5 Displaying Mass Chromatograms

In the following situations, displaying mass chromatograms (MC) makes it easier to analyze the data.

For instructions of how to display mass chromatograms, see "Appendix G Displaying Chromatograms" P.96.

Confirming the Purity of Peaks

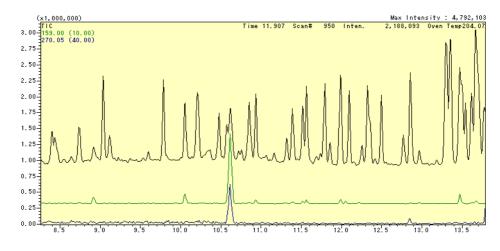
Displaying mass chromatograms can be used to check the presence of two or more overlapping peaks, or in other words, to check the purity of a peak in the chromatogram.



Looking for Target Compound Peaks Among Multiple Peaks

In some cases, peaks for target compounds cannot be confirmed in a total ion chromatogram (TIC).

If characteristic mass spectral peaks (i.e., m/z) of the target compounds are known, displaying the mass chromatograms makes it easier to check the position of the target compound's peaks in the chromatogram.



If characteristic spectral peaks are not known for the target compounds, see "Appendix F Index Searches" P.94 to check the mass spectra of target compounds.

4.4.6 Registering Spectra Displayed for Target Compounds

Register all the other target compounds using the procedure described in "4.4.2 Zoom in on a Peak in the Chromatogram and Displaying Mass Spectra" P.35.

4.4.7 Editing the Spectrum Process Table



Click the [Qualitative Table] icon on the [Qualitative] assistant bar. The [Qualitative Table] window opens.





Click 🔲 (Maximize).

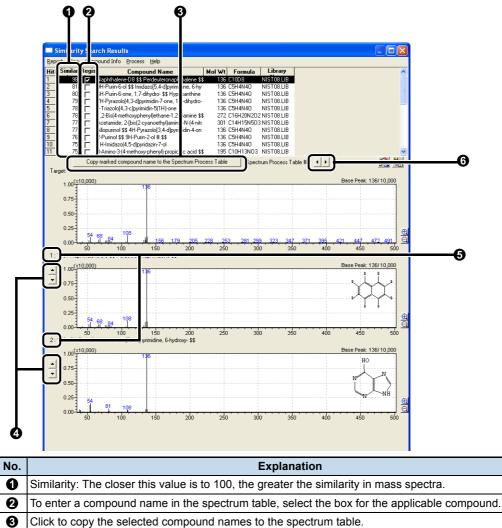
🗖 Q1	alitative Table								L	
Print	<u>E</u> dit <u>V</u> iew Similarit	y <u>S</u> earch							L. L	
	S	pectrum		Ba	ckground					
	Ret.Time	Start Tm	EndTm	Ret.Time	StartRT	EndRT	Search	Report	Name	
1		4.860	4.870	4.865	4.835	4.915	Done	•	Naphthalene-D8	
2		6.985	6.995	6.990	6.950	7.045		•	Acenaphthylene	
3		7.235	7.245	7.240	7.200	7.285	Done	•	Acenaphthene-d10	
4		8.200	8.210	8.205	8.160	8.250	Done	•	Fluorene	
5		10.250	10.260	10.255	10.205	10.280		V	Phenanthrene-D10	
6		10.305	10.315	10.310	10.280	10.365		V	Anthracene	
7		10.410	10.420	10.415	10.365	10.470		v	Anthracene	
8		14.210	14.220	14.215	14.160	14.290		v	Fluoranthene	
9		17.785	17.795	17.790	17.740	17.810		V	Triphenylene	
10		17.825	17.835	17.830	17.810	17.865		V	Chrysene-D12	
11		17.890	17.900	17.895	17.865	17.985		V	Benz[a]anthracene	
12		20.290	20.300	20.295	20.250	20.320		V	Benzo[e]pyrene	
13		20.340	20.350	20.345	20.320	20.455		V	Benz[e]acephenanthrylene	
14		20.915	20.925	20.920	20.875	20.995		V	Benz[e]acephenanthrylene	
15		21.035	21.045	21.040	20.995	21.140		V	Perylene-D12	
16		22.875	22.885	22.880	22.830	22.895		2	Benzo(ghi)perylene	
17		22.915	22.925	22.920	22.895	23.020		v	p-Bis(phenylethynyl)benzene	
18		23.325	23.335	23.330	23.290	23.410	Done	V	Benzo(ghi)perylene	
∢ 	\Spectrum Proce	ss (TIC /				•				



Double-click the first row in the spectrum table. The [Similarity Search Results] window opens.



Click the 🗾 buttons on the left of the mass spectra as appropriate to double-check the mass spectra for the compounds found.



No	Explanation				
0	Use to switch between the mass spectra for the compounds found.				
6	Hit numbers for the compounds found.				
6	Allows switching between search results for each row in the spectrum process table.				



After checking the mass spectra, close the [Similarity Search Results] window.

6

To edit compound names or other information in the spectrum process table, click the desired row, then select the [Edit] menu.

	ilitative Table							
rint	dit View Similarity Search	<u> </u>						
	Edit Compound Name	Ba	ckground					1
	Select All	Ret.Time	StartRT	EndRT	Search	Report	Name	1
		4.865	4.835	4.915	Done	ম	Naphthalene-D8	
2	Сору	6.990	6.950	7.045	Done	7	Acenaphthylene	
3	Delete Rows	7.240	7.200	7.285	Done	N	Acenaphthene-d10	
4	Delete Current Table	8.205	8.160	8.250	Done	2	Fluorene	
5		10.255	10.205	10.280	Done	ন	Phenanthrene-D10	
6	Delete All Peak Tables	10.310	10.280	10.365	Done	V	Anthracene	



Close the [Qualitative Table] window.

4.4.8 Saving Data Files

Click 📕 (Save) on the toolbar.

The qualitative table is saved in the data file.



4.5 Printing Qualitative Analysis Reports

The procedures are described below on how to use a template to create a report of analyzed data, how to edit the area of the chromatogram to display in the report, and how to edit the number of compounds to be displayed in the report of similarity search results.

4.5.1 Loading Report Formats



Click the [Report] icon on the [Qualitative] assistant bar.

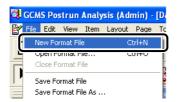
The [Data Report] window opens.





Click [New Format File] on the [File] menu.

The [File New] window opens.





Select [Use Template] and select the format [Qualitative Analysis Report].

File New	×
C New File	
Use Template	
Salibration Curve	^
Chromatogram-Spectrum	
DEFAULT Superstrum (10 Compounds)	
Qualitative Analysis Report	
Valuantitation (10 Lompounds)	
🔊 Quantitation (21 Compounds)	
C Duantitation (Chromato & CalCurve)	-
Comment	
Lomment:	
	<u>×</u>
OK Cancel <u>H</u> elp	



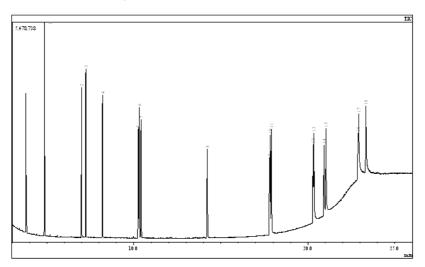
Click [OK].

The [Qualitative Analysis Report] format opens.

4.5.2 Editing Report Formats

Double-click on the chromatogram.

The [GCMS Chromatogram Properties] window opens.





Click the [Chromato] tab.

GCMS Chromatogram Pro	perties 🛛 🔁	
Genera Chromato Graph	File	
Position	Title	
Left 25.7 mm	Center 💌	
<u>T</u> op 98.2 mm	Chromatogram	
Size		
Width 165 mm	Font Name Times New Roman	
Height 100 mm	Size 8 Set	



In the [Area] area, deselect [Auto] for the X-axis and enter the time range.

GCMS Chromatogram Properties	×
General Chromato Graph File	
Iype Overlap ▼ ¥ 100 ↔ % ¥ 60 ↔ % Group 0 ↔ 0 ↔ Print out 1 ↔ TIC,MIC, <m r="" z@group-event="">, Separately</m>	
TIC	
Area X □ Auto 4 25 0 100000	
Line Width : 1 - GC(C) Detector Ch1	
OK Cancel Apply Help	



Click [OK].

Click the next page icon on the toolbar to display the second page.





Double-click on the [Library] display item.

The [GCMS Library Properties] window opens.

ny .
alget >>>
*1 R.Time * S*5(%can#37*) MassPeak 312
Mode:%mgle + 845(37+) BasePeak13+15(2390531)
Iode \$ 391(130) Group 1 - Event 1
6
26 ²⁴ 27 28 ²⁵ 10 10 10 10 10 10 10 10 10 10 10 10 10
1 Entry 9484 Library HIFI08 LIB
Formula C10ES CAS1144-45-2 MolWeight134 Befinder:0
pMame Maphfhalene-DS \$\$ Perdeutoronaphfhalene \$\$
16
54 63 78 108 D D
0 30 50 70 50 110 130 170 170 150 210 220 270 250 310 330 370 350 410 430 470 450
2 Entry 9937 Likeary MISTOS LIB
Formula C1H+N+O CAS93121-04-5 MolWeight134 Es Index1+21
pMame 9H-Pwine 4-ol\$\$ Imilaze [5,4-d]pyrimiline, 4-laylooxy- \$\$
· · · · · · · · · · · · · · · · · · ·
0 30 50 70 50 110 130 150 170 150 210 230 250 270 250 310 330 350 370 350 410 430 450 500 410 450 500 450





Click the [Result] tab.

GCMS Library Pro	operties	X
ResultTable General F	ResultColumn Post #Struct Position TargetSpectrum Result]	File ResultSpectrum
Position	7 mm	
<u>I</u> op 27.	8 mm	



Enter the [Maximum Compound Number] (maximum number of search results to display).

GCMS Library Prope	ties				X
ResultTable General Positi	ResultColumn on TargetSp) bectrum	ResultStruc Result		File ResultSpectrum
I √ Sp <u>e</u> ctrum	Position X 0 mm Y 0 mm	Size X	150 mm 35 mm	are no confir are w [Resu	checked items of displayed, m whether they ithin the [Size] of tt] in [Position]
☐ <u>I</u> able	Position X 0 mm Y 35.5 mm	X Y	150 mm 40 mm	tab.	
✓ Structure	Position X 120 mm Y 10 mm	Size X Y	30 mm 20 mm		
Print the Hit Print Only Sectors	Compounds	<u>M</u> aximum	i Compound I	Number	
	ОК	Canc	el	Apply	Help



Click [OK].

4

4.5.3 Outputting Reports



Click the [Preview] icon on the [Data Report] assistant bar.

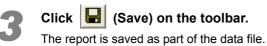
The print preview window opens.





After checking the report content, click [Print] to print the report.

Qu	ualitative Analysis Report	11/17/2009	Qualitative Analysis Report	11/17/2
And the second s	teptilement		<text></text>	2
	1/19		2 / 19	







5.1 Creating a Method File

With reference to "4 *Qualitative Analysis*" *P.20*, analyze standard samples and register the retention times and mass spectra of the target compounds in the spectrum process table.

5.1.1 Creating a Compound Table



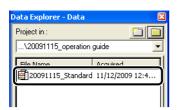
Start the [GCMS Postrun Analysis] program and click the [Compound Table] icon on the [Postrun] assistant bar.

The [Create Compound Table] window opens.





From Data Explorer, double-click the data file in which the spectrum process table for the target compounds was saved.



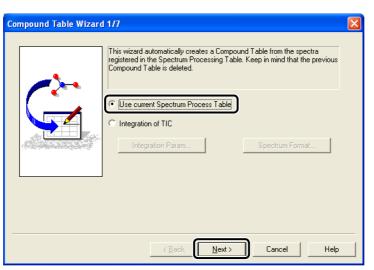


Click the [Wizard (New)] icon on the [Compound Table] assistant bar. The [Compound Table Wizard] window opens.





Select [Use current Spectrum Process Table] and then click [Next].





Click [Next].

Compound Table Wizard 2/7	×
Currently 18 of peaks are registerd in the Spectrum Process Table.	
# of <u>P</u> rocessed Peaks of Chromatogram:	
< Back Next > Cancel Help	



Select a row in the table, check the mass spectrum for each compound, and click [Next].

	Proc.	Ret.Time	Intensity	~	The wizard will create the Compound Table from
1	ম	4,865	5478738		this Spectrum Processing Table. Please deselect
2	না	6,990	3861699		any unnecessary peaks.
3		7.240	4319580		1
4	না	8.200	3666414		(×1,000,000) Base Peak: 164/933,553
5	না	10.250	2825621		1.00-164
6	ন	10.305	3365494		
7	ন	10.410	3061780		0.75
8	ন	14.215	2320214		
9	N	17.790	2124119		0.50
10	N	17.830	2679317		
11	N	17.895	2821427		80
12	N	20.295	2434062		0.25
13	N	20.340	2730652		
14	<u> </u>	20.920	2427288		
15	না	21.035	2833193	~	250 500

5 Quantitative Analysis



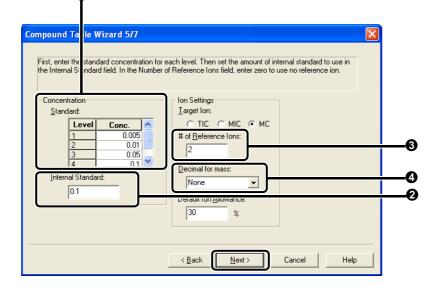
Specify the calibration curve type, the quantitative method, and other parameters as required, and click [Next].

Compound Tabl Wizard 4/7	3
Quantitative Method:	
Calculated by: • Area Height • Decimal Significant • Decimal Sign	6

No.	ltem	Explanation			
0	Quantitative Method	 External Standard:Quantitation is performed using a calibration curve obtained from the absolute quantity (concentration) and the area or height value of the target compound in a standard sample. Internal Standard:An internal standard is added to the sample, the sample is analyzed, and quantitation is performed using the relationship between the relative sensitivity and the quantitative ratio with respect to the internal standard compound. 			
0	Calculated by	Select [Area] or [Height]. Normally, select [Area].			
0	# of Calib. Levels	Input the number of concentration levels of the calibration curve.			
4	Unit	Set the concentration unit used for reports.			
0	Format of Concentration	Set the number of digits used to indicate concentrations.			

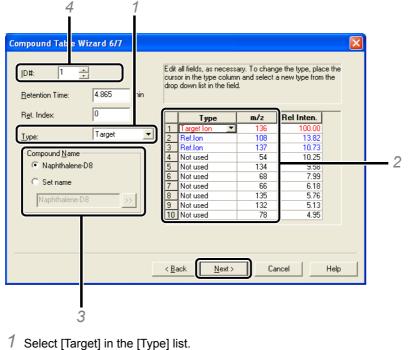


Make the appropriate settings for concentrations and measurement ions, and click [Next].



No.	ltem	Explanation
0	Standard	Set the concentrations of the standard samples. If the concentration varies with the compound, make the necessary corrections after completing the wizard procedure.
0	Internal Standard	Set the concentration of the internal standard.
€	# of Reference lons	Input the number of reference ions used to perform peak identification.
4	Decimal for mass	Determine the number of decimal places for target ion and reference ion m/z values. Selecting [1 Decimal] increases the sensitivity level.

Set the type, compound name, target ion, and reference ion for each substance. After entering the required information for all the compounds, click [Next].



- Select [I.S.] when setting for an internal standard.
- 2 Change the type and m/z value.

- To change the type, click cell for the type to be changed and select "Target Ion", "Ref. Ion", or "Not used".
- To change the *m*/*z* value, click the cell for the *m*/*z* value to be changed and click the arrow button that appears.

The mass spectrum is displayed. To set the m/z value, enlarge the area near the spectrum peak to be set by dragging the mouse and double-click on the spectrum peak. Switching the compound ID number also switches the mass spectrum.

Set Mass Ratio					
Int.(x1,000,000)				Peak: 136/2,	
- m/z 346.10 136	Abs. Inten.		21	Rel. Inten.	0.00
2.0-					
1.0					
					Æ
	207	253281	341	415	480
0.0- - , , , , , , , , , , , , , , , , , , 	200	30		400	m/z
				[Close

- 3 The names registered in the spectrum table are entered automatically. If there are blank spaces, enter the compound names.
- 4 Change the compound displayed by changing the ID number.

10

Click [Finish].

A compound table is created. Correct the contents of the compound table as required.

ID#	Name	Туре	ISTD G	m/z	Ret.Time	Ret. Index	Unit	Ref.lons	Conc.1	Conc.2	Conc.3	Conc.4	Event	STD Spec
1	Naphthalene-	ISTD	1	136.00	4.865	0	mg/L	108.00-13	0.1	0.1	0.1	0.1	1	Registered
2	Acenaphthyle	Target	1	152.00	6.990	0	mg/L	151.00-15	0.005	0.01	0.05	0.1	1	Registered
3	Acenaphthen	ISTD	2	164.00	7.240	0	mg/L	162.00-16	0.1	0.1	0.1	0.1	1	Registered
4	Fluorene	Target	2	166.00	8.200	0	mg/L	165.00-16	0.005	0.01	0.05	0.1	1	Registered
5	Phenanthrene	ISTD	3	188.00	10.250	0	mg/L	189.00-18	0.1	0.1	0.1	0.1	1	Registered
6	Phenanthrene	Target	3	178.00	10.305	0	mg/L	176.00-15	0.005	0.01	0.05	0.1	1	Registered
7	Anthracene	Target	3	178.00	10.410	0	mg/L	176.00-17	0.005	0.01	0.05	0.1	1	Registered
8	Pyrene	Target	4	202.00	14.215	0	mg/L	200.00-20	0.005	0.01	0.05	0.1	1	Registered
9	Benzo[a]anthr	Target	4	228.00	17.790	0	mg/L	226.00-22	0.005	0.01	0.05	0.1	1	Registered
10	Chrysene-D12	ISTD	4	240.00	17.830	0	mg/L	236.00-24	0.1	0.1	0.1	0.1	1	Registered
11	Chrysene	Target	4	228.00	17.895	0	mg/L	226.00-22	0.005	0.01	0.05	0.1	1	Registered
12	Benzo[b]fluor	Target	4	252.00	20.295	0	mg/L	250.00-25	0.005	0.01	0.05	0.1	1	Registered
13	Benzo[k]fluor	Target	5	252.00	20.340	0	mg/L	250.00-25	0.005	0.01	0.05	0.1	1	Registered
14	Benzo[a]pyre	Target	5	252.00	20.920	0	mg/L	250.00-25	0.005	0.01	0.05	0.1	1	Registered
15	Perylene-D12	ISTD	5	264.00	21.035	0	mg/L	260.00-26	0.1	0.1	0.1	0.1	1	Registered
16	Indeno[1,2,3-	Target	5	276.00	22.880	0	mg/L	274.00-27	0.005	0.01	0.05	0.1	1	Registered
17	Dibenz[a,h]an	Target	5	278.00	22.915	0	mg/L	279.00-13	0.005	0.01	0.05	0.1	1	Registered
18	Benzo[ghi]per	Target	5	276.00	23.330		mg/L	274.00-27	0.005	0.01	0.05	0.1	1	Registered
19		Target	5	TIC	0.000	0	ma/L		0.005	0.01	0.05	0.1	1	

To correct the compound table, enter edit mode by clicking 📝 Edit at the top-right corner of the

table. When editing is completed, return to display mode by clicking 63 View



Click the [Save Compound Table] icon on the [Compound Table] assistant bar.

The method file that was used to acquire the data will be selected automatically.





Click [Save].

Save Method As	X
Save jn: 🛅 20091115_operation guide 💽 🔶 🖻 🛒 🏢 🗸	
PAH_Scan	
File name: PAH_Scan	
Save as type: GCMS Method File (*.qgm)	\Box

If greater sensitivity is required, use the following procedure to create a quantitative analysis method for the SIM mode.

This completes the procedure for creating a quantitative method for Scan mode.

5.1.2 Creating a SIM Table



Click the [Create SIM Table [COAST]] icon on the [Compound Table] assistant bar. The [Select Method File] window opens.





Enter a file name and click [Save].

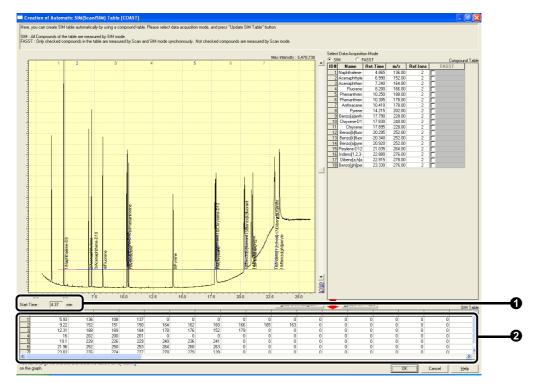
The [Create SIM Table [COAST]] window opens.

Select Method File	? 🗙
Save jn: 🗀 20091115_operation guide 💽 🗲 🗈 (* 🔳 *
PAH_Scan	
File name: PAH_SIM	<u>S</u> ave
Save as type: GCMS Method File (*.qgm)	Cancel



Click (Maximize) in the [Creation of Automatic SIM (Scan/SIM) Table [COAST]] window.

A SIM table is created automatically. Check the chromatogram and SIM table and, if necessary, modify the table with reference to the following procedure.



Modification Procedure

To ensure sufficient sensitivity, it is best to specify no more than 20 m/z values per row (i.e. per group). If necessary, modify the SIM table.

No.	ltem	Operation
0		Click within the frame next to [Start Time], then point the mouse pointer to the location on the chromatogram corresponding to the time when data acquisition is to be started, then click the left mouse button. Normally start time is set 0.5 to 1 minute before elution of the first target compound.
0	Each Group	Click the target row (i.e. group) and drag the mouse on the chromatogram to specify and enlarge the desired area. Next, click near the center of peaks labeled with compound names to specify the measurement end time for that group. This automatically sets the corresponding <i>m</i> / <i>z</i> values for the group at the same time.

- To edit table rows (i.e. groups), right-click on the desired row and select the following on the menu that appears.
 - · Add Row : Adds a row to the bottom of the table.
 - Insert Row : Inserts a new row above the selected row.
 - Delete Row : Deletes the selected row.
- To undo enlarging the chromatogram, right-click on the chromatogram and select [Undo Zoom] on the menu that appears.
- To split groups, use the following procedure. (Example: Splitting Group 3 into two groups)
 - **1.** Click the third row of the SIM table.
 - 2. Right-click on the table and select [Insert Row].
 - **3.** Click the inserted row and drag the mouse on the chromatogram to specify and enlarge the desired area.
 - Click near the center of peaks labeled with compound names. Group 3 is divided into two groups.



When finished, click [OK].

A method is created for SIM mode quantitative analysis.

5.2 Sequential Analysis

Create a batch file necessary for quantitative analysis and perform sequential analysis using the procedure described below.

5.2.1 Creating a Batch File

To use an existing batch file, follow the procedure starting in "5.2.2 Editing a Batch File Ver. 2.5" P.58.



Start the [GCMS Real Time Analysis] program and click the [Batch Processing] icon on the [Real Time] assistant bar.

The [Batch Table] window opens.

Data Analysis
Batch Processing
System Configuration



Select [New Batch File] on the [File] menu.

GCMS Re	al Tim	ie Analysis	(A dmi	n) - [B	latc
File Edit	View	Instrument	Batch	Tools	Wi
New Ba	atch File				
opend	accinicie	5	Cu	iτυ	Ê
Close E	Batch Fil	e			ple
Save B	atch File				Na
Save B	atch File	e As			
Save B	atch As	Template			
Select I	Project(Folder)			
File Sea	arch				
System	Admini:	stration			
	File Edit New Ba Open L Close E Save B Save B Save B Save B Save B	File Edit View New Batch File Open Data Thin Close Batch File Save Batch File Save Batch File Save Batch As Select Project(File Search	File Edit View Instrument New Batch File Open Decommen Close Batch File Save Batch File As Save Batch As Template Select Project(Folder)	File Edit View Instrument Batch New Batch File Open batch File Co Open batch File Save Batch File Co Save Batch File Save Batch File Save Batch File Save Batch File As Save Batch File As Save Batch File As Save Batch As Template Select Project(Folder) File Search	New Batch File Open Batch File Close Batch File Save Batch File Save Batch File As Save Batch As Template Select Project(Folder) File Search



Click the [Wizard] icon on the [Batch] assistant bar.

The [Batch Table Wizard] window opens.





Make the appropriate settings with the Batch Table Wizard and thereby create a batch table.

Batch Table Wizard	
Batch Table	1 101%Line2
Sample Type Standard & Unknown Standard Only Unknown Only	2
Method Method File: 20091115_operation guide\PAH_SIM.qgm Data Processing	 3
🔽 Quantitative	4
<u>Back</u> <u>Next</u> Cance	Help

- 1 Select [New].
- 2 Select [Standard & Unknown].
- 3 Click 🔎 and specify the method file to be used.
- 4 Select [Quantitative].
- 5 Click [Next].

Batch Table Wizard - Line1 Standard Sample (1)	
Standard Sample Vial #: 1: # of Calib. Levels: 4: Average Count: 1: Injection Volume: 1 uL Sample Name: Standard Sample Auto-increment Sample ID: STD-0001 ✓ Auto-increment	— 6 — 7 7
< <u>B</u> ack Next > Cancel Help	
9	

- 6 Input [Vial #].
 - The number of calibration points is loaded automatically from the method.
- 7 Input [Injection Volume].
- $\boldsymbol{8}$ Input [Average Count] (i.e., the number of repetitions).
- 9 Click [Next].

Batch Table Wizard - Li	ne1 Standard Sample (2)	
	Ata Create Filenames Automatically Data File Name: STD001 V Auto-increment Report Out Report Format File: pest.QGR Ata Description	10
	< <u>Back Next></u> Cancel Help 11	

10 Enter [Data File Name]. If the file name ends with a number, the files are named sequentially.

11 Click [Next].

Batch Table Wizard - Line1 Unknown Sample (1)	
Unknown Sample	12
Vial #: 4	-12
	<u> </u>
Sample Name:	
Unknown Sample	
Auto-increment	
Sample ID:	
UNK-0001	
Auto-increment	
< Back Next > Cancel Help	
15	
15	

- 12 Input [Vial #].13 Input [Sample Count].
- 14 Input [Injection Volume].
- 15 Click [Next].

Batch Table Wizard - Line1 Unknown Sample (2)	
Data File Name: sample1 V Auto-increment Report Dut Report Format File: Pest QGR	—16
Data Description	
< <u>B</u> ack Finish Cancel Help	
17	

- 16 Enter [Data File Name]. If the file name ends with a number, the files are named sequentially.
- 17 Click [Finish]. The batch table is displayed.

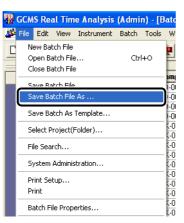
5.2.2 Editing a Batch File



5.2.3 Saving Batch Files



Select [Save Batch File As] on the [File] menu.





Open the folder where the method file is saved, enter a name, and save the file.

Save Batch F	File As
Save in: 🗀	20091115_operation guide 💽 🗲 🖻 📸 🗸
∰ 20091115_	1
File <u>n</u> ame:	20091115_2
Save as <u>t</u> ype:	GCMS Batch File (*.qgb)

5.2.4 Executing Sequential Analysis



Set the syringe rinse solvent and samples in the autosampler.



Click the [Start] icon on the [Batch] assistant bar. Analysis starts.



• To abort batch processing, click the

(Stop) icon on the [Batch] assistant bar.

• To modify or add batch files while analysis is in progress, see "Appendix H Editing and Adding Batch Files During Sequential Analysis" P.99.

 To execute only specified rows, select the rows by clicking or dragging the mouse and start the analysis.

Select Batch Execution Range	X
Execution Range	Start
C All Rows	Cancel
• Selected Row(s) 3-6,9-10	Help

5.3 Analyzing Data

5.3.1 Checking and Correcting Calibration Curves



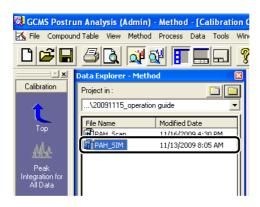
Start the [GCMS Postrun Analysis] program and click the [Calibration Curve] icon on the [Postrun] assistant bar.

The [Calibration Curve] window opens.





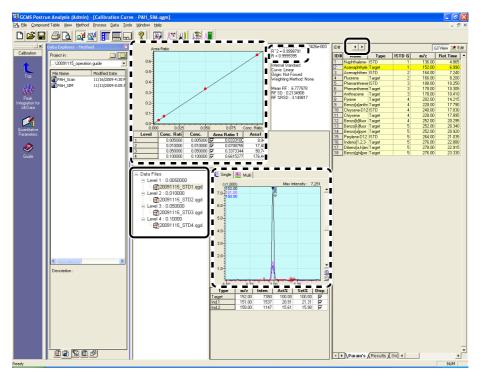
Double-click the method file used in analysis from Data Explorer.





Select a compound in the compound table and click the calibration curve level.

Check the calibration curve created and the chromatogram.



Reference

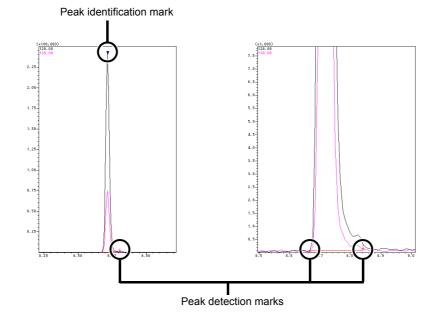
If no peaks are identified or detected, perform identification or peak integration with reference to *"Manual Identification and Manual Peak Integration" P.63.*

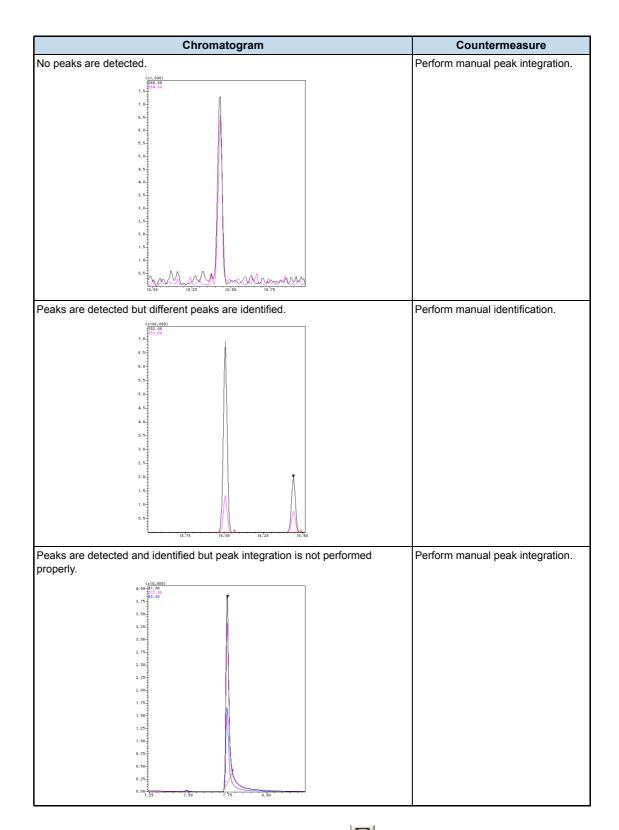
To change the method used to plot calibration curves, see "Changing Parameters for Quantitative Processing" P.65.

Peaks that are detected in the chromatograms after automatic peak integration, will have peak detection marks ($\uparrow \downarrow$).

The detected peaks are subjected to identification based on the retention times and ion ratios

(**v** peak identification mark).







Only after correcting the calibration curves, click 📕 (Save) on the toolbar to save the method file.



5

Manual Identification and Manual Peak Integration

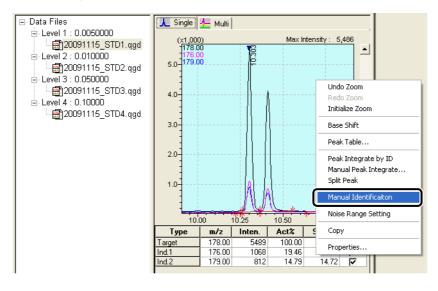
If no peaks are identified or detected, perform identification or peak integration using the procedure described below.

Manual Identification



Right-click in a chromatogram and select [Manual Identification] from the displayed menu.

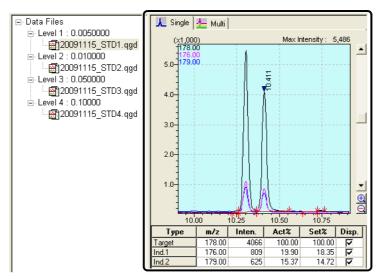
A bar is displayed.





Click the top of the peak to be identified.

The peak is identified.



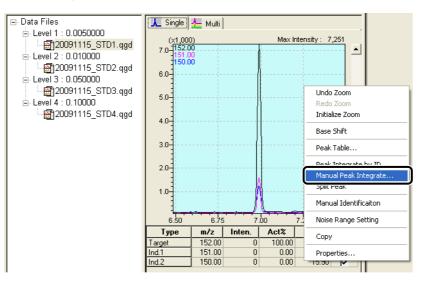


Manual Peak Integration



Right-click in a chromatogram and select [Manual Peak Integrate...] from the displayed menu.

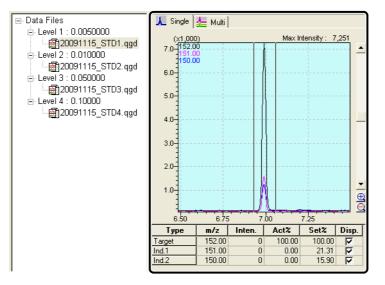
A bar is displayed.





Drag the mouse from the start point to the end point of the peak.

The [Base Line] window opens.





Select the baseline and click [OK].

The peak is integrated and identified.

Select Base Line	
C Link Point	
Horizontal	
⊂ <u>N</u> ew Baseline	_ <u>_</u>
OK Canc	el <u>H</u> elp

The same process can be accomplished by performing the following operations on the chromatogram.

Process	Operation	Explanation	
Manual Identification	[Shift] + [Ctrl] + right-click	Identifies integrated peaks.	
Manual Peak Integration		Connects start point and end point as baseline.	
Manual Peak Integration	[Ctrl] + right-click-drag	Connects points with horizontal baseline.	

Changing Parameters for Quantitative Processing

Change quantitative processing parameters as necessary.



Click the [Quantitative Parameters] icon on the [Calibration] assistant bar.

The [Quantitative Parameters] window opens.



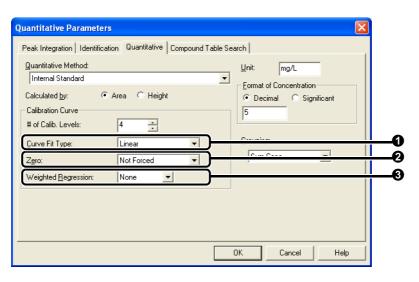


Click the [Quantitative] tab.

Quantitative Parameters	
Peak Integration Identificatio Quantitative Compound Table Se	arch
Quantitative Method:	Unit: mg/L
Calculated by:	Eormat of Concentration Occurrent Concentration Significant
of Calib. Levels: 4]9



Change the [Curve Fit Type], [Zero], and [Weighted Regression] settings, as necessary.



No.	Name	Explanation	
0	Curve Fit Type	 Specifies how to plot the calibration curve. Linear: Determines the calibration curve as a straight line from the obtained values. Point to point: Points are connected by a broken line. No formula is displayed for point to point calibration curves. Quadratic: Curve is fit to each point using a quadratic equation. This requires at least three points on the calibration curve. For two points or less, the curve is calculated as linear. Mean RF: First, it determines straight lines passing through the origin and each point. Then it finds the simple average of the slopes for each line. Consequently, the resulting calibration curve always passes through the origin. 	
0	Zero	Select either [Not Forced] or [Force Through]. Normally, select [Not Forced].	
0	Weighted Regression	 A typical least squares method of plotting calibration curves could result in a quantitation error that is larger the lower the concentration at the calibration point. In general, when the calibration curve has a large dynamic range (maximum concentration is at least 50 times higher than the minimum quantitation limit), formulas are weighted to reduce the weight of higher concentration points of the calibration curve. Typically, formulas are optimized by checking the correlation coefficient and contribution ratio. [1/C2]: Formulas are weighted by the inverse of the concentration value squared. [1/C2]: Formulas are weighted by the inverse of the area value squared (or height value when a height is specified for the data used). [1/A]: Formulas are weighted by the inverse of the area value (or height value when a height is specified for the data used). 	



After finishing making changes, click [OK].

Calibration curves are corrected according to the changed parameters.

5.3.2 Re-quantifying after Correcting a Calibration Curve

After correcting a calibration curve, re-quantify the data for samples with unknown concentrations.



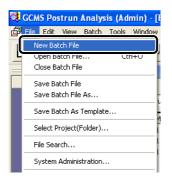
Click the [Batch Processing] icon on the [Postrun] assistant bar.

The [Batch Table] window opens.





Select [New Batch File] on the [File] menu.





Click the [Select Data File] icon on the [Batch] assistant bar.

The [Select Data File] window opens.







Click the data file for sample with unknown concentrations, for which re-quantification



The data file is selected.

Select Data File	? 🗙
Look jn: 🔁 20091115_operation guide 💽 🗲 🔁 (≝
20091115_PAH_Scan 20091115_STD3 20091115_Sample1 20091115_STD4 20091115_Sample2 20091115_STD4 20091115_Sample3 20091115_STD1 20091115_STD2 20091115_STD2	
Files of type: GCMS Data File (*.qgd)	OK Cancel
Selected Data File : Selected Data File : C:\20091115_operation guide\20091115_Sample1.ggd C:\20091115_operation guide\20091115_Sample2.ggd C:\20091115_operation guide\20091115_Sample3.ggd	<u>U</u> p <u>D</u> own



A batch table is displayed. Assign a name to the batch file and save it.

Fol	Folder: C:\GCMSsolution\20091115_operation guide								
		Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	Level#	ISTD Amt.
1		Unknown Sample	UNK-0001	0:Unknown	ITQT	PAH_SIM.qgm	20091115_Sample1.qgd	1	1111111
2		Unknown Sample	UNK-0002	0:Unknown	ITQT	PAH_SIM.qgm	20091115_Sample2.qgd	1	1111111
3		Unknown Sample	UNK-0003	0:Unknown	ITQT	PAH_SIM.qgm	20091115_Sample3.qgd	1	1111111



Click the [Start] icon on the [Batch] assistant bar.

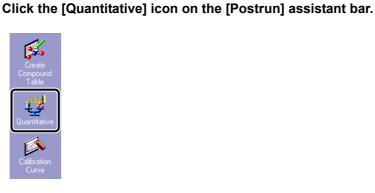
The data is re-quantified using the corrected calibration curve.



Click [OK].

5.3.3 Checking and Correcting Quantitation Results

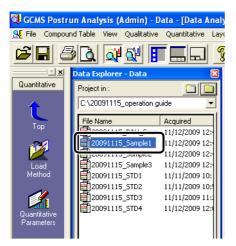
Check the quantitation results for the samples with unknown concentrations.





Double-click the data file to be checked from Data Explorer.

The data file being checked opens.





Click the [Results] tab in the [Compound Table View].

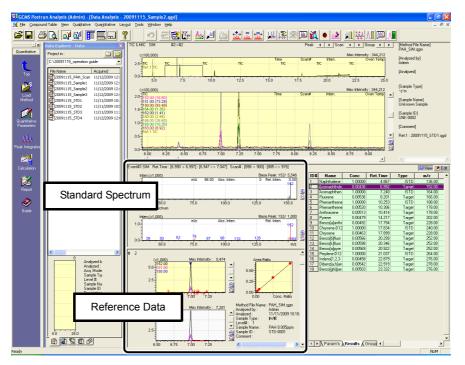
The quantitation results are displayed.

Naphthalene- Acenaphthyle	Туре	ISTD G	m/z	Ret.Time	Ret. Index	Unit	Ref.lons	Conc.
cenanhthule	ISTD	1	136.00	4.865	0	mg/L	108.00-13	
	Target	1	152.00	6.990	0	mg/L	151.00-15	0
cenaphthen	ISTD	2	164.00	7.240	0	mg/L	162.00-16	
luorene	Target	2	166.00	8.200	0	mg/L	165.00-16	0
henanthrene	ISTD	3	188.00	10.250	0	mg/L	189.00-18	
Phenanthrene	Target		178.00	10.305	0	mg/L	176.00-17	0
Anthracene	Target		178.00	10.410	0	mg/L	176.00-17	0
Pyrene	Target	4	202.00	14.215	0	mg/L	200.00-20	0
enzo[a]anthr	Target	4	228.00	17.790	0	mg/L	226.00-22	0
Chrysene-D12	ISTD	4	240.00	17.830	0	mg/L	236.00-24	
Chrysene	Target	4	228.00	17.895	0	mg/L	226.00-22	0
enzo[b]fluor	Target	4	252.00	20.295	0	mg/L	250.00-25	0
enzo(k)fluor	Target		252.00	20.340	0	mg/L	250.00-25	0
enzo[a]pyre	Target		252.00	20.920	0	mg/L	250.00-25	0
Perylene-D12	ISTD		264.00	21.035	0	mg/L	260.00-26	
ndeno[1,2,3-	Target		276.00	22.880	0	mg/L	274.00-27	0
)ibenz[a,h]an	Target		278.00	22.915	0	mg/L	279.00-13	0
enzo(ghi)per	Target	5	276.00	23.330	0	mg/L	274.00-27	0
	henanthrene henanthrene nthracene enzo[a]anthr hrysene-D12 hrysene enzo[b]fluor enzo[k]fluor enzo[k]fluor enzo[a]pyre erylene-D12 ideno[1,2,3- ibenz[a,h]an	henanthrene ISTD henanthrene Target nthracene Target yrene Target enzo[a]anthr Target hrysene-D12 ISTD	henanthrene ISTD 3 henanthrene Target 3 vence Target 3 vence Target 4 hysene 012 ISTD 4 hysene 012 ISTD 4 enco(bluor Target 4 enco(bluor Target 5 enco(a)pyer Target 5 enco(a)pyer Target 5 benc(a), 3 Target 5	henarthrene ISTD 3 198.00 henarthrene Tagel 3 178.00 rthracene Tagel 4 202.00 yrene Tagel 4 202.00 renocijalnih Taget 4 202.00 nyosene D12[S1D 4 228.00 nyosene D12[S1D 4 228.00 nenzlojihur Taget 4 228.00 nenzlojihur Taget 4 228.00 nenzlojihur Taget 5 252.00 nenzlojihur Taget 5 276.00 berga,hjan Taget 5 276.00	henarthment [STD] 3 188.00 10.250 henarthment Zyget 3 178.00 10.305 rbracer Target 3 178.00 10.415 rbracer Target 4 202.00 14.215 runger 4 228.00 17.780 17.835 runger 4 228.00 17.835 17.835 runger 4 226.00 17.835 22.00 20.205 runcib/luor Target 4 226.00 20.205 20.340 runcib/luor Target 5 25.00 20.340 21.055 runcib/luor Target 5 25.00 20.205 21.055 runcib/luor Target 5 25.00 22.055 26.00 21.055 dems(1.3.1) Target 5 27.600 22.895 27.600 22.895	benarthrene [STD] 3 188.00 10.250 0 reharthrene [age] 3 178.00 10.305 0 reharthrene [age] 3 178.00 10.410 0 vene [age] 4 202.00 14.215 0 rencalpathrit [age] 4 202.00 14.215 0 rysene [12]s1D 4 242.00 17.790 0 rysene [12]s1D 4 242.00 17.835 0 encol[biluot [age] 4 252.00 20.345 0 encol[biluot [age] 5 252.00 20.340 0 encol[biluot [age] 5 252.00 20.340 0 encol[biluot [age] 5 252.00 20.920 0 encol[biluot [age] 5 256.00 21.035 0 demo[a]haft [age] 5 276.00 22.880 0	henarthrene ISTD 3 188.00 10.250 0 mg/L henarthrene Target 3 178.00 10.305 0 mg/L rthracene Target 3 178.00 10.410 0 mg/L remarktinent Target 4 222.00 14.215 0 mg/L rupsene D12 STD 4 228.00 17.780 0 mg/L rupsene D12 STD 4 228.00 17.783 0 mg/L rupsene D12 STD 4 228.00 17.885 0 mg/L rupsene Target 4 228.00 17.885 0 mg/L runcib(lluor Target 4 228.00 17.885 0 mg/L runcib(lluor Target 5 255.00 20.390 0 mg/L runcib(lluor Target 5 255.00 20.390 0 mg/L runcib(lluor Target 5 256.00 20.390 0 mg/L runcib(lluor Target 5 256.00 <td< td=""><td>henarthrenk [STD] 3 198.00 10.250 0 mg/L 199.00-18 henarthrenk Taget 3 178.00 10.305 0 mg/L 176.00-17 rthxacer Taget 3 178.00 10.410 0 mg/L 126.00-12 vene Taget 4 222.00 14.215 0 mg/L 226.00-22 rysene 0.12[s1D 4 228.00 17.780 0 mg/L 228.00-22 rysene 0.12[s1D 4 228.00 17.880 0 mg/L 228.00-22 rysene 0.12[s1D 4 228.00 17.880 0 mg/L 228.00-22 encol(hunt Taget 4 228.00 17.880 0 mg/L 228.00-22 encol(hunt Taget 5 252.00 20.340 0 mg/L 280.00-25 encol(hunt Taget 5 252.00 20.340 0 mg/L 280.00-25 encol(hunt Taget 5 252.00 20.301 0 <t< td=""></t<></td></td<>	henarthrenk [STD] 3 198.00 10.250 0 mg/L 199.00-18 henarthrenk Taget 3 178.00 10.305 0 mg/L 176.00-17 rthxacer Taget 3 178.00 10.410 0 mg/L 126.00-12 vene Taget 4 222.00 14.215 0 mg/L 226.00-22 rysene 0.12[s1D 4 228.00 17.780 0 mg/L 228.00-22 rysene 0.12[s1D 4 228.00 17.880 0 mg/L 228.00-22 rysene 0.12[s1D 4 228.00 17.880 0 mg/L 228.00-22 encol(hunt Taget 4 228.00 17.880 0 mg/L 228.00-22 encol(hunt Taget 5 252.00 20.340 0 mg/L 280.00-25 encol(hunt Taget 5 252.00 20.340 0 mg/L 280.00-25 encol(hunt Taget 5 252.00 20.301 0 <t< td=""></t<>



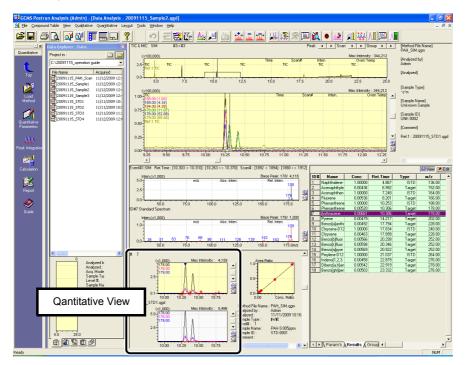
Display the standard spectra sub-window and reference data sub-window in the [Quantitative View] area.

If necessary, see "Displaying Standard Spectra" P.72, "Displaying Reference Data" P.72 to display information about identified compounds.



Click on a compound name in the compound table and check the chromatogram in the [Quantitative View].

Check the results while viewing the peak identification/detection marks and baseline in the chromatogram.



Reference

If necessary, perform identification or peak integration with reference to "Manual Identification and Manual Peak Integration" P.63.

The same process can be accomplished more easily by performing the following operations on the chromatogram.

Process	Operation	Explanation
Manual Identification	[Shift] + [Ctrl] + right-click	Identifies integrated peaks.
Manual Peak Integration		Connects start point and end point as baseline.
Manual Peak Integration	[Ctrl] + right-click-drag	Connects points with horizontal baseline.
Delete Identification Results	[Shift] + [Ctrl] + right-double-click	Voids identification and removes quantitative calculation results.



After checking the results, click 📕 (Save) on the toolbar.

The data file is saved.



When peaks are integrated for quantitation, concentrations calculated from the calibration curve are displayed.

However, if quantitation fails, character strings other than concentration values are displayed according to the cause of failure, as described below.

Displayed Character String	Explanation
No peak is detected.	Quantitative peak integration resulted in no peaks detected.
No peak is found in Window/Band range.	No peaks were detected within the retention time range specified for identification.
Ratio of reference ion does not match.	Peak is not identified due to the difference between specified and measured reference ion ratio values exceeding the allowable range.
Under the minimum similarity index.	Peak is not identified due to the measured similarity being less than the specified similarity setting, when mass pattern matching is specified in identification parameters.
No peak is identified.	Automatic identification results were manually deleted.

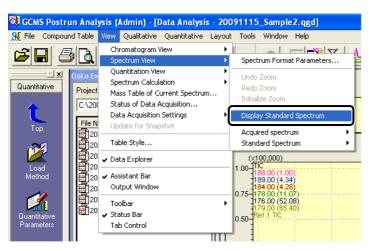
Displaying Standard Spectra

Data can be analyzed more easily by comparing the displayed spectrum with a standard spectrum.

1

Click [Spectrum View] on the [View] menu, then select [Display Standard Spectrum].

The standard spectrum is displayed.



The standard spectrum is a mass spectrum of a standard sample registered when the compound table was created.

The standard spectrum can be hidden by repeating step 1 above.

When the measured spectrum is enlarged by dragging, the standard spectrum is enlarged correspondingly.

Displaying Reference Data

Compounds can be identified from the shape of chromatograms, retention times, and other information obtained by referencing measurement data of standard samples or spiked samples.



Select [Open Reference Data File] on the [File] menu to open the data file being referenced.

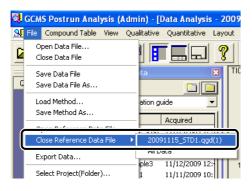
The reference data is displayed.

đ	GCM	S Postrun Anal	ysis (/	Admir
.	File	Compound Table	View	Qualit
		pen Data File lose Data File		ļ
	_	ave Data File ave Data File As		t
		oad Method ave Method As		a
	0	pen Reference Dat	a File	Ē
	E:	xport Data	a 1 110	- 6



Select [Close Reference Data File] on the [File] menu to specify the reference data file to close.

The reference data file closes.



Up to three reference data files can be displayed. Reference data peaks cannot be integrated.

5.4 Printing Quantitative Analysis Reports

5.4.1 Creating and Outputting Quantitative Analysis Reports



Click the [Report] icon on the [Quantitative] assistant bar. The [Data Report] window opens.





Click [New Format File] on the [File] menu.

The [File New] window opens.







Select [Use Template] and select the format [Quantitative Analysis Report].

File New	×
C New File	
Use Template	
🕲 Quantitation (10 Compounds)	^
🔯 Quantitation (21 Compounds)	
(Ve)	
🔯 Quantitative Analysis Report	
Quantitative Result (Table)	
	~
< · · · · · · · · · · · · · · · · · · ·	
Comment:	
	^
OK Cancel <u>H</u> elp	



Click [OK].

The [Quantitative Analysis Report] format opens.



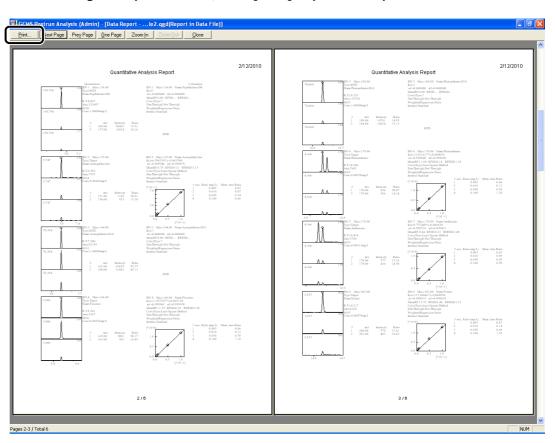
Click the [Preview] icon on the [Data Report] assistant bar.

The print preview window opens.





After checking the report content, click [Print] to print the report.





Click (Save) on the toolbar.

The report is saved as a data file.



Shutting Down GC/MS

6.1 Vacuum System Shutdown



6

Click the [Vacuum Control] icon on the [Real Time] assistant bar.

The [Vacuum Control] window opens.





Click [Auto Shutdown].

The vacuum system shuts down.

Vacuum Control	? 🛛
Auto Startup Auto Shutdown Cancel	Close
Ready 🕖 🔽 🛛 Vacuum Restart Mode	
	Advanced >>



When [Completed] is displayed, click [Close].

Vacuum Control	? 🔀
Auto Startup Auto Shutdown Cancel	
Not Ready 💟 🔽 Vacuum Restart Mode	
Completed.	Advanced >>

6.2 Turning OFF the Power

Turn OFF the power by performing the procedure for turning ON the power in reverse. If accessory/peripheral equipment is connected, switch OFF the accessory/peripheral equipment power last.

Reference

See "2.1 Turning ON the Power" P.3 for details on how to turn ON the power.



Quit the [GCMS Real Time Analysis] program and all other programs that are running.

Turn OFF the power to the PC, printer, and display.



Turn OFF the power to the MS unit.

Turn OFF the power to the GC unit.

Appendix File Format

GCMSsolution uses the file formats described below.

File type	lcon	Extension	File contents
Data file		.qgd	 In addition to the raw data acquired (e.g., chromatograms and spectra), the following information is saved. Calculation results such as area values and concentrations Status information such as the oven temperature and error status at the time data is acquired Contents of method files used in analysis (including configuration settings used for analysis) Contents of report format file (when reports are output) Contents of batch files (when batch processing is performed) Contents of tuning file used in analysis
Method file		.qgm	Analysis conditions, peak integration parameters, compound tables, etc. are saved. Because the configuration settings are saved when the method is edited, the configuration settings are checked when the method file is loaded to ensure that they agree with the current settings. Created calibration curves are also saved in the method file.
Report format file		.qgr	The report format information used to output a report, such as layout information and detailed settings, is saved. Once a report format file has been created, it can be used repeatedly to output reports of the same format.
Batch file		.qgb	Batch tables used to perform automatic sequential processing are saved. The same files can be used in both the [GCMS Real Time Analysis] program and the [GCMS Postrun Analysis] program.
Tuning file		.qgt	The conditions used to perform instrument adjustment (tuning) and the tuning results are saved.
Library file	Ű	.lib	These files are used to register the compound information and spectral data used to perform similarity searches. The libraries consist of public libraries (e.g., NIST and Wiley) and private libraries.



B.1 Viewing Help

If you do not know how to perform a procedure, refer to Help using one of the procedures described below.

B.1.1 Displaying Help from the Assistant Bar



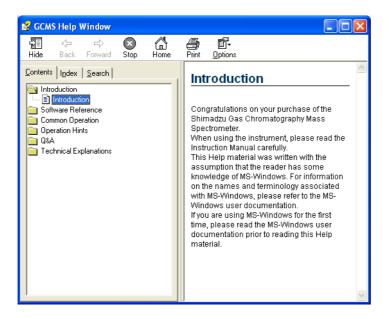
Click the [Guide] icon on the assistant bar in a window to display explanations for that window.



B.1.2 Displaying Help from the Menu Bar



Click [Contents] on the [Help] menu displayed in the menu bar of a window to display the [GCMS Help window].



Searching from the [Contents] Tab

1 Double-click the applicable topic.

Searching from the [Index] Tab

- Type the applicable word.
 The topic that matches the word is displayed at the top.
- 2 Select the applicable topic and click [Display]. Details on the selected topic are displayed.

If there are multiple instances of the word, the [Topics Found] window opens. Select the applicable topic from the list displayed and click [Display].

Searching from the [Search] Tab

- 1 Type the applicable word and click [Search]. The search results are displayed.
- 2 Select the applicable topic and click [Display]. Details on the selected topic are displayed.

B.1.3 Displaying Help with the F1 Key

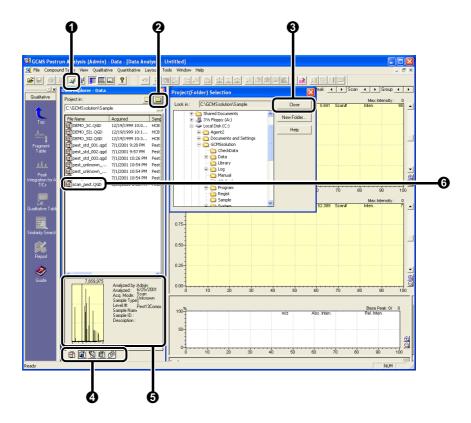


Press the [F1] key on the keyboard.

Help for the open window is displayed.



Using the data explorer function makes it easy to load files. For convenience, leave Data Explorer displayed at all times.



No.	Explanation
0	Click (Data Explorer) on the toolbar to open and close the [Data Explorer] window.
0	Click [[] (Project (Folder) Selection) to open the [Project (Folder) Selection] window and then click the applicable folder.
6	Click [Close] to close the [Project (Folder) Selection] window.
4	Click a tab to display the file of the corresponding type.
6	Click a file name (6) to display the corresponding file information.
6	Double-click the appropriate file to load the data.

[Create New Project (Folder)] can be used to copy files from the folder currently open in Data Explorer and to create new folders.

a Explorer - Metho iject in :		×	Create New Porject (Folder)
:\GCMSsolution\Sam	ple		Project <u>N</u> ame:
File Name	Acquired	Sample Name	· · · · · · · · · · · · · · · · · · ·
DEMO_SC.QGD	12/19/1999 9:00	HCB SCAN	Copy checked files in the current project to the new project
🗐 DEMO_SI1.QGD	12/19/1999 9:17	HCB SIM	Method Files
🗃 DEMO_SI2.QGD	12/19/1999 9:34	HCB SIM	🗖 Batch Files
pest_std_001.qgd	7/1/2001 8:28 PM	Pest13Compounds 1u	🔲 Report Format Files
DEMO_SI2.QGD pest_std_001.qgd	7/1/2001 8:57 PM	Pest13Compounds 1u	
pest_std_003.qgd	7/1/2001 9:26 PM	Pest13Compounds 1u	OK Cance
pest_unknown	7/1/2001 9:54 PM	Pest13Compounds 1	

This creates a new folder at the same directory level as currently open in Data Explorer.

Using this feature is especially useful in the following situation.

Example:

Folder A Quantitative Method File (calibration curve already created)	You want to use the same method file and batch file, but want to save the calibration curve.	Folder B Quantitative Method File (calibration curve already created)
Batch File		Batch File
Data files for standard samples used to create calibration curves and samples with unknown concentrations	Create a new project from Folder A.	

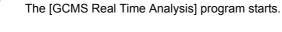


D.1 Maintenance

Replace or clean the consumable items and maintenance parts as necessary, referring to the [MS Navigator] window using the procedure described below.



(GCMS Real Time Analysis) icon.



Select [Maintenance] on the [Help] menu.

GCMS Real

Time Analysis

The [MS Navigator] window opens.

, U	ntitled, _default.qgt]	
wc	Help	
₩	Contents Maintenance	9.17
	About GCM5 Analysis	



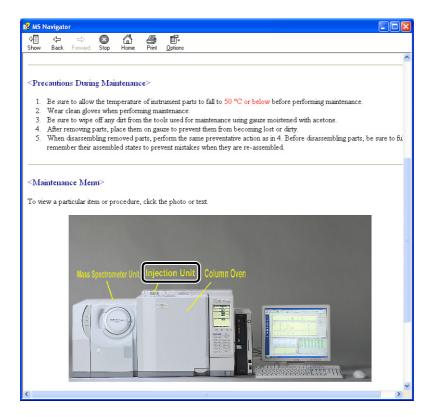
Click on the instrument for which maintenance will be performed.

💕 MS N	lavigator													×
수王 Show	< Back ∣	⊂> Forward	Stop	Home	Print	Detions								
					f S	hima Spo	dzu G ectron	neter	s		raph	M	as	^
					G	as Chrom	ntograph Ma	ss Spectr	ometers					
ſ	CMS-0	P2010			•	GCMS	QP2010 SE							
G	CMS-Q					GCMS				GCMS-Q	P2010S			
	el G	MS-GP201	OPTus				GCWS-GP20	10			Parvo	a2		
			1	For detai	ls on he	ow to judge	the type of C	C/MS you	u are usin	g, click <u>here</u> .				
						Per	ipheral Inst	uments						
A	himadzu Co uto-Injecto .OC- 20i o	or & Auto	o-Sample	91										
		A00-20	18205											~
<													>	





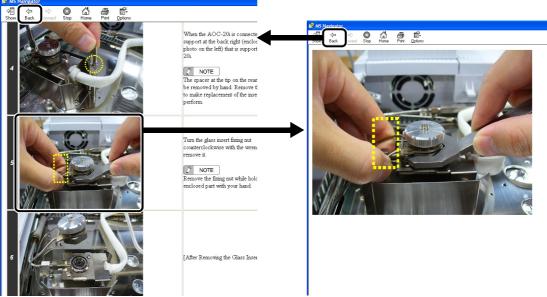
Read the precautionary information carefully and then click the applicable item under the maintenance menu.





Perform maintenance by following the instructions displayed on the screen.

Click an image to enlarge it. Click [Back] in the enlarged window to return to the original window.



To perform another maintenance item, click [Back] and repeat the procedure from step 3. After completing maintenance, close the [MS Navigator] window. After performing maintenance, reset the usage frequencies and usage times using the procedure described in *"Appendix D.3 Reset Procedure for Usage Frequencies and Usage Times* Ver.2.5" *P.87.*

D.2 Easy sTop (Applicable to QP2010 Ultra and QP2010 SE models)

Using Easy sTop allows replacing septa and glass inserts without stopping the vacuum system. Therefore, it significantly reduces the time required for stabilizing the system after replacement and eliminates the need for autotuning.

To protect columns, Easy sTop keeps the temperature of the sample injection unit, column oven, and interface at 70 °C or below. Consequently, it can take about 30 minutes until glass inserts and septa can be replaced.

Double-click one of the icons for consumables in the instrument monitor.

The [Consumable] tab page opens in the [Monitor Settings] window.



D Maintenance



Click [Easy sTop].

The [Easy sTop] window opens and the injection unit, column oven, and interface temperatures decrease. When each temperature reaches 70 °C or lower, the "Ready" status is displayed in the [Easy sTop] window.

onitor Settings		
🛈 Line1 🔁 Consumable		
GC Consumables Current/Rough Standard fo SPL1(INJ#1)	r Exchar	nge
	45/100	times
	45/500	times
- (INJ#2)		
Septum :		times
Glass Insert :	4/0	times
- (INJ#3)		
Septum :		times
<u>G</u> lass Insert :		times
CRG Coolant Time		
Col.Oven :		min
(INJ#2):		min
	ſſ	۵.
	E	asy sTop



Click [Replace], then replace septa or glass inserts in the sample injection unit.

For replacement procedures, refer to the septum replacement procedure or insert replacement procedure in the [MS Navigator] window.

Easy sTop
Ready
Temperatures are low enough. Please click the Replace button and then replace septa or glass inserts.
Beplace Cancel Help

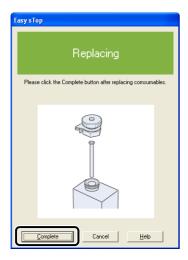
Clicking [Replace] stops the supply of carrier gas.

If left in that state for extended periods, it could reduce column performance. Therefore, replace septa and inserts as quickly as possible.



After replacement, click [Complete] in the [Easy sTop] window.

If there is no air leaking in, the sample injection unit, column oven, and interface temperatures return to their previous temperatures before Easy sTop started.





Reset the usage counter for the septum and glass insert.

For instructions on how to reset usage counters, see the procedure on page 88, starting with step 3.

D.3 Reset Procedure for Usage Frequencies and Usage Times Ver.2.5

The GCMSsolution's instrument monitor keeps track of the usage frequencies and usage times of the consumable items.

After replacing a consumable item or cleaning the ion source, reset the usage frequencies and usage times using the procedure described below.



Double-click one of the icons for consumables in the instrument monitor.

The [Consumable] tab page opens in the [Monitor Settings] window.

Ionization Mode
GC Consumables
1
MS Consumables
m 🔤 🦗
Detail





Click [Reset Consumables].

The [Reset Consumables] window opens.

Monitor Settings				
🔟 Line1 🔚 Consum	able			
GC Consumables Current/Rough Standar SPL1(INJ#1)	d for Exchar	nge	MS Consumables Current/Rough Standard for I	Exchange
Septum :	45/100	times	Filament #1 :	74/1000 hr
Glass Insert :	45/500		Filament #2 :	3/1000 hr
			Ion Source :	77/1500 hr
[INJ#2]			Detector :	77/6000 hr
Septum :		times	Turbo Molecular Pump1 :	1059 hr
Glass Insert :	4/0	times	Turbo Molecular Pump2 :	1059 hr
(INJ#3)				
		times	Rotary Pump 1 :	1060/15000 hr
<u>G</u> lass Insert :		times	Rotary Pump 1 Oil :	1060/3000 hr
			Rotary Pump 2 :	0/0 hr
			Rotary Pump 2 Oil :	0/0 hr
(INJ#2):				
	E	🧿 asy sTop		
			Total Run :	1065 hr Reset Consumables
			OK Cancel	Apply Help



Click [Clear] for the consumable items subjected to maintenance or input "0" in the usage time cells as appropriate, and click [OK].

The previous window returns.

eset Consumables				×		
GC		MS				
SPL1(INJ#1) Septum :	45 times	Clear	Filament # <u>1</u> :	74 Hour		
Glass Insert :	45 times	Clear	Filament # <u>2</u> :	3 Hour		
			Ion <u>S</u> ource :	77 Hour		
Septum :	0 times	Clear	Rotary Pump 1 <u>O</u> il :	1060 Hour		
Glass Insert :	0 times	Clear				
(INJ#3)						
Septum :	0 times	Clear				
Glass Insert :	0 times	Clear				
CRG Coolant Uesd Time	8					
Column Oven :	0 min	Clear				
(INJ#2):	0 min	Clear				
, , , , , , , , , , , , , , , , , , ,			<u>ОК</u> Са	ancel <u>H</u> elp		



Click [OK] in the [Monitor Settings] window.

The window closes.

D.4 Changing Replacement Guidelines for septa and Glass Inserts

For septa, replacement frequency varies depending on the syringe needle diameter. Glass insert replacement frequency varies depending on the sample. Set replacement guidelines based on the sample.



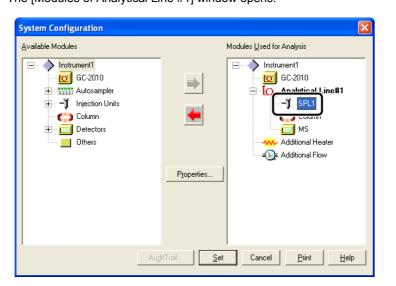
Click the [System Configuration] icon on the [Real Time] assistant bar.

The [System Configuration] window opens.





Double-click [SPL1] under [Modules Used for Analysis]. The [Modules of Analytical Line #1] window opens.







Click [Injection Port Maintenance].

The [Injection Port Maintenance (SPL1)] window opens.

odules of Analytical Line	#1						×
SPL1 Column MS							
<u>N</u> ame :	SPL1						
Injection Unit <u>Type</u> :	SPL						
Carrier <u>G</u> as :	He						
	ſ	Injection	n Port	Maintenar	nce	n	
- Heater	Ľ					J	
Zone:	INJ1						
<u>M</u> aximum Temperature :	470	°C					
- Flow]	
Elow Unit Type :	AFC-2010						
Z <u>o</u> ne :	CAR1	Sļot	:	SLOT1			
Primary Pressure :	500.0-900.0	▼ kPa					
- Setting for No Purge APC -							
Purge Flow :	3	mL/min					
[nlet Pressure :	100	kPa					
			_				
				OK	Car	cel	Help



Input [Septum Used Counts] and [Insert Used Counts] settings.

To restore default settings, click [Default].





Click [OK].

The [Modules of Analytical Line #1] window returns.

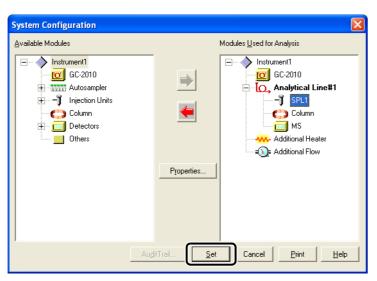


Click [OK].

The [System Configuration] window returns.



Click [Set].



The replacement guidelines for septa and glass inserts are changed.



Appendix E Single Analysis (Manual Injection)

Use the procedure described below when analyzing samples one-by-one using the autosampler or when performing analysis using manual injection.



Start the [GCMS Real Time Analysis] program, then click the [Data Acquisition] icon on the [Real Time] assistant bar.

The [Acquisition] window opens.





Double-click the method file to be used in Data Explorer.





Click the [Sample Login] icon on the [Acquisition] assistant bar.



The [Sample Login] window opens.

Sa	mple Login - C:\G	CMSsolution\20091115_operation guide\PAH_Sc 🛛	
ſ	Line1		
	Acquisition Information		
	<u>S</u> ample Name :	UNK-001	
	Sample <u>I</u> D :		1
	<u>D</u> ata File :	20091115_PAHmix_1.QGD	
	<u>B</u> aseline Data :		
	Data Des <u>c</u> ription :	PAH 13 Compounds Mix 1mg/L Analysis Condition 1	
	Sampler		
	<u>V</u> ial # :		-2
	Injection Volume :	1 uL Syringe Capacity : 10 uL	
	<u>M</u> ulti Inj. Times :	1	
	<u>T</u> uning File :	E	
		Advanced >> OK Cancel Help	
		3	·

- 1 Enter [Sample Name] and [Data File].
- 2 When using an autosampler, input [Vial #] in which the sample is set and [Injection Volume].
- 3 Click [OK].



When using an autosampler, set syringe rinse solvent and samples in the specified positions.



Click the [Download] icon on the [Acquisition] assistant bar.

The method file settings are transferred to the instrument.

When preparation for GC and MS has been completed, the [Start] icon turns green, indicating that it can be selected.

If using autosampler model AOC-20i, the analysis starts automatically.





Inject the sample and press the [START] button on the keyboard at the GC unit.

If using accessory/peripheral equipment, start such equipment first, then click the (Start) icon.

To abort analysis before completion, click the 🔞 (Stop) icon on the [Acquisition] assistant bar.



It is possible to search for information related to the target compounds (e.g., spectra and information on the structure) in the library.



Click the [Library Editor] icon on the [Postrun] assistant bar.

The [Library Editor] window opens.





Click [Open Library] on the [File] menu to open the library to be used. The library opens.

GCMS Postrun Analysis (Admin) - [Library Editor File View HitList Target Info. Compound Info. Index Contact Detects Library... Open Library... Ctrl+0



Click the second row cell in the [Index] column to select an item.

	Parameters									
		Index		Parameter						
	1	Joenar Humber	-191436				No need to set	191436		
	2	No Setting 📃 💌					No need to set	0		
	3	Serial Number					No need to set	0		
	4	Mol Wt					No need to set	0		
	5	Formula					No need to set	0		
	6	Umpd Name					No need to set	0		
		Base Peak						-		
		Ret.Index								
	1	Class Flags	d Name	Mol Wt		Formula				
		CAS Number NoSetting	r gen \$\$ o∙Hydrogen \$\$ p•	2	H2					
. r	$\overline{2}$	NO Seturiy	INI 10E7 ##	4	D2					



Enter information for the index item in the [Parameter] column for the row where the index item was selected.

Para	meters			
	Index	Parameter	Upper/Lower	# of Hit 🔺
1	Serial Number	1-191436	No need to set	191436
2	Cmpd Name	hexa	🔲 Match Case	0 🔤
3	No Setting		No need to set	0
4	No Setting		No need to set	0
5	No Setting		No need to set	0
6	No Setting		No need to set	0 🤜
- 1	he car		AL 11 1	o 🛄



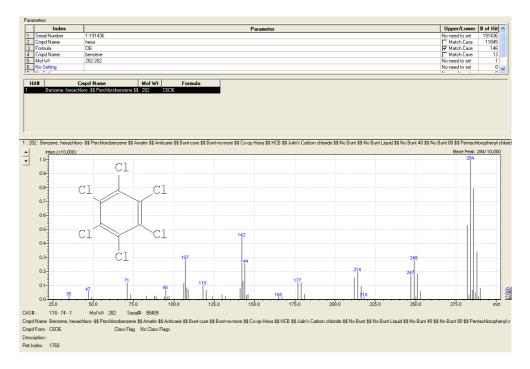
Click [Start] on the [Index Search] menu.

The results are displayed. Add index items until the target compound is found.

n /	٨na	ılysis (Admin) - [Lib	rary Editor - NISTOB.LIB (191,436 Spectrum)]
:List	: 1	arget Info. Compound	Info. Index Search Tools Window Help
Ę	Ę	🕰 💐 💱 🚺	
P	ara	meters	Export Search Results
		Index	Parameter
	1	Serial Number	1-191436
	2	Cmpd Name	hexa
	3	Formula	CI6
	4	Cmpd Name	benzene



Confirm the applicable information (e.g., spectrum or structure).



Appendix G Displaying Chromatograms

Displaying the appropriate mass chromatogram while analyzing data for qualitative analysis makes analysis easier.

If the *m/z* value for which the chromatogram is to be displayed is not known, search for it beforehand using the procedure described in "*Appendix F Index Searches*" *P.94*.

G.1 Displaying Chromatograms from Fragment Tables



Click the [Fragment Table] icon on the [Qualitative] assistant bar.

The [MC Fragment Table] window opens.

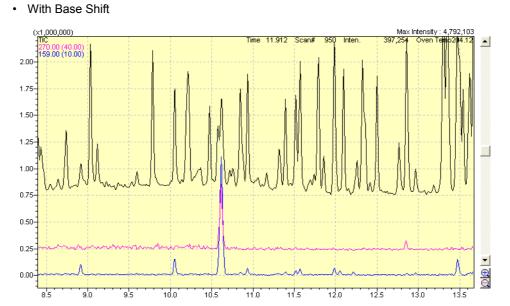




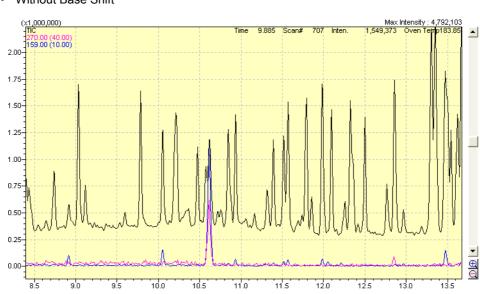
Enter the applicable values in the [m/z] and [Factor] columns, select the corresponding cells in the [Disp.] column, and click [OK].

A mass chromatogram is displayed in the MC window.

MC F	ragmer	nt Table		
Gro	up#1	• •	[ОК
				Cancel
	<u>T</u> IC MIC			
10	Page	1 -		Help
C	None	· ·		
	- Base SI	oift		
_	10.000 01			`
	Disp.	m/z	Factor	~
1	<u> </u>	270.00	40.00	
2		159.00	10.00	=
4				_
5				
1 2 3 4 5 6 7				
<u>/</u> 8				
<u>8</u> 9				
10				
11 12				
13				
14				~



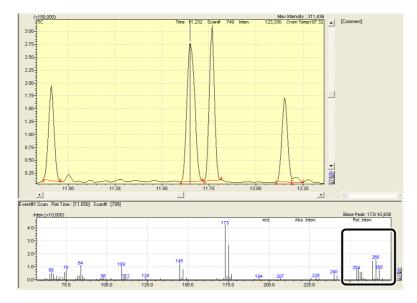
The display can be changed as shown below by enabling/disabling [Base Shift] in the table.



· Without Base Shift

G.2 Displaying Chromatograms from Mass Spectra

In the mass spectrum, specify and enlarge the range containing the desired peaks by dragging the mouse.



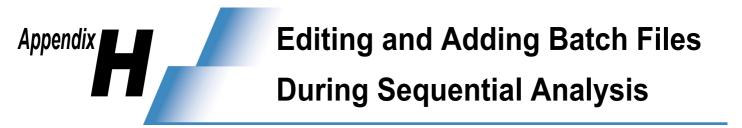


Move the mouse pointer to the spectral peak to be displayed and double-click.

A mass chromatogram is displayed in the MC window, enlarged by an automatically set enlargement rate.

Event#1:Sca	an Ret.Time:[11.65	50] Scan#:[799]							
	(×10,000)							Base	Peak: 173/42,638
2.0						m/z	267.90 Abs. Inten.	8,528 F	Rel. Inten
1.5						264			
1.0-									
		-	5					1.1	
0.5			256						
0.0				258					€ O
0.0				1			1 I I		Q
2	50.0 25	2.5 25	5.0 2	57.5 26	0.0 26	2.5 2	65.0 2	67.5 2	70.0

- To hide the mass chromatogram, deselect the applicable cell in the [Disp.] column in the [MC Fragment Table] window.
- To undo enlarging, right-click on the mass spectrum and select [Undo Zoom] on the menu that appears.

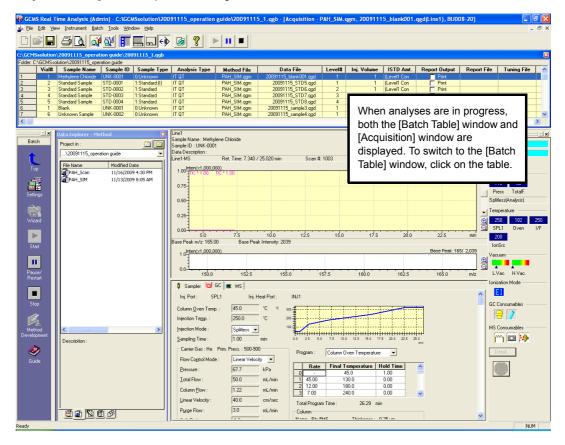


During sequential analyses, the batch file being executed can be edited while the analysis is still in progress. In addition, a separate batch file can be added for processing after the current batch file is finished, by specifying a batch queue.

H.1 Editing Batch Files

Click on the batch table, then after the window switches, click the [Pause/Restart] icon on the [Batch] assistant bar.

The [Batch Table] window opens, allowing unexecuted rows to be edited.



Analysis of rows currently being analyzed will continue to be executed.

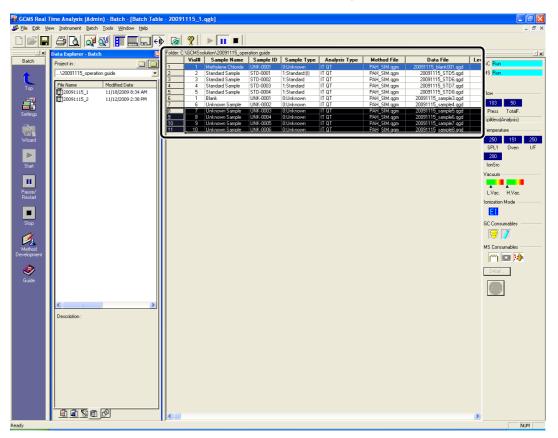
H Editing and Adding Batch Files During Sequential Analysis



Edit the batch table.

Right-click on the row to be edited, then select [Add Row], [Delete Row], or other action on the menu that appears.

The vial number, data file name, or other information can be changed as well.





Click 📕 (Save) on the toolbar.





Click the [Pause/Restart] icon on the [Batch] assistant bar. The analysis restarts.

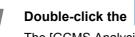




Some accessory/peripheral equipment may prevent using this function.

H.2 Adding Batch Files (Batch Queue)

H.2.1 Creating Batch Files to Add





GCMS Analysis Editor) icon.

The [GCMS Analysis Editor] program starts.



Click the [Batch Processing] icon on the [Real Time] assistant bar. The [Batch Table] window opens.





Create the batch file to be added.

rer - Batch
colution\20091115_operation guide
colution\20091115_operation guide
Madified Date
115_1 11/18/2009 8:34 AM
13_1 11/10/2009 0.34 /44
n:

H

H Editing and Adding Batch Files During Sequential Analysis



Name and save the batch file.

Save Batch I	File As
Savejn: 🗀	20091115_operation guide 💽 👉 🗈 📸 🕶
∰20091115_	1
File <u>n</u> ame:	20091115_2 Save
Save as <u>typ</u> e:	GCMS Batch File (*.qgb)



Quit the [GCMS Analysis Editor] program.

- The analysis will not start if the same data file name is used more than once or the specified method file does not exist.
- The batch queue is not activated until the [GCMS Analysis Editor] program is closed.

H.2.2 Adding Batch Files

Start the [GCMS Real Time Analysis] program.

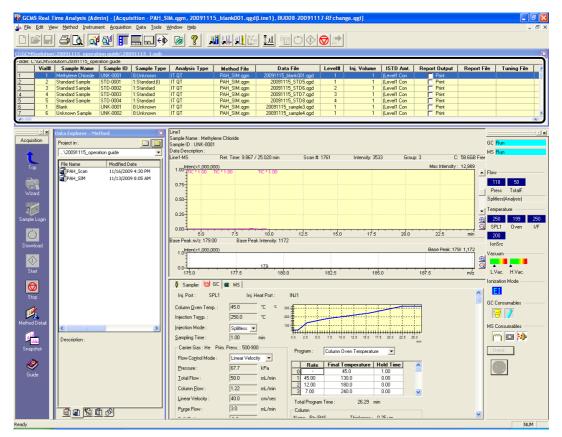
During analysis, both the [Acquisition] and [Batch Table] windows are displayed simultaneously.

🎇 GCMS Real Time Analysis (Admin) - [Acquisition - PAH_SIM.ggm , 20091115_blank001.ggd(Line1), BU008-20091117-RFchange.ggt]	- 2 🛛
Ja Elie Edit Yiew Method Instrument Acquisition Data Iools Window Help	- 8 ×
23.6CMScolution/20001115_noneration.unde/20001115_1.onb	X
Folder: C:\GCMS:obution/20091115_operation guide]
Vialit Sample Name Sample ID Sample Type Analysis Type Method File Data File Leveltt Ini Volume IST0 And. Report Duty Report File Network Strategy and Sample Sampl	le Tuning File
2 2 Standard Sangle IST0 40001 1.5 Andradrill) IT 0.7 PAH_SIM.ggm 2001115_STD5.ggd 1 1 ILevel Topo — Paor 3 3 Standard Sangle IST0.40001 1.5 Andradrill IT 0.7 PAH_SIM.ggm 2001115_STD5.ggd 1 1 ILevel Topo — Paor	
4 4 Standard Sample STD-0003 1:Standard IT QT PAH_SIM.ggm 20091115_STD7.ggd 3 1 Levell C [Batch Table] Wi	ndow
5 5 Standard Sample STD-0004 1:Standard IT 0T PAH_SIM.gam 20091115_STD8.god 4 1 [Level1 C] 6 1 Blank UNK-0001 0.UVrk/rown IT 0T PAH_SIM.gam 20091115_STD8.god 4 1 [Level1 C]	
7 6 Unknown Sample UNK-0002 0:Unknown IT QT PAH_SIM.agm 20091115_sample4.agd 1 1 [Levell Con Pink	
Acquisition Children - Method C Sample Name : Methylene Chloride	<u></u>
[Acquisition] Window	3C Run VIS Run
Line1 MS Ret. Time: 9.667 / 25.020 min Scan # 1761 Inter	
Top File Name Modified Date Impart_Scan 11/16/2009 4/30 PM 1.00 ⁻¹ (10 ⁻¹) 10 ⁻¹ (10 ⁻¹)	Flow
Пран_SIM 11/13/2009 8:05 АМ 0.75	118 50
Varia	Press TotalF.
0.50-1	Splitless(Analysis)
	Temperature
Sample Logn E	250 199 250 SPL1 Oven I/F
0.00 50 7.5 100 12.5 150 17.5 20.0 22.5 mm	200
Base Peak m/z 179.00 Base Peak Intensity: 1172 Downloadterr(x1.000.000) Base Peak Intensity: 1172terr(x1.000.000) Base Peak Intensity: 1172	lonSrc
10 ^{Men(x1,000,000)} Base Peak: 179/ 1,172	√acuum
179	
	L.Vac. H.Vac. onization Mode
Image:	EI
Stop	GC Consumables
Column Qven Temp : 450 °C * 30	
Method Detai	
C Injection Mode : Spitless -	MS Consumables
Description: Sampling Time: 1.00 min c.a. 25 56 7.5 10.6 22.5 25.6 min	m 🔤 🕪
Sinspehot Carrier Gas: He Prim: Press: 500-300 Program: Column Oven Temperature	Detail
Flow Coghol Mode: Linear Velocity Rate Final Temperature Hold Time Pressue: 67.7 kPa 45.0 1.00 1.00	
Guide Telesure (0.7, 4.7, 0) - 45.0 1.00	
Column Flow: 122 ml /min 2 12.00 180.0 0.00	
Purea resolution interesting i	
	NUM

2

Click the [Batch Table] window.

The content of the toolbar, menu bar, and assistant bar changes.





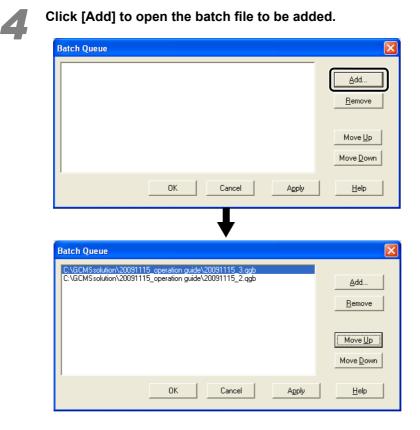
Select [Batch Queue] on the [Batch] menu.

The [Batch Queue] window opens.

e Analysis	(Admi	n) - Ba	tch - [B	atch T	able - 200	91115_1.
Instrument	Batch	Tools	Window	Help		
∌ ∆	Star Pau	•				
ta Explorer	Stop)				
roject in :	Bato	:h Queu	e			
\20091115_	Sett	ings				
File Name 120091115	Ente	ers Ecolo	ogy Mode (when en	ding Realtime	Batch

Η

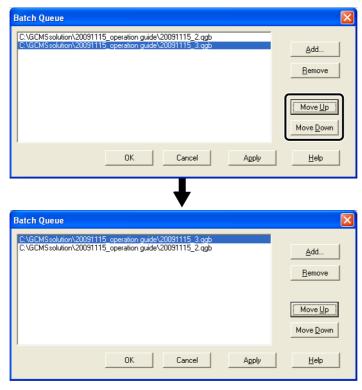
H Editing and Adding Batch Files During Sequential Analysis





If multiple batch files were added, change their order by clicking to select the desired batch file, then clicking [Move Up] or [Move Down].

Files are executed consecutively from the top.





When finished editing, click [OK].

Appendix Reducing the Carrier Gas Flow Rate After Sequential Analysis and Using the Ecology Mode

Reducing the carrier gas flow rate after analysis is finished is recommended to reduce carrier gas consumption.

I.1 Reducing the Carrier Gas Flow Rate After Sequential Analysis

For models other than QP2010 Ultra and SE, perform the following operations.

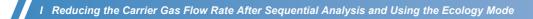
I.1.1 Creating a Method File That Reduces the Carrier Gas Flow Rate

As an example, the following describes how to create a method file that reduces the total flow rate to 20 mL/min.



Start the [GCMS Real Time Analysis] program, then in Data Explorer, double-click the method file to be used for sequential analysis.

🚻 GCMS Real 1	'ime Analysis (Admin) - Method - [Acquisitio	ı - PAH_SIM.qgm, Untitled]	
	ew Method Instrument Acquisition Data Iools	and the second se	_ & ×
Logical Control Contro	Data Explorer - Method Co Project in: - Coupling_operation guide Project in: - Coupling_operation guide Project in: - Coupling_operation guide Project in: - Coupling_operation guide - Coupling - Coupl	Image: Point Sector Image: Point Sector Image: Point Sector Image: Point Sector 100 ¹ Point Sector Point Sector Point Sector Point Sector Point Sector 100 ¹ Point Sector Point Sector Point Sector Point Sector Point Sector 100 ¹ Point Sector Point Sector Point Sector Point Sector Point Sector 100 ¹ Point Sector Point Sector Point Sector Point Sector Point Sector 100 ¹ Point Sector Point Sector Point Sector Point Sector Point Sector 101 Point Sector Point Sector Point Sector Point Sector Point Sector 101 Point Sector Point Sector Point Sector Point Sector Point Sector 101 Point Sector Point Sector Point Sector Point Sector Point Sector 101 Point Sector Point Sector Point Sector Point Sector Point Sector 101 Point Sector Point Sector Point Sector Point Sector Point Sector 102 Point Sector Point Point Se	GC Ready MS Ready Flow
			lines (
Ready			NUM





Change [Total Flow] to 20 mL/min, then name and save the method file.

🏮 Sampler 🔯 GC 🗧	🔹 MS						
Inj. Port : SPL1	Inj. He	at Port :	INJ1				
Column <u>O</u> ven Temp. :	45.0	°C °C	300				
Injection Temp. :	250.0	°C	200	<u>}</u>			
Injection Mode :	Splitless 💌		10	<u> </u>	-+	-++	
Sampling Time :	1.00	min	0.0	2.5 5.0	7.5 10.0 12.5 15.0	17.5 20.0 22	5 25.0
Carrier Gas : He Prim.	Press. : 500-900		Bree	gram :	Column Oven Temperat		
Flow Control Mode :	Linear Velocity		riug	giani .	Column Oven Temperal	ure 💌	
Pressure	67.7	kPa		Rate	Final Temperature	Hold Time	^
C					45.0	1.00	
		1.1.1		45.00			
Lotal Flow :	20.0	mL/min	JĪ	45.00	130.0	0.00	
Lotal Flow : Column Elow :	20.0	mL/min mL/min		12.00	130.0 180.0	0.00	
-	1		3	12.00 7.00	130.0 180.0 240.0	0.00 0.00 0.00	~
Column Elow :	 1 .22	mL/min	3	12.00 7.00 al Program	130.0 180.0 240.0	0.00	
Column Elow : Linear Velocity :	1.22 40.0	mL/min cm/sec	3 Tota Cok	12.00 7.00 al Program	130.0 180.0 240.0 Time : 26.29	0.00 0.00 0.00 min 0.25 um	

Save Method	l File As					? 🗙
Save jn: 隘	20091115_operation guide	•	+	£	Ċ	•
PAH_Scan						
File <u>n</u> ame:	PAH_SIM_low					<u>S</u> ave
Save as <u>typ</u> e:	GCMS Method File (*.qgm)	_		•		Cancel

I.1.2 Creating Batch Files



Click the [Batch Processing] icon on the [Real Time] assistant bar. The [Batch Table] window opens.





In Data Explorer, double-click the batch file to be used for sequential analysis.

Data Explorer - Bato	ch 🛛 🔀
Project in :	🔟 🔟
\20091115_operat	ion guide 📃 💌
File Name	Modified Date
File Name	Modified Date 11/18/2009 8:34 AM
and the second se	



Right-click on the batch table and select [Table Style] on the menu that appears. The [Table Style] window opens.

115_1.qgl	~1			
0	?			
Folder: C:\GC	CMSsol	lution\20091115_ope	eration guide	
	'ial#	Sample Name	Sample ID	Sample Type
1	1	Methylene Chloride	UNK-0001	0:Unknown
2	2	Standard Sample	Fill Series	4.61 1.00
3		Standard Sample	Fill Down	
2 3 4 5 6	4	Standard Sample	THEOWIT	
5	5	Standard Sample Blank	Cut	Ctrl+X
7	6	Unknown Sample	Сору	Ctrl+C
<u> </u>	0	Unknown Sample	Paste	Ctrl+V
			Clear Select All Copy Row Add Row Insert Row Paste Row Delete Row Input Col. Dat. Browse Data Edit Method Edit Method Edit Report Fo Wizard Settings Table Style	



Click [Run Mode] in the [Hide Items] list, then click [Add>>] and [OK].

A [Run Mode] column is added to the end of the batch schedule.

Table Style	
Column Order Font Hide Items Promoty Sample Amt, Dil. Factor System Check, User Prog Sampler File Action Barcode Baseline Data F Option 1 Option 2 Option 3 Option 3	Display Items Vialt Sample Name Sample ID Sample Type Analysis Type Method File Levelt Ini, Volume ISTD Amt. Report Dutput Report File Tuning File Data Decorimina
	OK Cancel



Edit the batch file.

Add a row at the end and select a method file created in "*Appendix I.1.2 Creating Batch Files*" *P.106*. Vial number, level number, and injection volume settings do not need to be changed from their default values. Enter a data file name that is not the same as any other row.

Folder: C:\GCMSsolution\20091115_operation guide									
	¥ial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File		
1	1	Methylene Chloride	UNK-0001	0:Unknown	ITQT	PAH_SIM.qgm	20091115_blank.qgd		
2	2	Standard Sample	STD-0001	1:Standard:(I)	ITQT	PAH_SIM.qgm	20091115_STD1.qgd		
3	3	Standard Sample	STD-0002	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD2.qgd		
4	4	Standard Sample	STD-0003	1:Standard	ITQT	PAH_SIM.ggm	20091115_STD3.qgd		
5	5	Standard Sample	STD-0004	1:Standard	ITQT	PAH_SIM.ggm	20091115_STD4.qgd		
6	1	Blank	UNK-0001	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample1.qgd		
7	6	Unknown Sample	UNK-0002	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample2.qgd		
8	1			0:Unknown	ITQT	PAH_SIM_low.qgm	20091115_low.qgd 😎		



Click the [Run Mode] cell for the row that specifies the method file that reduces the flow rate, then click the arrow button that appears.

The [Run Mode] window opens.

Folder: C:\GCMSsolution\20091115_operation guide								
	Level#	Inj. Volume	ISTD Amt.	Report Output	Report File	Tuning File	Data Description	Run Mode
1	1	1	(Level1 Con	🗖 Print				DL AQ DP
2	1	1	(Level1 Con	🗖 Print				DL AQ DP
3	2	1	(Level1 Con	🗖 Print				DL AQ DP
4	3	1	(Level1 Con	🗖 Print				DL AQ DP
5	4	1	(Level1 Con	🗖 Print				DL AQ DP
6	1	1	(Level1 Con	🗖 Print				DL AQ DP
7	1	1	(Level1 Con	🗖 Print			(
8	1	1	(Level1 Con	Print				DL AQ DP 耳
9	1	1	(Level1 Con	🗖 Print				DEAGDI



Configure [Run Mode] settings as shown below, then click [OK].

Run Mode		
Mode		
Eun(Default)		
Mait before download	P <u>e</u> riod:	1 [min]
Pause before download		
Process		
Download of Instrument Parame	ters	
Data Acquisition		
🗖 Data Processing		
OK Cancel		<u>H</u> elp

Name and save the batch file, then click the [Start] icon on the [Batch] assistant bar.

This results in loading the method file that reduces flow rate after the analysis for the seventh row is finished, which ends the sequential analysis with the carrier gas flow rate at 20 mL/min.



I.2 Ecology Mode (This feature applies to QP2010 Ultra and QP2010 SE models.)

Using the ecology mode reduces power consumption and carrier gas consumption during standby for analysis.

I.2.1 Setting the Mode Manually



Click the [Ecology Mode] icon in the instrument monitor.

A message window opens.

Vacuum
L.Vac. H.Vac.
Ionization Mode
EI
GC Consumables
9
MS Consumables
(m) 🔤 🥬
Detail



Click [Yes].

The [Ecology Mode] window opens and the mode switches to the ecology mode. After switching to the ecology mode, the column oven temperature and the total carrier gas flow rate decrease.

GCMS Real Time Analysis							
(1)	135] Do you want to g	o into the ecology mode?					
	s <u>N</u> o	Help					

The [Ecology Mode] window is displayed when in the ecology mode. Cancel the ecology mode before using [GCMS Real Time Analysis] to perform operations in other windows.

To cancel the ecology mode, click [Cancel] in the [Ecology Mode] window.

When the ecology mode is canceled, settings before switching to the ecology mode are restored.



I Reducing the Carrier Gas Flow Rate After Sequential Analysis and Using the Ecology Mode

I.2.2 Setting the Mode Using Batch Processing

This allows switching the instrument to the ecology mode after the entire sequential analysis is finished.

Click the [Batch Processing] icon on the [Real Time] assistant bar.

The [Batch Table] window opens.





Create and save a batch file.

			8	III III						
Data Explorer - Bate		Folder: C	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	Let an Participation
Project in :		1	Tialw	Methylene Chloride	UNK-0001	0:Unknown	IT QT	PAH_SIM.qgm	20091115_blank.qgd	GC Ready
\20091115_operat	ion guide 🗾 👻	2	2	Standard Sample			IT QT	PAH_SIM.qgm	20091115_STD1.qgd	MS Ready
		3	3	Standard Sample			IT QT	PAH_SIM.qgm	20091115_STD2.qgd	
op File Name	Modified Date	4	4	Standard Sample			IT QT	PAH_SIM.qgm	20091115_STD3.qgd	
20091115_1 20091115_2	11/18/2009 8:34 AM	5	5	Standard Sample Blank			IT QT IT QT	PAH_SIM.qgm PAH_SIM.qgm	20091115_STD4.ggd 20091115_sample1.ggd	Flow
20091115_2	11/18/2009 9:00 AM	7	6	Unknown Sample			ITQT	PAH_SIM.ggm	20091115_sample2.ggd	68 50
		8	7	Unknown Sample			IT QT	PAH SIM.ggm	20091115_sample3.qgd	Press TotalF.
ings		9	8	Unknown Sample			IT QT	PAH_SIM.ggm	20091115_sample4.qgd	Split(Valve:Open)
~ III		10	9	Unknown Sample			IT QT	PAH_SIM.qgm	20091115_sample5.qgd	
		11	10	Unknown Sample	UNK-0006	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample6.qgd	Temperature
≥ ade										200 IonSic Vacuum CVac HVac Ionization Mode GC Consumables ♥ Vacuum GC Consumables ♥ Vacuum MS Consumables ♥ Detail



Select [Enters Ecology Mode when ending Realtime Batch] on the [Batch] menu.

ne Analysis	(Admin) - Batch - [Batch Table - 20091115_1	
Instrument	Batch Tools Window Help	
50	Start Pause	
ata Explorer	Stop	Ы
Project in :	Batch Queue	h
\20091115_	Settings	H
File Name	Enters Ecology Mode when ending Realtime Batch	J



Click the [Start] icon on the [Batch] assistant bar.





When the ecology mode confirmation message appears, click [Yes].

The mode switches to the ecology mode after the sequential analysis is completely finished, including the batch queue.

GCMS Re	eal Time Analysis
2	[1136] Do you want to go into the ecology mode after batch processing ends?
	<u>Yes</u> <u>N</u> o Help

The setting can be canceled by repeating step 3, but leave the setting as it is.

The [Ecology Mode] window is displayed when in the ecology mode. Cancel the ecology mode before using [GCMS Real Time Analysis] to perform operations in other windows.

To cancel the ecology mode, click [Cancel] in the [Ecology Mode] window.

When the ecology mode is canceled, settings before switching to the ecology mode are restored.

Ecology Mode	2
	2 eco
Can	cel Help



Reports can be output from GCMSsolution using the two methods described below.

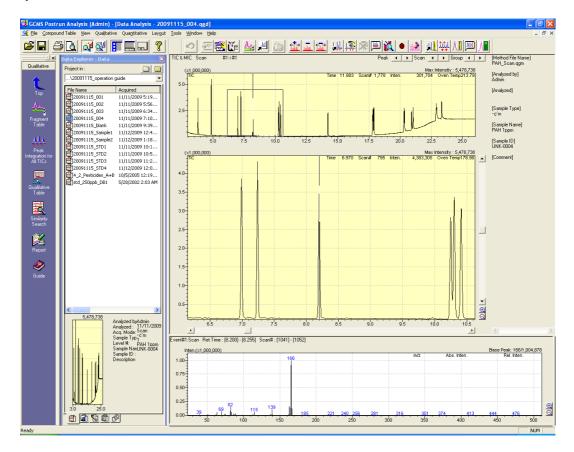
- Image printing : The image in the displayed window is automatically converted to a report.
- Report creation : A report format is set and output manually.

J.1 Printing Images (Printing Spectra and Chromatograms Displayed in Windows)

Call up the applicable data in the [Data Analysis] window in the qualitative or quantitative processing modes of the [GCMS Postrun Analysis] program.



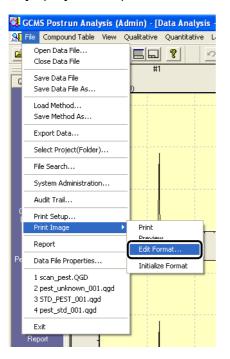
Display the chromatogram and mass spectrum in the window in the way desired for the report.





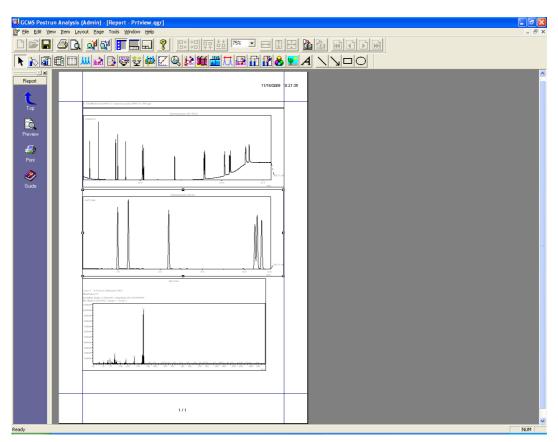
Point to [Print Image] on the [File] menu and select [Edit Format].

The [Report] window opens.





Adjust the size as necessary.



Ŋ

J Printing Reports



After editing, click the [Print] icon on the [Report] assistant bar. The report is output.





After outputting the report, close the [Report] window.

J.2 Creating Reports

With report creation, reports are output after setting report formats or using previously created templates.

Process and save the results to be output (such as spectral information) in advance.



Open the applicable data in the [GCMS Postrun Analysis] - [Data Analysis] window. The same report is output for both the qualitative and quantitative windows.

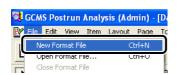


Click the (Report) icon on the [Qualitative] or [Quantitative] assistant bar. The [Data Report] window opens.

J.2.1 Using Templates



Select [New Format File] on the [File] menu.





Select [Use Template], select the applicable template, and click [OK].

File New	×
○ New File	
Salibration Curve	J
S Chromatogram-Spectrum	
M DEFAULT	
MSSpectrum (10 Compounds)	
🔊 Quantitation (10 Compounds)	
🔊 Quantitation (21 Compounds)	
🔊 Quantitation (Chromato & CalCurve)	
Curantitative Result (Granh)	
Comment:	
Chroamtgram in a Framgment Table settings.	
Spectrum in a Spectrum Process Table settings of the Qualitative Tabl	
≥	P
OK Cancel <u>H</u> elp	

If this selection window is not displayed, select [Option] on the [Tool] menu to display the [Setting Options] window and, on the [File New] tab, select [Prompt on File New] for the report format file.

J.2.2 Using Previously Created Report Files

Project in :	
\20091115_operation	guide
File Name	Modified Date
🔊 Calibration Curve	7/9/2001 1:57 PM
Chromatogram-S	11/11/2005 10:10 AM
MSSpectrum (10	11/22/2005 3:03 PM
🔊 nida	2/3/2006 6:15 PM
Spest	1/24/2006 9:58 AM
🔊 Quantitation (10	1/24/2006 9:59 AM
🔊 Quantitation (21	1/24/2006 9:59 AM
🔊 Quantitation (Ch	1/24/2006 10:00 AM
Quantitative Res	1/24/2006 10:00 AM
Quantitative Res	7/17/2001 3:24 PM
Similarity Search	11/11/2005 10:11 AM
Similarity Search	11/11/2005 10:11 AM

In Data Explorer, double-click the report file to be used.

J.2.3 Manually Setting Report Content

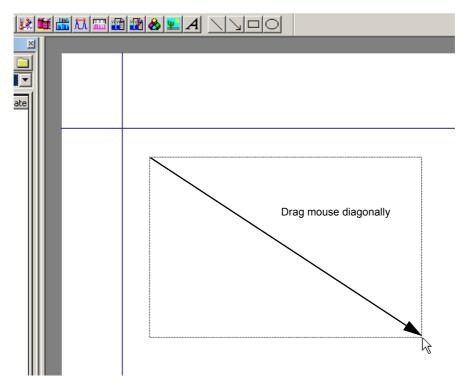
Click the buttons on the toolbar for the information to be printed or select the desired items on the [Item] menu.

lcon	Name	Explanation				
	Sample information	Select to print sample information.				
	Method	Select to print methods.				
	Peak table	Select to print the peak tables in qualitative tables.				
WY	Chromatogram	Select to print the chromatograms (TIC, MIC, and MC).				
шÀ	Spectrum graph	Select to print the mass spectra registered in spectrum processing tables.				
	Mass table	Select to print the mass tables for the spectra registered in spectrum processing tables.				
<u>k</u> a	Quantitative graph	Select to print the chromatograms and quantitative values obtained in quantitative results.				
Ŷ	Quantitative table	Select to print the tables obtained in quantitative results.				
K	Calibration curve	Select to print calibration curves.				
<u>Q</u>	Tuning	Select to print the tuning results obtained when data acquisition is executed.				
	Library search	Select to print the library search results obtained for the mass spectra registered in spectrum tables.Searches must be performed in the spectrum tables.				



Drag the mouse in the layout view to specify the print range.

The properties window for the item being laid out opens.





Set [Properties] and click [OK].

GCMS Chromatogram Properties	×
General Chromato Graph File Position It It Left 20.3 mm It It Iop 35.2 mm It Chromatogram Size Size Sample Name Data File Vidth 169.6 mm Font Name Times New Roman Leight 61.6 mm Size Set Color Back Ground Set Set	
Def <u>M</u> axLine 1 ≟ OK Cancel Apply Help	

Reference

Refer to Help for details on property settings.



To display a properties window again, double-click on the corresponding item.

J Printing Reports



Click the [Preview] icon on the [Data Report] assistant bar and check the contents of the report being output.





After the checking the report content, click [Print] to output the report.

Qualitative Analysis Report	11/18/2009	Qualitative Analysis Report	11/18/200
<text><text><text><text><text><text></text></text></text></text></text></text>	Set an	<text></text>	2 1
17.19		2 / 19	



Select [Save Format File As] on the [File] menu to name and save the report file. This allows loading the report format in the future to create reports easily.

😋 G	СМ	S Po	strun	Analy	sis (Adr	nin) -	Re
F 🎽	ile	Edit	View	Item	Layout	Page	То
Г	New Format File			Ctrl+N		1	
L	Open Format File Ctrl+O						
	Close Format File						
	Save Format File As Save Format As Template						
D					Ī		