

Gas Chromatograph Mass Spectrometer

GCMS-QP Series GCMS-TQ Series

Compatible with GCMSsolution Ver. 4.4 or later

Operation Guide

Basic Operation Guide

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

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Introduction

Read this Instruction Manual thoroughly before using the product.

Thank you for purchasing the GCMS-QP series and GCMS-TQ series gas chromatograph mass spectrometer.

This manual is intended to explain basic operations to first-time users. Read this manual thoroughly before using the product and operate the product in accordance with the instructions in this manual.

Also, keep this manual for future reference.

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

Important

• If the user or installation location changes, ensure that this Instruction Manual is transferred with the product.

• If this manual is lost or damaged, immediately contact your Shimadzu representative to request a replacement.

• To ensure safe operation, read all Safety Instructions before using the product.

• To ensure safe operation, contact your Shimadzu representative if product installation, adjustment, or reinstallation (after the product is moved) is required.

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Introduction

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• Information in this manual is subject to change without notice and does not represent a commitment on the part of the vendor.

• Any errors or omissions which may have occurred in this manual despite the utmost care taken in its production will be corrected as soon as possible, although not necessarily immediately after detection.

• Shimadzu Corporation is not responsible for errors or injuries resulting from following the instructions in this document.

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The TM and R symbols are omitted in this manual.

• Replacement parts for this product will be available for a period of seven (7) years after the product is discontinued.

Product Warranty

Shimadzu Corporation provides the following warranty for this product.

Details

1. Period:	Please contact your Shimadzu representative for information about the period of this warranty.		
2. Description:	If a product/part failure occurs for reasons attributable to Shimadzu during the warranty period, Shimadzu will repair or replace the product/part free of charge. However, in the case of products which are usually available on the market only for a short time, such as personal computers and their peripherals/parts, Shimadzu may not be able to provide identical replacement products.		
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. 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. Exceptions:	Failures caused by the following are excluded from the warranty, even if they occur during the warranty period.		
	1) Improper product handling		
	 Repairs or modifications performed by parties other than Shimadzu or Shimadzu designated companies 		
	 Product use in combination with hardware or software other than that designated by Shimadzu 		
	 Computer viruses leading to device failures and damage to data and software, including the product's basic software 		
	 Power failures, including power outages and sudden voltage drops, leading to device failures and damage to data and software, including the product's basic software 		
	6) Turning OFF the product without following the proper shutdown procedure leading to device failures and damage to data and software, including the product's basic software		
	Reasons unrelated to the product itself		
	8) Product use in harsh environments, such as those subject to high temperature or humidity levels, corrosive gasses, or strong vibrations		
	 Fires, earthquakes or any other act of nature, contamination by radioactive or hazardous substances, or any other force majeure event, including wars, riots, and crimes 		
	10)Product movement or transportation after installation		
	11) Consumable items		
	Note:Recording media, such as floppy disks and CD-ROMs are considered consumable items.		

If there is a document such as a warranty provided with the product, or there is a separate contact agreed upon that includes warranty conditions, the provisions of those documents shall apply.
 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, may result in minor to moderate injury or equipment damage.	
	Indicates additional information that is provided to ensure the proper use of this product.	
Reference	Indicates the location of related information.	
-Ò́- Hint	Indicates information provided to improve product performance.	
[]	Indicates items displayed on the screen, such as buttons, menu selections, settings, windows, and icons. Example: Click [OK].	

Safety Precautions

To ensure safe product operation, read these important safety instructions carefully before use and follow all DANGER, WARNING and CAUTION instructions given in this section.

- For repairs, contact Shimadzu or your Shimadzu representative. Not doing so could cause a fire, electrical shock, or injury.
- Do not modify or disassemble the instrument without the express approval of an authorized Shimadzu representative.
 Doing so could cause an accident from electric shock or a short circuit. It could also cause injury or instrument failure.
- 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

- 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 install this instrument in a location with flammable or explosive gases or liquids. Because this product is not designed to be explosion proof, doing so could cause a fire or explosion.
- Do not place flammable materials near the column oven exhaust at the back of the instrument, as they could ignite and cause a fire.
- The lab table or other surface on which this instrument is installed should be level, stable, and sufficiently strong to support the instrument's weight. Otherwise, the unit could tip over or fall off the surface.

Do not install the instrument in a location with corrosive gases, gases containing organic solvents, halogen compounds, or siloxanes, oil mist, or high levels of debris/dust. The instrument performance could be affected and its service life hortened.

Do not operate the instrument in an environment where condensation may form. Doing so could cause it to malfunction.

High-Pressure Gas Precautions

🕂 WARNING

- A high-pressure gas cylinder will be used to supply the carrier gas. When handling the gas cylinders, observe the following suggestions.
 - Keep gas cylinders in a well-ventilated area outside of the instrument installation site. Avoid exposure to direct sunlight. Use lines to transport the gas from the cylinders to the instrument. For flammable gases, this precaution is required by law.
 - Do not place the high-pressure gas cylinder in a location where the temperature can exceed 40 °C.
 - Choose an instrument installation site with sufficient ventilation, and include checking for gas leaks using an electronic gas leak detector in your daily inspection procedure. Do not smoke or use open flames within 5 m of the instrument when using highly combustible gases, such as acetylene and hydrogen, or potentially combustible gases, such as oxygen and nitrous oxide. Install and maintain effective fire extinguishers.
 - Secure the high-pressure gas cylinder with a cylinder stand or chain, etc., so that it does not fall over.
 - Be sure to use a pressure release valve specified as "not to be used with oil." Also, do not use a pressure release valve having piping, that is in contact with gas, whose inner surface is oily.
 - · When finished using the gas, immediately close the main cylinder valve.
 - Verify that the pressure gauges are functional at least once every three months.
 - Warning signs (adhesive aluminum plates) are available to indicate hydrogen gas use. Ask your Shimadzu representative for more details. Signs are supplied free of charge to sites in which they are mandatory.
- Legal authorization is required to use cylinders with a capacity of 300 m3 or greater.

Operation Precautions

- Always wear safety glasses or goggles when handling solvents. If solvent gets into the eyes, blindness could result. Should solvent get into the eyes, immediately flush with large amounts of water and seek medical attention.
- Do not place solvents near PCs, printers or other instruments, as fire or instrument damage could result.
- Do not use flammable sprays (hair sprays, insecticide sprays, etc.) near this instrument, as they could ignite and cause a fire.

Handling Emergencies

The following measures should be taken in the event of an emergency such as a malfunction of the gas chromatograph mass spectrometer.

Take adequate precautions and contact your Shimadzu representative as necessary before resuming use of the instrument.

Emergency Shutdown Procedure

- 1 Turn OFF the gas chromatograph mass spectrometer.
- 2 Turn OFF all accessories.
- 3 Close the valves for the pipes supplying carrier gas, CID 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.

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Two operation guides, Basic Operation Guide and Method Development Guide, are available for the GCMS-QP series and TQ series models.

This document covers the basic operations related to the QP series and TQ series.

Name	Contents
Basic Operation Guide	Covers the procedures to perform analysis using the existing method files for the GCMS-QP series or TQ series models and to create new method files (for Scan mode or SIM mode).
Method Develop- ment Guide	Mainly covers the procedures to create method files (for SIM mode or MRM mode, etc.) using the Smart database.

Icons and windows for functions that can only be used on the TQ series, QP2100 Ultra, QP2100 SE or QP2020 will not be displayed on the software if the GCMS model used is QP2010, QP2010 Plus or PARVUM2.

Indicates the procedure that can be used on the GCMS-TQ series models.

Indicates the procedure that can be used on the GCMS-QP2010 Ultra, GCMS-QP2010 SE or GCMS-QP2020 models.

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.

lcon	Name	Description
GCMS Browser	GCMS Browser	Used to perform qualitative and quantitative processing, print reports, and perform other data processing tasks for multiple data files.

1.2 Routine Analysis Operation Flowchart



1.3 Flowchart of Qualitative and Quantitative Analyses

1.3 Flowchart of Qualitative and Quantitative Analyses





2.1 Turning ON the Power

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

Switch ON any sample pretreatment unit connected to the system before switching ON the GCMS system.

When using a TQ series model, open the CID gas (argon gas) supply valve and supply the CID gas required for measurements in MRM mode.

Turn ON the power to the GC.





Turn ON the power to the MS.





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





(GCMS Real Time Analysis) icon.

The [GCMS Real Time Analysis] program starts.

Double-click the



2.2 Layout of Operating Areas



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.
0	Toolbar	Real Time Analysis, Analysis Editor, Postrun Analysis, and Browser	Displays command tool buttons corresponding to the window currently open.
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.
0	Instrument Monitor	Real Time Analysis	Displays analytical instrument parameter values in real time.

No.	Name	GCMS Program	Explanation
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.

2 Starting GCMS

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 GCMS 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 K Maintenance*" *P.104*.

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

2

2.4 System Configuration

Check and set the modules used for analysis using the procedures described below. If the column has been changed, enter the column information using the procedure in the [MS Navigator] window.

2.4.1 Setting the Modules Used for Analysis

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





1

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 is to register the module in [Modules Used for Analysis].
- 3 Click [Set].





Setting the CID Gas

For the GCMS-TQ series model, the default is set to use CID gas (argon gas). Turn OFF the CID gas to perform analysis using only the Q3 Scan or Q3 SIM mode.

- 1 Double-click 🔟 (MS) icon under [Modules Used for Analysis].
- 2 Deselect the [Use CID Gas] checkbox.

DC-20i SPL1 Co	olumn MS			
<u>N</u> ame :	MS			
Detector Type :	MS			
<u>S</u> erial # :	O20705100198J1	ROM V	ersion :	1.10
Model :	Dual Stage TMP (TQ80	40) <u>M</u> anufad	ctured Year-Month :	2013-08
<u>U</u> nit ID :				
Interface	CID Gas	as (Initial value of tu	ining) : 200	kPa
<u>H</u> eat Port :	DET1	Max <u>T</u> emp.:	350 °	С
Ion Source		Reag	ent Gas	
Typ <u>e</u> :	El 🔻	Por	1: None	Ŧ
Temperature :	200 °C	Port	l2∶ None	Ŧ
Vacuum Unit				
Tu <u>r</u> bo Molecular Pu	ump1: 200	Pirani <u>G</u> au	ge(Lower Vacuum) :	Present
Tur <u>b</u> o Molecular Pu	ump2 : 200	lo <u>n</u> Gauge	(Higher Vacuum) :	Present
Rot <u>ary</u> Pump 2 :	None 🔻			
Jet Separator : (Present None	Vacu	uum <u>U</u> nits : F	a 🔻
0 <u>I</u> Type : Nor	ne		Test Value of Sy	ste <u>m</u> Check

3 Click [OK].

Returns to the [System Configuration] sub-window.

4 Click [Set].

The configuration has now been set to use no CID gas. From now on, parameters regarding CID gas will not be displayed.

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	<u>C</u> lose
Not Ready 🕖 🔽 Vacuum Restart Mode	
	Advanced >>



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

? 🛛
Advanced >>

2 Starting GCMS

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

5 Click (Filament ON/OFF) to turn OFF the filament.

Click 🔀 button in the top-right corner to close the [Tuning] window.

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

	[×
_ ć	j'	×

GCMS Real Ti	ne Analysis					
(0311] Save current Tuning File? C:\GCMSsolution\System\Tune1_default.qgt						



Click the [Top] icon on the assistant bar.

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.

Perform autotuning periodically, even with the vacuum system operating.

Create calibration curves again after performing autotuning.

2.7.1 Setting Analysis Conditions

If no analysis conditions have been created, start from "2.7.2 Executing Autotuning" P.13.

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 崖 (Open) on the toolbar.

The [Open Method File] sub-window opens.





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

The method file is loaded.

🔐 Open Method File 🛛 💽							
Look in:	📗 Training	•	G 🍺 📂 🛄 🛪				
Ca.	Name	*	Date modified	Туре			
	Herbicide_S	Scan_example.qgm	12/02/2014 7:16 PM	GC/MS M			
Recent Places	Herbicide S	SIM example.ggm	12/02/2014 2:15 PM	GC/MS M			
Desktop							
Computer							
	•			4			
Network			(=				
	File <u>n</u> ame:	Herbicide_Scan_example.qgm		<u>O</u> pen			
	Files of type:	GCMS Method File (*.qgm)	- T	Cancel			

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] and click (Save) on the toolbar.



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

'alve:Openì

The set parameters are transferred to the instrument. When the parameter values become equal to the settings, [GC: Ready] and [MS: Ready] are displayed.

dmin)	- Method	- [Acc	juisiti	on - PAH	_Sc
ment	Acquisition	Data	Tools	Window	Hel
<u>.</u> K	Plot			i i	9
<u> </u>	Sample L	ogin		1	
letho	Download	Н		a	me :
	Start			,	:
eration	Extend			c	riptioi
	Stop				níx1
	Download	d Initial	Parame	ters	

2.7.2 Executing Autotuning



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

The [Tuning] window opens.



2 Starting GCMS



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

The [Peak Monitor] window opens.





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

The [Select Tuning Mode] sub-window opens.





Select Tuning Mode appropriate for the application



When using a TQ series, QP2010 Ultra, QP2010 SE or QP2020 model and 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.

- TQ series, QP2010 Ultra or QP2020: 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 Tuning Mode							
<u>T</u> uning Mode:	C High <u>C</u> onc.		C High <u>S</u> ens.				
	[<u>0</u> K	Help				

Perform Autotuning Even with CID Gas OFF

When using a TQ series model, a tuning method can be chosen depending on the measurement mode.



Tuning Information	
Target Condition	
Perform Auto Tuning Even with	h CID Gas OFF

Table: Estimated Time Required for Autotuning

System Configuratio n	System onfiguratio Tuning Condition Acquisition Mode n				Time	
Use CID Gas	Perform Autotuning Even with CID Gas OFF	Q3 Scan	Q3 SIM	MRM		
		Possible	Possible	Impossible	About 5 min	
		Possible *1	Possible *1	Possible	About 7 min	
	V	Possible	Possible	Possible	About 7 min (Recommended time)	

*1 : High sensitivity analysis

For GCMS-QP series models, autotuning takes about 3 minutes.



Select the filament to be used.

Detector	1.00 📫	kV
	Advanced	I
(
Filament	• #1 O	#2
Filament Low Vacuum	• #1 • • • • • • • • • • • • • • • • • •	#2 Pa



Click the [Start Auto Tuning] icon on the [Tuning] assistant bar.





Enter a file name and click [Save].

Autotuning starts.

When autotuning is completed, a report is printed.

Save Tuning F	ile As			×
Save <u>i</u> n:	🐌 Tune1	•	G 🤌 📂 🛄 -	
P	Name	*	Date modified	Туре
Recent Places	adefault.qgt		18/02/2014 10:06	GC/MS Tι
Desktop				
Libraries				
Computer				
Network C	•			4
	File <u>n</u> ame:	20131128.qgt	- [<u>S</u> ave
	Save as type:	GCMS Tuning File (*.qgt)		Cancel



2.7.3 Checking Autotuning Results

Check the results of autotuning.





- 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 relative intensity ratio for *m*/*z* 502 is at least 2 % (for QP2010S and SE : 1 %).
- 4 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 K Maintenance" P.104 to implement corrective measures.

3

Routine Analysis Flow

This chapter describes a series of routine analysis operations using the existing method files and batch files.

3.1 Preparing for Analysis

TQQP

When the ecology mode is set in the [GCMS Real Time Analysis] program, click [Cancel].

Ecology Mode
eco
I I I I I I
Cancel



Inspect consumable items and maintenance parts.

When a consumable item has passed its recommended replacement point, or when the column requires maintenance, perform maintenance with reference to "*Appendix K Maintenance*" *P.104*.





Perform autotuning.

Perform autotuning periodically (once every two weeks, for example) even with the vacuum system operating, referring to "2.7.2 *Executing Autotuning*" P.13. When quantitative analysis is to be performed, create calibration curves again after autotuning.



Create a new folder.

[Create New Project (Folder)] can be used to create a new folder at the same directory level as currently open in Data Explorer and to copy the target files.

Data Explorer - Batch	h 🛛 🛛	Create New Porject (Folder)
Project in :		Project <u>N</u> ame:
D:\20131127	•	20131128
File Name	Modified Date	Copy checked files in the current project to the new project
Qual	2/7/2014 11:29 PM	V Method Files
Quan	3/4/2014 7:18 PM	Batch Files
		Report Format Files
il i		OK Cancel

3.2 Editing a Batch File

For routine analyses, it may be more convenient to load an exiting batch file and partially edit it. The following procedure describes how to edit information in specified rows(s) collectively.



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





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

The [Batch Table] window opens.



(Example of a batch table for qualitative analysis)

Folder: D	:\20131127						
	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File
1	1	Methylene Chloride		0:Unknown		Herbicide_Scan.ggm	Methylene Chloride
2	2	Sample1	UNK-0001	0:Unknown		Herbicide_Scan.ggm	Sample
3	3	Sample2	UNK-0002	0:Unknown		Herbicide Scan.ggm	Sample

(Example of a batch table for quantitative analysis)

Fol	lder: D	:\2013112	27					
		Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File
1		1	Methylene Chloride		0:Unknown	ΠΩΤ	Herbicide_SIM.ggm	Methylene Chlo
2		2	STD 5ppb	STD-0001	1:Standard:(I)	IT QT	Herbicide_SIM.ggm	STD 5
3		3	STD 10ppb	STD-0002	1:Standard	IT QT	Herbicide_SIM.ggm	STD 10
4		4	STD 50ppb	STD-0003	1:Standard	IT QT	Herbicide_SIM.ggm	STD 50
5		5	STD 100ppb	STD-0004	1:Standard	IT QT	Herbicide_SIM.ggm	STD 100
6		6	Sample1	UNK-0001	0:Unknown	ΠΩΤ	Herbicide_SIM.ggm	Sam
7		7	Sample2	UNK-0002	0:Unknown	IT QT	Herbicide SIM.ggm	Sam



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

1 Click on the row number to be edited to highlight the whole row.

Folde	er: D:\20131	127					
	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File
1	1	Methylene Chloride		0:Unknown	IT QT	Herbicide_SIM.ggm	Methylene Chloride
2	2	STD 5ppb	STD-0001	1:Standard:(I)	IT QT	Herbicide_SIM.ggm	STD 5ppb
3	3	STD 10ppb	STD-0002	1:Standard	IT QT	Herbicide_SIM.ggm	STD 10ppb
4	4	STD 50ppb	STD-0003	1:Standard	IT QT	Herbicide_SIM.ggm	STD 50ppb
5	5	STD 100ppb	STD-0004	1:Standard	IT QT	Herbicide_SIM.ggm	STD 100ppb
6	6	Sample1	UNK-0001	0:Unknown	IT QT	Herbicide_SIM.ggm	Sample1
17		Sample2	UNK-0002	U:Unknown	ារបា	Herbicide SIM.ggm	Sample2

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.



Drag the mouse from the row of the unknown sample to the row specified with serial numbers.

Folder: D	:\2013112	7					
	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File
1	1	Methylene Chloride		0:Unknown	IT QT	Herbicide_SIM.ggm	Methylene Chloride
2	2	STD 5ppb	STD-0001	1:Standard:(I)	IT QT	Herbicide_SIM.ggm	STD 5ppb
3	3	STD 10ppb	STD-0002	1:Standard	IT QT	Herbicide_SIM.ggm	STD 10ppb
4	4	STD 50ppb	STD-0003	1:Standard	IT QT	Herbicide_SIM.ggm	STD 50ppb
5	5	STD 100ppb	STD-0004	1:Standard	IT QT	Herbicide_SIM.ggm	STD 100ppb
ß	ГК	Sample 1	บทห-บบก	1:Unknown	าเซเ	Herbicide_SIM.ggm	Samplel
7	7	Sample2	UNK-0002	0:Unknown	IT QT	Herbicide_SIM.ggm	Sample2
8	1			0:Unknown	IT QT		
9	1			0:Unknown	ПОТ		
10	L 1			0:Unknown	IT QT		



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

The entire content of the first row is copied.

GCMS	6 Real '	Time Aı	nalysis (Admir	n) - [Bato	h Table
👺 File	Edit	View	Instrument	Batch	Tools
D 🗲		Fill Seri	es		
		Fill Dov	vn		



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

Edited parameters will be appended with serial numbers. Modify the sample name, etc. if necessary.

🙀 GCMS	Real Time Analysis (Admin) - [Batch Table -
👋 File	Table Mission Terretorium Databa Terretori
	Fill Series
	Fill Down

1	1.
-()-
U	Hint

To collectively edit specified rows without changing other rows, right-click the cell in the first row and click [Fill Down] or [Fill Series].

Folder: D:\20131127								
	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	
1	1	Methylene Chloride		0:Unknown	ΠQT	Herbicide_SIM.ggm	Methylene Chloride	
2	2	STD 5ppb	STD-0001	1:Standard:(I)	ΠQT	Herbicide_SIM.qgm	STD 5ppb	
3	3	STD 10ppb	STD-0002	1:Standard	ΠQT	Herbicide_SIM.qgm	STD 10ppb	
4	4	STD 50ppb	STD-0003	1:Standard	ITQT	Herbicide_SIM.ggm	STD 50ppb	
5	5	STD 100ppb	510 A			Herbicide_SIM.ggm	STD 100ppb	
6	6	Sample1	Fill Series			Herbicide_SIM.ggm	Sample1	
7	7	Sample2	Fill Down			Herbicide_SIM.qgm	Sample2	
8	1							
9	1		Cut	(Ttrl+ Y			
10	1		Cut	`				
			Copy	(trl+C			



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.





Set the syringe rinse solvent and samples in the autosampler.

3 Routine Analysis Flow



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

Analysis starts. When the "Do you want to go into the ecology mode after batch processing ends?" message appears, click [Yes].





- To abort batch processing, click the (Stop) icon on the [Batch] assistant bar.
- To execute only specified rows, select the rows by clicking or dragging the mouse, then start the analysis.

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

 For details on how to create data file names automatically or how to change settings for continuous data acquisition during the measurement, refer to "Appendix D Batch File" P.74.

3.3 Dana Analysis

Reference

Refer to "4.5 Analyzing Data" P.34 when performing qualitative analysis. Refer to "5.3 Analyzing Data" P.54 when performing quantitative analysis. Refer to "Appendix L Quantitative Browser" P.110 when quantitating multiple samples.


4.1 Selecting a Folder

1	Start up the [GCMS Real Time Analysis] program.
2	Click the 🛛 🕺 (Data Explorer) icon on the toolbar to display Data Explorer.
	GCMS Real Time Analysis (Admin) - Batch - [Acquisition File Edit View Method Instrument Acquisition Defined File Name Modified Date Acquisition
3	Click (Project (Folder) Selection). The [Project (Folder) Selection] window opens.
	Data Explorer - Batch Image: Complementary of the second seco
4	Click the folder to be used.
	Project(Folder) Selection
	Look m: C:\LLMS solution\Sample\Training Close New Folder QP2010 Plus QP2010 Plus QP2010 SE QP2010 Ultra QP2010 Ultra QP2010 Ultra QP2010 SE Description SampleData(TQseries) SampleData(TQseries) Description SampleData(TQseries) Description Descrip
5	Click [Close].

4



Creating a Folder

Click the desired hard drive or folder and then click [New Folder].
 The [Create New Folder] window opens.

Project(Folder) Selection	—	
Look in : C:\2013		Close
<u> </u>	25	New Folder
	27 28	
⊕	ion la	

2 Type a folder name and click [OK].

A folder is created in the drive or folder selected in step 1, and the [Project (Folder Selection)] window returns.

Create New Folder
Create New Folder under the
C:\2013
Please input new folder name
20131129
OK Cancel Help

4.2 Creating a Method File

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



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

The [Acquisition] window opens.





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



4.2.1 Setting Autosampler Parameters



Click the [Sampler] tab and specify the number of rinses appropriate for the sample.

# of <u>R</u> inses with Solvent (Pre-run) :	1	ן		
# of Rinses with Solvent (Post-run) :	3			
# of Rinses with <u>S</u> ample :	1	J		
Plunger Speed(Suction) :	High	C Middle	C Low	
⊻iscosity Comp. Time :	0.2	sec		
Plunger Speed(Injection) :	High	C Middle	C Low	
Syringe Insertion Speed :	High	C Low		
Injection Mode :	0: Normal			S <u>e</u> t
Advanced				

4.2.2 Setting GC Parameters



Click the [GC] tab and set the analysis conditions.

- 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.

Middle bore ca (I.D. 0.2	ipillary column 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		

Typical Pressure Settings for Carrier Gas

- 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.

4.2.3 Setting MS Parameters

3 🔿 MS 🖣 Sampler 🔟 G GCMS-QP2010 200 Ion Source Temp 250 Absolute Interface Temp Detector Voltage Relative to the Tuning Resul 2.5 Solvent Cut Time 02 kV ro Scan Width 0 Threshold 0 Use MS Program Set... GC Program Time 19.67 min #2 - Event#1 Start Tin Ch1 Enc (min) m/7 m/7 5 2 6

Click the [MS] tab and set the analysis conditions.

- 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 24).

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. Increasing the detector voltage by 0.1 kV increases the peak intensity by 2 to 4 times.

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



- 5 Select [Scan]. (For TQ series models, select Q3 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).

4.2.4 Setting Similarity Search Parameters

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

The [Qualitative Parameters] window opens.

🙀 GCMS Real Ti	me Analy	sis (Admin)	- [Acquis	ition -	Untit	led, l
File Edit Viev	v Method	Instrument	Acquisition	Data	Tools	Wind
0 🖻 🖬 🖨	Instru	iment Parame	ters			
X	Qualit	ative Paramet	ers			
Acquisition	Quart	atative naram	C(C) 3			
rioquintion	Data	view Paramete	ers			



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

Qualitative Parameters					×
Peak Integration Spectrum Pr	oces: Sir	nilarity Search	etention Index Colu	mn Performance	
Library File Name:		Min.SI:			
C:\GCMSsolution\Library\NIS	ST11.lib	[] <u>-</u>	Search Denth:	No PreSearch	1
C:\GCMSsolution\Library\NIS	ST11s.lib	0	Max.Hit#:	25	
		0	Do not include	duplicate hits	3
		0	Reverse Search	n	
		0	- 10	+ 10	
Post-search: 🔲 Match (Case				
			Parameter		
Index 1 No Setting			Parameter		
Index No Setting			Parameter		
1 No Setting			Parameter		
Index 1 No Setting ∢			Parameter		•
Index I No Setting			Parameter		,
Index 1 No Setting ∢ ™			Parameter		•
Index 1 No Setting			OK	Cancel H	elp
Index I No Setting			Parameter OK	Cancel H	elp
Index 1 No Setting			OK 4	Cancel H	Þ

The [Open File] window opens.

🏭 Open					×
Look in:)) library		•	G 🦻 🖻 🛄 -	
æ	Name	*		Date modified	Туре
Recent Places	MIST11			6/20/2011 4:39 PM 6/20/2011 4:19 PM	Library Fil Library Fil
Desktop					
Libraries					
Network	•				۴
	File name:	NIST11		-	Open
	Files of type:	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.

4.2.5 Saving the Method File





Enter a file name and click [Save].

🙀 Save Method I	File As			×
Save in:	📗 Training	•	G 🌶 📂 🛄 🕶	
en	Name	*	Date modified	Туре
Recent Places		No items match your	search.	
Desktop				
Libraries				
Computer				
	•	III		4
Network	File name:	Herbicide_Scan	-	Save
	Save as type:	GCMS Method File (*.qgm)	▼	Cancel

4.3 Repeating Autotuning

If autotuning has not been performed under the analysis conditions, perform the procedures described under "2.7 Autotuning" P.12.

4.4 Sequential Analysis

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

4.4.1 Creating a Batch File



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

Batch Table Wizard - Line1 Unknown Sample (1)	
Unknown Sample	5
Sample Count: 1	<u> </u>
Sample Name: Unknown Sample	
Auto-increment Sample ID: UNK-0001	
V Auto-increment	
< Back Next >	7

- 5 Input [Vial #] and [Sample Count].
- 6 Input [Injection Volume].
- 7 Click [Next].

Batch Table Wizard - Line1	Unknown Sample (2)	
	Data Create Filenames Automatically	8
	< Back Finish	9

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



It is recommended to measure the blank (solvent, etc.) before starting analysis.

- 1. Insert a row above the first row.
- 2. Copy a row for the unknown sample and paste it on the first row.
- 3. Edit the vial #, sample name and data filename.

Folder: C:	:\GCMSso						
	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File
1	10	Methylene Chloride	UNK-0001	0:Unknown		Herbicide_Scan.qgm	Methylene Chloride.qgd
2	1	Unknown Sample	UNK-0001	0:Unknown		Herbicide_Scan.qgm	Sample1.qgd

4.4.2 Saving Batch Files

S	el	ect	t [S	ave	Batch	File	As]	on	the	: [Fi	ile]	mer	ıu.
	-	GCN	IS Re	al Tim	e Analysis	(Admi	n) - [B						
	10	File	Edit	View	Instrument	Batch	Tools						
		N C	ew Bal pen Ba lose Ba	tch File atch File atch File	e	Ctrl+O							
		_ <	ava Ra	stoh File			n S						
		S	ave Ba	atch File	As		n S						
		S	ave Ba	atch As	Template		vn S						



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

🙀 Save Batch File	e As			×
Save in:	20131127	•	G 🤌 📂 🛄 🗸	
C	Name	*	Date modified	Туре
Recent Places	∰ Qual ∰ Quan		2/10/2014 2:18 AM 3/4/2014 7:15 PM	GC/MS Ba GC/MS Ba
Desktop				
Libraries				
Computer				
Network	•	III		4
	File <u>n</u> ame:	20131128_1	-	<u>S</u> ave
	Save as type:	GCMS Batch File (*.qgb)	•	Cancel

4.4.3 Executing Sequential Analysis

Set the syringe rinse solvent and samples in the autosampler.



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



4.5 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

4.5.1 Loading Data Files



Double-click the data file to analyze.

The data file opens. If the required folder is not found, refer to "4.1 Selecting a Folder" P.23.

Data Explorer - Data	X						
Project in :							
C:\GCMSsolution\Sample\Training							
File Name	Modified						
Bi Sample1	1/29/201						
Scan_STD	2/12/201						

4.5.2 Displaying Mass Spectra



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

- 2 Move the mouse pointer to the peak top and double-click.
- 3 Click <u>[</u> (Spectrum Subtraction) on the toolbar.
- 4 Double-click at the background processing position.

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

Example 2)



Example 3)

Background spectrum can be subtracted from one of positions.

If a red peak appears on a mass spectrum, it indicates that the peak is saturated. This spectrum has a different pattern (intensity ratio) from the mass spectrum for the target compounds. In such a case,

click the left and right arrow buttons Scan \checkmark to select a mass spectrum that shows no red peaks.

4.5.3 Searching for Similarity

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





Check the similarity search results.



- 1 Use to switch between the mass spectra for the compounds found.
- 2 Select the checkbox for the applicable compound to enter a compound name in the spectrum table.
- 3 After checking the mass spectra, click (Register Target Spectrum to Spectrum Process Table). The mass spectrum is registered.

-PHint

By registering the target mass spectrum in the spectrum process table, you can re-check the similarity search results or output them in reports.

4 Close the [Similarity Search Results] window.

4.5.4 Editing the Spectrum Process Table

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

The [Qualitative Table] window opens.





Click 🔲 (Maximize).

Double-click [Done] in the first row of the spectrum process table.

Qualitative Table Drint Edit View Similarity Search											
Spectrum Background								^			
	Ret.Time	Start Tm	End Tm	Ret.Time	StartRT	EndRT	Carmh	Report	Event	Name	1 🗆
1	5.480			5.545		-	Done	~	1	Hexachlorocyclopentadiene	
2	6.495			6.540				V	1	Acenaphthene-d10	1
3	8.290			8.325			Done	V	1	Simazine	1
1	8.365			8.395			Done	V	1	Atrazine	=
i i	8.730			8.760			Done	V	1	Anthracene-D10-	1 1
	9.690			9.725			Done	V	1	Alachlor	
	10.300			10.335			Done	1	1	Metolachlor	
	11.470			11.520			Done	1	1	Butachlor	
											-
											Ŧ
I 🕨	Spectrum Proce	ss /			•				111		. F

The [Similarity Search Results] window opens.



¹

To sort the spectrum process table in chronological order, click [Sort Table] on the [Edit] menu.

Select All Copy Delete Rows Delete Current Table Delete All Peak Tables Register to Spectrum Process Table Register to Library	Edit Compound Name	Backgroun
Select All Copy Delete Rows Delete Current Table Delete All Peak Tables Register to Spectrum Process Table Register to Library	•	StartRT
Copy Delete Rows Delete Current Table Delete All Peak Tables Register to Spectrum Process Table Register to Library	Select All	-
Delete Rows Delete Current Table Delete All Peak Tables Register to Spectrum Process Table Register to Library	Сору	
Delete Rows		
Delete Current Table	Delete Rows	
Delete All Peak Tables	Delete Current Table	
Register to Spectrum Process Table Register to Library	Delete All Peak Tables	
Register to Spectrum Process Table Register to Library		
Register to Library	Register to Spectrum Process Table	
	Register to Library	



-Ď-Hint

After check is complete, close the [Similarity Search Results] window.

• To edit a compound name, select the desired row and click [Edit Compound Name] on the [Edit] menu. Enter the compound name in the [Edit Compound Name] window displayed and click [OK].

 yiew similarity search							
Edit Compound Name	Background						
	StartRT	EndRT	Search	Report	Event	Name	
Select All			Done	V	1	Hexachlorocyclopentadiene	
Conv			Done	V	1	Acenaphthene-d10	
copy			Done		1	Simazine	
Delete Rows			Done		1	Atrazine	
Delete Rows	Done 📝 1 Phenanthrene-D10					Phenanthrene-D10	
Delete Current Table			Done		1	Alachlor	
Delete All Peak Tables	Edit Compound Name						
Register to Spectrum Process Table	Compound Name - Line# 5						
Register to Library	Phenar	nthrene-D10					
Sort Table					0	K Cancel	

 To delete a row in the spectrum processing table, select the desired row and click [Delete Rows] on the [Edit] menu.





Close the [Qualitative Table] window.

4.5.5 Saving Data Files



Click 📕 (Save) on the toolbar.

The qualitative table is saved in the data file.



4.6 Printing Qualitative Analysis Reports

It is convenient to use a template to create a report of analyzed data. Depending on the data, edit the area of the chromatogram to display in the report, or edit the number of compounds to be displayed in the report of similarity search results.

4.6.1 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.

Q.	GCMS	S Postr	un Ana	lysis (A	dmin) - R	eport Fo	ormat - [l		
Ľ	File	Edit	View	Item	Lavout	Page	Tools		
		New F	ormat	File	Ctrl+N				
		Open	rumai	riie		Cur	tv E		
		Close	Format	File			5		



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

le New		-
🔿 New File		
Use Template		
S Calibration Curv	e	
Chromatogram-	- Spectrum	
M DEFAULT		
A		
🔊 Qualitative Anal	ysis Report	:
Lel ringunurganou (Le	Compounds)	
No. 11. 11. 104	c 1)	
🔊 Quantitation (21	Lompoundsj	
🔊 Quantitation (21	Lompoundsj romato & CalCurve)	
Quantitation (21 Quantitation (CP Quantitative An	Lompounds) nromato & CalCurve) alysis Report	
Quantitation (21 Quantitation (CP Quantitative An Quantitative Re	compounds) nomato & CalCurve) alysis Report sult (Graph)	
Quantitation (21 Quantitation (Cf Quantitative An Quantitative Re	Lompounds) rromato & CalCurve) alysis Report sult (Graph) auth (Table)	
Quantitation (21 Quantitation (21 Quantitation (Cf Quantitative An Quantitative Re	Compounds) rromato & CalCurve) alysis Report sult (Graph) m	4
Quantitation (21 Quantitation (CF Quantitative An Quantitative Re Quantitative Re	Lonpounds) romato & CalCurve) alysis Report sult (Graph) m	
Ya Quantitation (21 Ya Quantitation (CF Ya Quantitative An Ya Quantitative Re	Lonpounds) romato & CalCurve) alysis Report sult (Graph) auth (Table) III	
Comment:	Lonpounds) romato & CalCurve) alysis Report sult (Graph) m	
Comment:	Compounds) rromato & CalCurve) alysis Report sult (Graph) 	•
A Quantitation (21 Q Quantitative An Q Quantitative An Q Quantitative Re Quantitative Re Comment:	Compounds) romato & CaCurve) alysis Report sult (Graph) avit (T-bla) III	 4
A Quantitation (21 Q Quantitative An Q Quantitative An Q Quantitative Re Comment:	Compounds) romato & CalCurve) alysis Report sult (Graph) me (T-bbb) m	4
Quantitation [2] Quantitation [2] Quantitation [2] Quantitative An Quantitative An Quantitative Re Comment:	Compounds) romato & CalCurve) alysis Report sub (Graph) are fit able) III	4



Click [OK].

The [Qualitative Analysis Report] format opens.

4.6.2 Editing Report Formats

Double-click on the chromatogram.

The [GCMS Chromatogram Properties] window opens.





Click the [Chromato] tab.





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

GCMS Chromatogram Properties	×
General Chromato Graph File	
Iype Overlap ▼ X 100 % X 50 % Image: Comp in the state of the stat	
Area X □ Auto 4 25 min	
Line With: 1 🚽 CCC Detector Cht 💌	
OK Cancel Apply Help	



Click [OK].

5

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.





Click the [Result] tab.

GCMS Library Properties	s	X
ResultTable General Position	ResultColumn Possibilities	File ResultSpectrum
Position	Title	
<u>T</u> op 27.8 mm	Library	



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

GCMS Library P	roperties					×			
ResultTable General	R Position	esultColumn TargetSp) bectrum	ResultSti Resul	uct t	File ResultSpectrum			
⊽ Sp <u>e</u> c	trum Posit X Y	ion 0 mm 0 mm	X X Y	150 mm 35 mm	lf th are con are [Re:	e checked items not displayed, firm whether they within the [Size] of sult] in [Position]			
☐ <u>T</u> able	× Posit	0 mm 35.5 mm	X Y	150 mm 40 mm	tab.				
√ St <u>r</u> uc	ture Posit X Y	120 mm 10 mm	X X Y	30 mm 20 mm					
 Print f Print f 	Print the Hit Compounds Maximum Compound Number:								
				. 1		1			
		UK	Canc	el	Apply	Help			

-Ĥ-Hint

- Selecting [Print the Hit Compounds] prints the report for the maximum number of search results to display in order starting with the highest similarity.
- Selecting [Print Only Specified Compound] prints the report for the compounds selected for registration in the similarity search.



Click [OK].

4.6.3 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.

CCMS Poetrun Analysis (Admin) - [Data Report - Sample1.qgd(Report in Data File)]	
Print [lext Page Prev Page One Page Zoom In Zoom Out Close	
Carset Coveryn Analysis (Admin) - [Data Report - Sample1.agd(Report in Data File)] Pert. Pert. Rea Page. Prov Page. One Page. Zoon In. Zoon Ou. Gose Guardiative Analysis Report Guardiative Analysis	Gualitative Analysis Report Series The main series The
1/9	2/9
Pages 1-2 / Total 9	NUM



Click 📕 (Save) on the toolbar.

The report is saved as part of the data file.





5.1 Creating a Method File

With reference to "4 Qualitative Analysis" P.23 analyze standard samples (including internal standard substances when using the internal standard method for analysis) 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.



Table Wizard 1/7] window.

Click [Next] in the [Compound Table Wizard 2/7] window.

Select a row in the table, check the mass spectrum for each compound, and click [Next] in the [Compound Table Wizard 3/7] window.

Select [Use current Spectrum Process Table] and then click [Next] in the [Compound

7

6

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

Compound Tab Wizard 4/7	
Quantitative Method: Unit: mg/L Internal Standard Eormat of Concentration Calculated by: Area Height Calculated by: Oncentration Calculated by: Image: Concentration Calculated by: Oncentration Calculated by: Image: Concentration Calculated by: Image: Concentration Calculated by: Image: Concentration Calculated by: Image: Concentration Carcel Help	- 4 5
0	

No.	Item	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.
0	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.	Item	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.
0	# of Reference lons	Input the number of reference ions used to perform peak identification.
0	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].

Retention Time:	5.480 min	urop	down list in the ne	au.		
Ret. Index:	0	ſ	Туре	m/z	Rel Inten.	
	T		Target Ion	237 🗨	100.00	
Туре:	Target	2	Ref.lon	239	66.12	
Compound Name		3	Ref.lon	235	58.83	
Compound Name		4	Not used	241	20.83	
Hexachlorocy	clopentadiene/	5	Not used	272	10.00	
Cet name		6	Not used	130	18.63	
O Set name		7	Not used	118	16.57	
Hexachlorocy	clopentadien 🕟	8	Not used	274	15.89	
		9	Not used	95	14.62	
		10	Not used	141	14.61	

- 1 Change the compound displayed by changing the ID number.
- 2 Select [Target] in the [Type] list. Select [I.S.] when setting for an internal standard.

- 3 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 mass value, click in the cell containing that value, click the resulting arrow button, point your cursor at the desired peak on the mass spectrum, and then double-click it.



Click [Finish].

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

														00 1101
ID#	Name	Туре	ISTD Gr	m/z	Ret.Time	Ret. Index	Unit	Ref.lons	Conc.1	Conc.2	Conc.3	Conc.4	Event	STD
1	Hexachlorocyclopentadiene	Target	1	237.00	5.480	0	mg/L	239.00-235.00	0.005	0.01	0.05	0.1	1	Regis
2	Acenaphthene-D10	ISTD	1	164.00	6.495	0	mg/L	162.00-160.00	0.1	0.1	0.1	0.1	1	Regis
3	Simazine	Target	1	201.00	8.290	0	mg/L	173.00-186.00	0.005	0.01	0.05	0.1	1	Regis
4	Atrazine	Target	2	215.00	8.365	0	mg/L	200.00-202.00	0.005	0.01	0.05	0.1	1	Regis
5	Phenanthrene-D10	ISTD	2	188.00	8.735	0	mg/L	189.00-184.00	0.1	0.1	0.1	0.1	1	Regis
6	Alachlor	Target	2	237.00	9.690	0	mg/L	160.00-188.00	0.005	0.01	0.05	0.1	1	Regis
7	Metolachlor	Target	2	162.00	10.300	0	mg/L	238.00-240.00	0.005	0.01	0.05	0.1	1	Regis
8	Butachlor	Target	2	237.00	11.470	0	mg/L	176.00-160.00	0.005	0.01	0.05	0.1	1	Regis
9		Target	2	TIC	0.000	0	mg/L		0.005	0.01	0.05	0.1	1	

11

Click 63 View to set the compound table to the display mode.

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



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.



6.316au





Click [Save].

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

🔇 Save Method /	As			—
Save in:	鷆 Training		- G 🤌 📂 💷-	
(Ba	Name	*	Date modified	Туре
Recent Places	Herbicide_S	can	2/12/2014 7:16 PM	GC/MS M
Desktop				
Libraries				
Computer				
	•	m		4
Network	File name:	Herbicide_Scan	[Save
	Save as type:	GCMS Method File (*.qgm)	•	Lancei

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

5.1.2 Creating a SIM Table



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





Enter a file name and click [Save].

The [Creation of Automatic MS Table [COAST]] window opens.

💐 Select Method	l File				- ×-
Look in:	📗 Training	•	• 🎯 🦻	>⊞ و	
æ	Name	*	Date mo	dified	Туре
Recent Places	Herbicide_Sc	an	2/12/201	4 7:16 PM	GC/MS M
Desktop					
Libraries					
Computer					
Q	•	III			4
Network	File name:	Herbicide_SIM		•	Save
	Files of type:	GCMS Method File (*.qgm)		•	Cancel

Click (Maximize) in the [Creation of Automatic MS 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.



-Ò-

• To ensure sufficient sensitivity:

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.

• To edit table rows (i.e. groups):

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 split groups:

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].
- Click the inserted row and drag the mouse on the chromatogram to specify and enlarge the desired area.
- 4. 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



Start the [GCMS Real Time Analysis] program and 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.





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

Batch Table Wizard				—
	Batch Table	@ Ad		
	Batch Type	Append		
	Line1	Line2	Line1&Line2	
	Sample Type			
	 Standard Standard 	& Unknown Only		
Concertant?)	O Unknown	Only		
	Method File:			2
	Data Processing	lwi.qgm		
	Quantitati	ve	Qualitative	
	< Back	Next >		

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

Batch Table Wizard - Line	L Standard Sample (1)	
	Standard Sample	5 7 6
	Auto-increment Auto-inc	_ 8

5 Input [Vial #].

The number of calibration points is loaded automatically from the method.

- 6 Input [Injection Volume].
- 7 Input [Average Count] (i.e., the number of repetitions).
- 8 Click [Next].

Batch Table Wizard - Line1 Standard Sample (2)	
Data Create Filenames Automatically Data File Name: STD1 Auto-increment Report Out Peport Format File: Data Description	9
< Back Next >	- 10

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

Batch Table Wizard - Line1 Unknown Sample (1)	
Unknown Sample Vial #: 5 - 1 Sample Count: 2 - 1 Sample Count: 2 - 1 Sample Name: Unknown Sample Auto-increment Sample ID: UNK-0001	—11 —12 —13
✓ Auto-increment ✓ Auto-increment < Back	_14

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

Batch Table Wizard - Line1 Unknown Sample (2)	
Data Create Filenames Automatically Data Tile Name: UNK1 PALCO-INCREMENT Report Out Data Description	15
< Back Finish Cancel Haln	16

15 Enter [Data File Name].

If the file name ends with a number, the files are named sequentially.

16 Click [Finish].

The batch table is displayed.

Folder: C:\GCMSsolution\Sample\Training									
	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	Level#	Inj. Volume
1	1	Standard Sample	STD-0001	1:Standard:(I)	ITQT	Herbicide_SIM.qgm	STD1.qgd	1	1
2	2	Standard Sample	STD-0002	1:Standard	ITQT	Herbicide_SIM.qgm	STD2.qgd	2	1
3	3	Standard Sample	STD-0003	1:Standard	IT QT	Herbicide_SIM.qgm	STD3.qgd	3	1
4	4	Standard Sample	STD-0004	1:Standard	IT QT	Herbicide_SIM.qgm	STD4.qgd	4	1
5	5	Unknown Sample	UNK-0001	0:Unknown	ITQT	Herbicide_SIM.qgm	UNK1.qgd	1	1
6	6	Unknown Sample	UNK-0002	0:Unknown	ITQT	Herbicide_SIM.qgm	UNK2.qgd	1	1

It is recommended to measure the blank (solvent, etc.) before starting analysis.

- 1. Insert a row above the first row.
- 2. Copy a row for the unknown sample and paste it on the first row.
- 3. Edit the vial #, sample name and data filename.

Fol	Folder: C:\GUMSsolution\Sample\Training							
Г		Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File
1		10	Blank	UNK-0001	0:Unknown	ITQT	Herbicide_SIM.qgm	Blank.ggd
2		1	Standard Sample	STD-0001	1:Standard:(I)	ITQT	Herbicide_SIM.qgm	STD1.qgd
3		2	Standard Sample	STD-0002	1:Standard	ITQT	Herbicide_SIM.qgm	STD2.qgd
4		3	Standard Sample	STD-0003	1:Standard	ITQT	Herbicide_SIM.qgm	STD3.qgd
5		4	Standard Sample	STD-0004	1:Standard	ITQT	Herbicide_SIM.qgm	STD4.qgd
6		5	Unknown Sample	UNK-0001	0:Unknown	ITQT	Herbicide_SIM.qgm	UNK1.qgd
7		6	Unknown Sample	UNK-0002	0:Unknown	ITQT	Herbicide_SIM.qgm	UNK2.qgd

5.2.2 Saving Batch Files



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

Ctrl+O

Ŵ

•





÷

•

Save

Cancel

5.2.3 Executing Sequential Analysis

Save as type

Quant

GCMS Batch File (*.qgb)



Set the syringe rinse solvent and samples in the autosampler.



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



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.57*.

To change the method used to plot calibration curves, see "Appendix I Editing Parameters for *Quantitative Analysis*" P.96.



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



--Phint

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

The detected peaks are subjected to identification based on the retention times and ion ratios (**v** peak identification mark).



Chromatogram	Countermeasure		
No peaks are detected.	Perform manual peak integration.		
(c1, 604) (64, 60 (34, 60 ((P.58)		
7.0.			
6.5- 6.0-			
3.5			
5.6-			
4.6			
3.6			
2.5			
2.0			
1.0			



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 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.

	120					
⊟ Data Files	🔥 Single	🛵 Multi				
	(x10,000) Max			Intensity : 22,160		
Level 2 : 0.010000	2.0-239.0	<u>.</u>		Undo Zoom		
	-235.0	U	5	Redo Zoom		
STD3.QGD	1.0			Initialize Zoom		
Level 4 : 0.10000	-		Λ	Base Shift		
<u></u> 0104.400	5.00	5.25	5.50 * *	Peak Table		
	Туре	m/z	Inten.	Dask Integrate by ID		
	Target	237.00	21404	Manual Peak Integrate		
	Ind.1	239.00	13685			
	Ind.2	235.00	13156	Split Peak		



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

The [Select Base Line] window opens.




Select the baseline and click [OK].

The peak is integrated and identified.

Select Base Line	×
C Link Point	
• Horizontal	
C New Baseline	
OK Cancel <u>H</u> el	>

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	[Shift] + right-click-drag	Connects start point and end point as baseline.
Manual Peak Integration	[Ctrl] + right-click-drag	Connects points with horizontal baseline.

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.



2

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



5 Quantitative Analysis



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

is to be performed and click (Add). The data file is selected.

🔃 Select Data Fi	le			— X—)
Look in:	鷆 Training	•	G 🤌 📂 🛄 -	
Recent Places Desktop Libraries	Name Sample1 Scan_STD STD1 STD2 STD3 STD3 STD4 Unk2 Unk2	-	Date modified 1/29/2014 12:30 PM 2/12/2014 2:14 PM 3/4/2014 3:22 PM 3/4/2014 3:22 PM 3/4/2014 3:22 PM 3/4/2014 3:22 PM 3/4/2014 2:21 PM	Type GC/MS [GC/MS [GC/MS [GC/MS [GC/MS [GC/MS [
Network	<	III		OK
Selected Data Fil C:\GCMSsolutior C:\GCMSsolutior	e : NSample\Training\L NSample\Training\L	Ink1.ggd	Up Down	Caricel



Click [OK].

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

Folder: C:	:\GCMSsolution\Sample	\Training					
	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	Level#
1	Unknown Sample1	UNK-0001	1:Standard	ITQT	Herbicide_SIM.qgm	Unk1.qgd	1
2	Unknown Sample2	UNK-0002	1:Standard	ITQT	Herbicide_SIM.qgm	Unk2.qgd	1



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

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



Wizard

5.3.3 Checking and Correcting Quantitation Results

Check the quantitation results for the samples with unknown concentrations.



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

Create Compound Table
Quantitative
Calibration Curve



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

The data file being checked opens.

🔇 GCMS Postru	n Analysis (Admin) -	Data - [Data Ana
👫 File Comp	ound Table View	Qualitative Qu
🖻 🖬 🖉	3 🖪 醚 🖓	
X	Data Explorer - Data	
Quantitative	Project in :	
↑	\Sample\Training	•
Тор	File Name	Modif
	Million 10	3/4/20
2	🔠 Unk1	: 4/20
Load Method		3/4/20



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

The quantitation results are displayed.

							63	View 📝 E	dit
ID#	Name	Туре	ISTD Gr	m/z	Ret.Time	Ret. Index	Unit	Ref.I	-
1	Hexachlorocyclopentadiene	Target	1	237.00	5.480	0	mg/L	239.00-2	
2	Acenaphthene-D10	ISTD	1	164.00	6.495	0	mg/L	162.00-1	
3	Simazine	Target	1	201.00	8.290	0	mg/L	186.00-1	
4	Atrazine	Target	2	215.00	8.365	0	mg/L	200.00-2	
5	Phenanthrene-D10	ISTD	2	188.00	8.735	0	mg/L	189.00-1	E
6	Alachlor	Target	2	237.00	9.690	0	mg/L	160.00-1	
7	Metolachlor	Target	2	238.00	10.300	0	mg/L	162.00-2	
8	Butachlor	Target	2	237.00	11.470	0	mg/L	160.00-1	
								-	
✓ ► \Param': {Results } FroupParam's {Group <									



5

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

If necessary, see "Displaying Standard Spectra" P.63, "Displaying Reference Data" P.64 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.57.

-Hint

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	[Shift] + right-click-drag	Connects start point and end point as baseline.

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

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

However, if no concentration is displayed, character strings shown below are displayed according to the cause.

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.
	When the calibration curve is quadratic and the area is larger than the local maximum value (or smaller than the local minimum value), "" is displayed since the concentration cannot be calculated. The target component may be out of the measurement range. Confirm the peak.



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

The data file is saved.





Displaying Standard Spectra

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

When scan mode is used for measurements, data can be analyzed more easily by comparing the displayed spectrum with a standard spectrum.

1 Click [Spectrum View] - [Display Setting] on the [View] menu. If the [Spectrum Graph Display Setting] window is displayed, select [Display Standard Spectrum].

The standard spectrum is displayed.

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.



-Ú-Hint

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.

1 Select [Open Reference Data File] on the [File] menu to open the data file being referenced. The reference data is displayed.

🔇 GCM	S Postrun Analysis (A	(dmin)	Data - [Data	Analys
🔒 🗜 File	Compound Table	View	Qualitative	Quar
E	Open Data File Close Data File			
Q	Save Data File Save Data File As			TIC
	Load Method Save Method As			
	Open Reference Dat	a File		
	Close hererence par	a i iic	,	

Closing Reference Data

1 Click [Close Reference Data File] on the [File] menu and specify the reference file to close. The reference data file closes.

🔆 GCN	1S Postrun Analysis (A	\dmin) ·	- Data - [Data	Analysis - Unk	1.qgd]
🔒 🔣 File	Compound Table	View	Qualitative	Quantitative	Layout Tools V
E	Open Data File Close Data File			- ?	n 1
Q	Save Data File Save Data File As			TIC & MIC 8 3 ^{(x100,}	#4->#4
L	Load Method Save Method As			0.0 4	.5 5.0
	Close Reference Dat	ta File	•	STD1.q	gd(1)
	Export Data			All Dat	a
				240	00 (4.00)

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

Fixing the Intensity Axis

1 Right-click in [Quantitative View] and select [Fix the Intensity Axis to this Data] on the menu displayed to fix the intensity axis.



5.4 Printing Quantitative Analysis Reports

It is convenient to use a template to create a report of analyzed data.

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.

🔆 GCN	//S Postrun Analysis (Admin) - [Data Report - l	Jn
E File	Edit View Item Layout	Page Tool	5
Г	New Format File	Ctrl+N	J
	Open Format File	Ctrl+0	Ë
	Close Format File		
	Save Format File		ŀ





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

	_
File New	×
O <u>N</u> ew File	
• Use Template	
🕲 Quantitation (10 Compounds)	^
🙀 Quantitation (21 Compounds)	
ve)	
Uuantitative Analysis Report	
Cuantitative Result (Table)	
Similarity Search Result	
	×
Comment:	
	^
	\mathbf{v}
<u><</u>	
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.







Click (Save) on the toolbar.

The report is saved as a data file.



Shutting Down GCMS

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	
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

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.4 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.



4

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	Ĩ	.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.



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

B.1 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

- 1 Type the applicable word.
- 2 Select the applicable topic and click [Display].

Searching from the [Search] Tab

- 1 Type the applicable word and click [Search].
- 2 Select the applicable topic and click [Display].

B.2 Displaying Help with the F1 Key



Press the [F1] key on the keyboard.

Help for the open window is displayed.

Appendix C 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.

1

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.

Data Explorer - Method	I 🗵
Project in :	
\Sample\Training	•
File Name	Modifie
Herbicide_Scan	2/12/20



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



The [Sample Login] window opens.

ne1		(in a long (in a long a	an_examp		
cquisition Information					
Sample Name :	Sample1				
Sample ID :					
Data File :	Sample1.qgd			2	
Baseline Data :				2	
Data Description :					
				~	
ampler	•			•	
Vial # :	1				
Injection Volume :	1 ul	Syringe Capacity :	0	uL	
Multi Inj. Times :	1				
uning File :					

- 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].

-PHint

[Tuning File] is not set usually. If it is left blank, the tuning file saved in the previous tuning will be used.



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.





- In manual injection mode, inject the sample and then press [START] on the GC unit keyboard.
- 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.



D.1 Generating Filenames Automatically

In the [Settings] window displayed when clicking [Settings] on the [Batch] assistant bar, data filenames can be generated automatically. The settings are saved in the batch file.



Start the [GCMS Real Time Analysis] program. Click the [Settings] icon on the [Batch] assistant bar.





Specify the format of the data file names to be automatically created.



- 1 Click the [Data Filename] tab.
- 2 Select the [Create filenames automatically with] checkbox.
- 3 Add or delete items in the [Selected Items] box.
- **4** Click [OK].

When the settings are complete, the [Data File] column in the batch table is highlighted in yellow. Example: Automatically generating data filenames by putting [Batch Start Date] and [Sample Name] in the [Selected Items] box

Batch Start Date	Sample Name	Datafile (.qgd)		
	Standard 1ppb	20131220_Standard 1ppb_1		
00404000	Standard 10ppb	20131220_Standard 10ppb_2		
20131220	Standard 100ppb	20131220_Standard 100ppb_3		
	Unknown	20131220_Unknown_4		
	Unknown	20131220_Unknown_5		

Symbols that cannot be used in a data filename, such as "/" should not be included in the sample names.

D.2 Editing a Batch File



Modify a batch file.

GCMS Real Time Analysis (Admin) - C:\GCMSsolution	N20091115_operation guide\20091115_1.qgb - [Acquisition - PAH_5MA.qgm, 20091115_Mark001.qgd(Line1), BU008.20]
C:\GCMSsolution\20091115_operation guide\20091115_1.4 Folder: C:\GCMSsolution\20091115_operation guide Vial# Sample Name Sample ID Sample	op Type Analysis Type Method File Data File Levelli Ini, Volume ISTD AmL Report Output Report File Tuning File 🖉
1 Methytens Dixtode UNI-S0011 Oldraces 2 Standard Sample STD-0001 Standard 3 Standard Sample STD-0001 Standard 4 Standard Sample STD-0001 Standard 5 Standard Sample STD-0001 Standard 6 Istandard Standard Standard 7 Blank UNK-0002 Outnizow 6 Unk-0001 UNK-0002 Outnizow	ITOT PM4_SM age 2008THS_MIXED agd 1 Level Con Pint ITOT PM4_SM age 2008THS_ST06 agd 1 Level Con Pint ITOT PM4_SM age 2008THS_ST06 agd 2 1 Level Con Pint ITOT PM4_SM age 2008THS_ST06 agd 2 1 Level Con Pint ITOT PM4_SM age 2008THS_ST06 agd 2 1 Level Con Pint ITOT PM4_SM age 2008THS_ST06 agd 2 1 Level Con Pint ITOT PM4_SM age 2008THS_ST06 agd 4 1 Level Con Pint ITOT PM4_SM age 2008THS_ST06 agd 4 1 Level Con Pint ITOT PM4_SM age 2008THS_ST06 agd 4 1 Level Con Pint ITOT PM4_SM age 2008THS_ST06 agd 4 1 Level Con Pint ITOT PM4_SM age 2008THS_ST06 agd 4 1 Level Con Pint
Balch Project in :	Table] window and [Acquisition] window are displayed. To switch to the [Batch Table] window,
To The Name Modified Date PAH_San 11/15(2009-8:05 AM Date Sales Settings Vicand Vicand	1 1.00
Case	Image: 1,000000 Description: 150,0000 Description: 150,00000
	Uman Dis Di€ Teleforment 0.18 mm

- 1 Click on the table.
- 2 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.

D Batch File



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.

🙀 GCMS Real Tir	me Analysis	(A drr
👺 Eile Edit View	Instrument	Batch
	B	



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

The analysis restarts.



Some accessory/peripheral equipment may prevent using this function.

D.3 Adding Batch Files (Batch Queue)

D.3.1 Creating Batch Files to Add



GCMS Analysis Editor (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.

🖁 GCMS Analysis Editor (Admin) - [Batch Table - Untitled]												
👺 Eile Edit Vie	💯 Efe Edit View Instrument Batch Iools Window Help 🛛 🖉 🛪											
0088												
X	Data Explorer - Batch 🛛 🔀	Folder: C	\GCMSso	lution\20091115_op	peration guide							
Batch	Project in :		Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	Level#	Inj. Volume	ISTE
		1	6 🚖	Unknown Sample	UNK-0001	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample3.qgd	1	1	(Level1
	C:\GCMSsolution\20091115_operation guide 🗾	2	7	Unknown Sample	UNK-0002	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample4.ggd	1	1	(Level1
	[3	8	Unknown Sample	UNK-0003	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample5.qgd	1	1	(Level1
Top	File Name Modified Date	4	9	Unknown Sample	UNK-0004	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample6.qgd	1	1	(Level1
Top	20091115_1 11/18/2009 8:34 AM	5	10	Unknown Sample	UNK-0005	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample7.ggd	1	1	(Level1
		6	11	Unknown Sample	UNK-0006	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample8.ggd	1	1	(Level1
		7	12	Unknown Sample	UNK-0007	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample9.ggd	1	1	(Level1
California		8	13	Unknown Sample	UNK-0008	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample10.qgd	1	1	(Level1
Seturigs		9	14	Unknown Sample	UNK-0009	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample11.qgd	1	1	(Level1
		10	15	Unknown Sample	UNK-0010	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample12.qgd	1	1	(Level1



Name and save the batch file.

🙀 Save Batch File	e As			×
Save in:	鷆 Training	-	G 🏚 📂 🛄 -	
(An	Name	*	Date modified	Туре
Recent Places		No items match you	r search.	
Desktop				
Libraries				
Computer				
Network	•	m		Þ
	File name:	Quant	- (Save
	Save as type:	GCMS Batch File (*.qgb)	-	Cancel



- 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.



Quit the [GCMS Analysis Editor] program.

D.3.2 Adding Batch Files

1	
2	

Start the [GCMS Real Time Analysis] program.

Click the [Batch Table] window.

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

🚻 GC	MS Real T	'ime Analysis (Ad	min) - [Acqui	sition - PAH_SI	M.qgm, 2009111	5_blank001.qgd	l(Line1), BU008-2009111	7-RFchar	ge.qgt]					3 X
An Ele	A Effe Edit Yew Method Instrument Acquisition Data Iools Window Help _ B ×													
C:\GCN	Ssolution	\20091115 opera	tion quide\200	91115 1.ggb				*******	******			******		×
r older:	C:\GEMSsc	Sample Name	ration guide	Cample Tupe	Analusis Tuno	Mash ad File	Data File	Lought	Ini Volumo	ICTD Amt	Penert Output	Papart File	Tuning File	
-	Vidi#	Jampie Maine	Saliple ID	Sample Type	Analysis Type	Method File	Data File	LCVCI#	mi. Volume	1310 Allic.	nepoli output	neport rile	Tuning File	
1		Meinviene Unionde	UNK-0001	U:Unknown	IT OT	PAH_SIM.ggm	20031115_blank001.ggd			Level Lon	Pint			
2	4	Standard Sample	STD-0001	1:Standard:(I)	ITUT	PAH_SIM.qgm	20091115_STD5.qgd	1	1	Levell Lon	E Print			-
3	3	Standard Sample	510-0002	1:Standard	11 Q1	PAH_SIM.qgm	20091115_STD6.qgd	2		Level Lon	Print			-
4	4	Standard Sample	STD-0003	1:Standard	11 41	PAH_SIM.qgm	20091115_STD7.qgd	3	1	[Level1 Lon	Print			
5	5	Standard Sample	STD-0004	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD8.qgd	4	1	(Level1 Con	Print			
6	1	Blank	UNK-0001	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample3.qgd	1	1	(Level1 Con	Print			
7	6	Unknown Sample	UNK-0002	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample4.qgd	1	1	(Level1 Con	Print			
	X	Data Explorer - Me	sthod	×	Line1									
Aca	initian				Sample Name : Methy	lene Chloride								
Acqu	ISIOUT	Project in :			Sample ID · LINK-000	1						GC	Run	



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

The [Batch Queue] window opens.

e Analysis	(Admi	n) - Ba	atch - [B	atch 1	Table - 2	2009111	5_1.
Instrument	Batch	Tools	Window	Help			
5 🖪	Star Pau:	t se					
ta Explorer	Stop)					0
roject in :	Bato	:h Queu	ie				
\20091115_	Sett	ings					Ī
File Name 1120091115	Ente	ers Ecolo	ogy Mode (when ei	nding Real	time Batch	Ĵ



Click [Add] to open the batch file to be added.

Batch Queue	
C:\GCMSsolution\20091115_operation guide\20091115_3.ggb C:\GCMSsolution\20091115_operation guide\20091115_2.ggb	<u>A</u> dd <u>R</u> emove
	Move <u>Up</u> Move <u>D</u> own
OK Cancel Apply	Help

-P-Hint

If multiple batch files were added, change their order by clicking the desired batch file, then clicking [Move Up] or [Move Down]. Then analysis starts in that order from the top.



When finished editing, click [OK].

Appendix E Reducing the Carrier Gas Flow Rate During Standby

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

E.1 Ecology Mode TQ QP

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

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.

X
_

E.1.1 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. (For the TQ series model, CID gas supply stops.)



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.

E.1.2 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.

🎆 GCMS Real 1	lime Analysis (Admin) - Batch - [Batch Tabl	e - 2009	1115_1.	qgb]							- 7 🛛
🖉 Eile Edit Vie	ew Instrument Batch Tools Window Help										_ 8 ×
	/ 🖓 🖓 🚺 🗖 🖬 📢	> 🧔	?								
X	Data Explorer - Batch 🛛 🔀	Folder:	C:\GCMSsc	lution\20091115_ope	ration guide						X
Batch	Defection III -		Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File	Lev	CC Prote
		1	1	Methylene Chloride	UNK-0001	0:Unknown	ITQT	PAH_SIM.qgm	20091115_blank.ggd		dc neauy
	\20091115_operation guide 🔹	2	2	Standard Sample	STD-0001	1:Standard:(I)	ITQT	PAH_SIM.qgm	20091115_STD1.qgd		MS Ready
	· · · · · · · · · · · · · · · · · · ·	3	3	Standard Sample	STD-0002	1:Standard	IT QT	PAH_SIM.qgm	20091115_STD2.qgd		
Top	File Name Modified Date	4	4	Standard Sample	STD-0003	1:Standard	ITQT	PAH_SIM.qgm	20091115_STD3.qgd		
100	20091115_1 11/18/2009 8:34 AM	5	5	Standard Sample	STD-0004	1:Standard	IT QT	PAH_SIM.qgm	20091115_STD4.qgd		Flow
	11/18/20091115 2 11/18/2009 9:00 AM	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.ggd		68 50
California (California)		8	7	Unknown Sample	UNK-0003	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample3.qgd		Press TotalF.
Settings		9	8	Unknown Sample	UNK-0004	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample4.ggd		SoB(value:Open)
19 8 -		10	9	Unknown Sample	UNK-0005	0:Unknown	IT QT	PAH_SIM.qgm	20091115_sample5.qgd		opidvave.openj
rei 🔁		11	10	Unknown Sample	UNK-0006	0:Unknown	ITQT	PAH_SIM.qgm	20091115_sample6.ggd		Temperature
Wizard											250 45 250
											SPLI Uven I/F



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

ne Analysis	(Admin) - Batch - [Batch Table - 20091115_	1.0
Instrument	Batch Tools Window Help	
B	Start Pause	
ata Explorer	Stop	ol
Project in :	Batch Queue	╏
\20091115_	Settings	_
File Name	Enters Ecology Mode when ending Realtime Batch]



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



Wizard



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?

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

E.2 Reducing the Carrier Gas Flow Rate During Standby

For models QP2010, QP2010 Plus and QP2010S, perform the following operations.

E.2.1 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.



E Reducing the Carrier Gas Flow Rate During Standby



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

Inj. Port :	SPL1	Inj. Heat Port :	INJ1		
ан о т	00				· · · ·
Joiumn Oven Ter	mp.: ou.		300		
njection Temp.:	200		200		1
njection Mode :	Spl	tless 🔻	100 + + + + + + + + + + + + + + + + + +		+++++++++++++++++++++++++++++++++++++++
Sampling Time :	1.0) min	0.0 2.5	5.0 7.5 10.0 1	12.5 15.0 17.5
Carrier Gas : He	e Prim. Press	: 500-900	Program :	Column Oven Temperate	ure 🔻
Flow Control Mo	ode : Line	ear Velocity 🔷 👻			
Pressure :	113	.8 kPa	O -	80.0	1.00
Total Flow :	20.	0 mL/min	1 20.00	180.0	0.00
Column Flow :	1.6	7 mL/min	2 10.00	220.0	0.00
Linear Velocity :	47.	6 cm/sec	Total Pro-	Time : 10.07	
Purge Flow :	3.0	mL/min		19.67	
Split Ratio :	-1.0		Name Rtx-5	MS Thickness :	0.25 um
					s or Set
Save Method F	File As		Length : 30.0) m Diameter :	0.25 mm
Save Method F Save in:	File As		Length : 30.0) m Diameter :	0.25 mm
Save Method R Save in:	File As	*	Length : 30.0	Diameter :	Type
Save Method R Save in:	File As Training Name Mame	•	Length : 30.0	Diameter :	Type File folder
Save Method I Save in:	File As Training Name Name Herbici	^ de_Scan	Length : 30.0	Diameter : Date modified 3/4/2014 1:18 PM 2/12/2014 7:16 PM	Type File folder GC/MS M
Save Method I Save in:	File As Training Name Mame Mame Mame	^ de_Scan	Length : 30.0	Date modified 3/4/2014 1:18 PM 2/12/2014 7:16 PM	Type File folder GC/MS M
Save Method I Save in: Cecent Places	File As Training Name Litizi	^ de_Scan	Length : 30.0	Date modified 3/4/2014 1:18 PM 2/12/2014 7:16 PM	Type File folder GC/MS M
Save Method R Save in:	File As Training Name Mitizi	^ de_Scan	Length : 30.0	Date modified 3/4/2014 1:18 PM 2/12/2014 7:16 PM	Type File folder GC/MS M
Save Method R Save in: Save in	File As Training Name Mame Mame Mame Mame Mame Mame Mame Mame Mame Mame	^ de_Scan	Length : 30.0	Date modified 3/4/2014 1:18 PM 2/12/2014 7:16 PM	Type File folder GC/MS M
Save Method H Save in: Save in	File As Training Name Jitizi Training Name	^ de_Scan	Length : 30.0	Date modified 3/4/2014 1:18 PM 2/12/2014 7:16 PM	Type File folder GC/MS M
Save Method H Save in: Save in	File As Training Name Litzi Herbici	∽ de_Scan	Length : 30.0	Date modified 3/4/2014 1:18 PM 2/12/2014 7:16 PM	Type File folder GC/MS M
Save Method H Save in: Save in: Desktop Libraries Computer Computer Save in: Save in	File As Training Name Itizi Itizi Itizi Itizi	∽ de_Scan	Length : 30.0	Date modified 3/4/2014 1:18 PM 2/12/2014 7:16 PM	Type File folder GC/MS M
Save Method I Save in: Save in: Desktop Libraries Computer Save in: Save in	File As Training Name Training Name Training Name Name	∽ de_Scan	Length : 30.0	Date modified 3/4/2014 1:18 PM 2/12/2014 7:16 PM	Type File folder GC/MS M
Save Method I Save in: Save in: Desktop Libraries Computer Save in: Save in	File As Training Name Training Training Training Training Training Training Training Training Name	∽ de_Scan		Date modified 3/4/2014 1:18 PM 2/12/2014 7:16 PM	U_25 mm Vertex
Save Method I Save in: Save in: Save in: Save in: Save in: Save Method I Save Method I Save Method I Save Method I Save Method I Save in: Save in: Desktop Libraries Computer Network	File As Training Name Training Itzi Training Name Vame File name:	de_Scan Herbicide_Sc	"" an_low	Date modified 3/4/2014 1:18 PM 2/12/2014 7:16 PM	Type File folder GC/MS M

E.2.2 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 - Ba	tch 🗵
Project in :	
\Sample\Traini	ng 🔻
File Name	м
File Name	M



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

The [Table Style] window opens.





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	\mathbf{X}
Column Order Font Hide Items Sample Amt. Dil. Factor System Check. User Prog.	Add >> Display Items Vialt Sample Name Sample ID Sample ID Sample Type Analysis Type Method File Data File Data
Action Barcode Baseline Data F Option 1 Option 2 Option 3	<
	DK Cancel



Edit the batch file.

Add a row at the end and select a method file created in "Appendix E.2.1 Creating a Method File That Reduces the Carrier Gas Flow Rate" P.81.

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.

older: C:	\GCMSsolution\Sample\Tra	aining				
	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File
1	Methylene Chloride	UNK-0001	0:Unknown		Herbicide_Scan.qgm	Blank.ggd
2	Unknown Sample	UNK-0001	0:Unknown		Herbicide_Scan.qgm	Sample1.qgd
3	low		0:Unknown		Herbicide_Scan_low.qgm 🕄	low.qgd
4			0:Unknown	ITQT		



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.

	Data File	Report File	Tuning File	Data Description	EPA Sample#	Ext. Volume	Run Mode
1	Blank.ggd					1	DL AQ DP
2	Sample1.qgd					1 6	DEMAD
3	low.qgd					1	DL AQ DP 💽
4						1	Derigor



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





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

During this process, the method file for reducing the carrier gas flowrate is loaded when the final row is reached, and continuous data acquisition ends when the flowrate reaches 20 mL/min.



Appendix F Peak Integration for Total Ion Current Chromatogram (TIC)

When qualitatively analyzing multiple components, perform peak integration as described below to make the analysis operation easier.



Double-click the

(GCMS Postrun Analysis) icon.

The [GCMS Postrun Analysis] program starts.



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

GCMS Postrun

Analysis





Open the data file.





Set the peak integration parameters and perform peak integration for the entire TIC.

1 Click the [Peak Integration for All TICs] icon on the [Qualitative] assistant bar.



2 Click the [Peak Integration] tab in the [Quantitative Parameters] window.

ntegration			Smoothing Method Standard	i 👻	
Auto(Area)	-		# of Constitute Theorem	0	
# of Peaks:	8			0	
Slope:	100	/min	Smoothing Width:	0 sec	
Width:	2	sec			
Drift:	0	/min		Im	
T.DBL:	1000	min		Program	
Min.Area/Height:	0				
Base (Area	Height			

- 3 Click [Auto(Area)].
- 4 Set a value in [# of Peaks].
- 5 Click [OK].

Open the TIC peak table and check the peaks detected.



- Click the [Qualitative Table] icon on the [Qualitative] assistant bar.
 The [Qualitative Table] window opens.
- 2 Click the [TIC] tab.

The results for peak integration now can be checked.



Click [Select All] on the [Edit] menu.

	Edit Compound Name	Area	Area%	Height	Height %	A/H	Mark	Name
		89354	10.56	1919995	9.13	1.66		
	Select All	24812	4.06	968692	4.61	1.26		
-	1.000	.58529	14.44	3361668	15.98	1.30		
	сору	5594414	18.53	4299313	20.43	1.30	V	
	Delete Rows	973202	3.22	703014	3.34	1.38		
	Delete nons	5037710	16.69	3545673	16.86	1.42		
	Delete Current Table	5472339	18.13	3208920	15.26	1.71		
	Delete All Peak Tables	4337919	14.37	3025606	14.39	1.43		
	Register to Spectrum Process Table							
	Register to Library							
	Sort Table							
~	Copy Compound Name to TIC Peak Table							



Click [Edit] menu again and then click [Register to Spectrum Process Table].

	Edit Compound Name	Area	Area%	Height	Height%	A/H	Mark	Name
		3189354	10.56	1919995	9.13	1.66		
	Select All	1224812	4.06	968692	4.61	1.26		
	Conv	4358529	14.44	3361668	15.98	1.30		
	copy	5594414	18.53	4299313	20.43	1.30	V	
	Delete Rows	973202	3.22	703014	3.34	1.38		
	DING STU	5037710	16.69	3545673	16.86	1.42		
	Delete Current Table	5472339	18.13	3208920	15.26	1./1		
	Delete All Peak Tables	4337313	14.37	3025606	14.39	1.43		
	Register to Spectrum Process Table							
	register to cionary	_						
	Sort Table							
1	Conv Compound Name to TIC Peak Table							



Perform similarity search for every row.

💷 Qu	alitative Table	_									- 0 -	<	
Print	Edit View	-) <u> </u>				_	2
	Ret. Tim		Search All	Table				Search	Report	Event	Name		2
1]	Search Sele	ected Rows				_	7	1			
2			Stop						V	1			
3			C	and Manager	I David an Country			<u> </u>	7	1			
4			Copy Com	pound Name of	Hit #1 to spectru	m Process 1	Die		V	1		Е	
6		-	9.685	9.695	9.690	9.655	9.735		3	1			
7			10.295	10.305	10.300	10.260	10.350		7	1			
8			11.465	11.475	11.470	11.435	11.520		7	1			
			_					~				-	1
	\ Spectrum P	roce	ss (U/			1					,		1

- 1 Click the [Spectrum Process] tab in the [Qualitative Table] window.
- 2 Click [Search All Table] on the [Similarity Search] menu. [Done] is displayed in the [Search] cell.





Double-click the first row and check the similarity search results in order.



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	Click to copy the selected compound names to the spectrum table.
4	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.



Modifying the TIC Table

If peaks cannot be detected properly by automatic peak integration, take the following actions.



Copying the Hit #1 Compound Name in the Spectrum Process Table

Print Edit	View Sir	milarity Search							
		Search All Table							
Ret	.Time	Search Selected Power				port	Event	Name	
1		Search Selected Rows				1	1	Hexachlorocyclopentadiene	
2		Stop				1	1	Acenaphthene-d10	
3	-6						1	Simazine	
4	- 1	Copy Compound Nam	e of Hit #1 to S	pectrum Pr	ocess Table		1	Atrazine	
5	-	8 7 91 1 8 7411 1	8 / 10 1	8 /1811	8 /60 11000	i	1	Anthracene-D10-	
0		0.000 1 0.000 1	0.000.1	0.000.1	0.700 1.0	100	1	AL LL	

If [Copy Compound Name of Hit #1 to Spectrum Process Table] is selected, the name of the compound that was hit first in the similarity search can be automatically entered. However, it is necessary to confirm that the first hit compound is actually the target compound because it might not be.

Appendix G Index Searches

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 Create Divide Library... Open Library... Ctrl+O



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





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

Para	meters	
	Index	Parameter
1	Serial Number	1-212961
2	Cmpd Name	Atrazine
3	CAS Number	1912 -24-9
4	No Setting	



ł

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

The results are displayed.

GCMS Postru	n Analysis (Admin) - [L	library Editor - NIST	11.li	b (212	961 Spectrum)]		
🍳 File 🛛 View	HitList Target Info.	Compound Info.	In	dex Sea	arch Tools Windo	w Help	
🗅 🚅 🔒	a 🔂 🕹			Sta	t		P
<u> </u>	Data Explorer - Data	8	1	Sto Exp	p ort Search Results		
Postrun	Project in :						
		ople\Training 💌			Index		
JAAL I		ipiestraining +		1	Serial Number	1-212961	
<u>Illiid.</u>	CT N	M 100 10		2	Cmpd Name	Atrazine	
Qualitative	File Name	Modified L		3	CAS Number	1912 -24-9	
-	Sample1	1/29/2014		4	No Setting		



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



Appendix Chromatograms (MC)

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

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.



Perform the operation as described below.

- 1 Perform "Index Searches" P.90 to check the mass spectra of the target compounds.
- 2 Check one to three ions in the high m/z region.
- 3 Enter *m/z* values in the fragment table and display the mass chromatograms.
- 4 Perform similarity searches for the mass spectra of the target peaks.

H.1 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:Scan Ret.Time: [11.650] Scan#: [799]			

In	ten.(x10,000)								Base Peak: 173	/ 42,638
2.0							m/z .267.90	Abs. Inten.	8,528 Rel. Inten.	- 20.00
1.5						2	64			
1.0			255							
0.5										
0.0	250.0	252.5	255.0	257.5	260.0	262.5	265.0	267.5	270.0	ē

- 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.

H.2 Displaying Chromatograms from Fragment Tables

1

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 Fragment Table				
Gro	up#1	•	ОК	
0	TIC MIC Page None Base S	. 1 ×	Apply Help	
F	Dien	m/2	Englar	
1		TIC	1.00	
2	V	200.00	2.00 =	
3	V	215.00	4.00	
4				
	1000			
<u>0</u> 8				
3 6 7				
5 6 7 8				
5 6 7 8 9				
3 6 7 8 9 10				
0 6 7 8 9 10 11 12				
3 6 7 8 9 10 11 12 13				
The display can be changed as shown below by enabling/disabling [Base Shift] in the table. • With Base Shift



Without Base Shift



Appendix

Editing Parameters for Quantitative Analysis

Change quantitative processing parameters as necessary.



Start the [GCMS Postrun Analysis] Program and open the method file.







Click the [Quantitative] tab.

Quantitative Parameters	
Peak Integration Identification Quantitative Compound Table Sec	arch
Internal Standard Calculated by: Calculated by: Calculated by:	Eormat of Concentration
tailbration Lurve # of Calib. Levels: 4	5



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



No.	Item	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.
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



After finishing making changes, click [OK].

Calibration curves are corrected according to the changed parameters.



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].







Adjust the size as necessary.





After editing, click the [Print] icon on the [Report] assistant bar.







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 (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	×
C New File	
Calibration Curve	^
Chromatogram-Spectrum	
MSSpectrum (10 Compounds)	
Quantitation (10 Compounds)	
Quantitation (21 Compounds)	
Quantitation (Chromato & CalCurve)	~
Constitutive Recult (Graph)	
Comment	
Chroamtgram in a Framgment Table settings. Spectrum in a Spectrum Process Table settings of the Qualitative Tabl	~
	~
OK Cancel <u>H</u> elp	

) Hin

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

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

Data Explorer - Report	t Format 🛛 🛛 🛛
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
Sinida	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

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.
YYY	Chromatogram	Select to print the chromatograms (TIC, MIC, and MC).
Ш <mark>я</mark> н	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.
Sa	Quantitative graph	Select to print the chromatograms and quantitative values obtained in quantitative results.
R	Quantitative table	Select to print the tables obtained in quantitative results.
X	Calibration curve	Select to print calibration curves.
S.	Tuning	Select to print the tuning results obtained when data acquisition is executed. Select [GC/MS Tuning] or [GC/MS/MS Tuning] icon.
and and a second	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.

J Printing Reports



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 Pro	perties	×
General Chromato Graph	File	
Position Left 20.3 mm Iop 35.2 mm Size Wight 169.6 mm	Title ✓ Enable Center ▼ Chromatogram ✓ Sample Name □ Data File Font Name Times New Roman Size 8 Set	
Color Back Ground		
	OK Cancel Apply Help	

Reference

Refer to Help for details on property settings.

-Hint

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



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

Data Report
Return
Preview
5
Print



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>	30*1.00 20*1.00	<text></text>	
1 / 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.

Q.	GCM	S Po	strun	Analy	sis (Adı	nin) -	Re
Ľ	File	Edit	View	Item	Layout	Page	То
Г	New Format File				C	trl+N	
<u> </u>	Open Format File				C	trl+0	
	Close Format File						
1	Court Courter File					-	
	S	ave Fo	rmat Fi	ile As			
0	Si	ave Fo	rmat A	s Temp	late		Ĩ



K.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 Double-click the Time Analysis

(GCMS Real Time Analysis) icon.

The [GCMS Real Time Analysis] program starts.



Select [Maintenance] on the [Help] menu.

The [MS Navigator] window opens.

, U	ntitled, _default.qgt]	
wc	Help	
₩.	Contents Maintenance	917
	About GCM5 Analysis	



Click on the instrument for which maintenance will be performed.

😵 MS Navigator		x	
Show Back Forward Pint			
Maintena	nce of Shimadzu Gas Chromatograph Mass Spectrometers Click the thumbnail image of your instrument.		
	Gas Chromatograph Mass Spectrometers		
GCMS-TQ Serie GCMS-TQ8040	es GCMS-TQ8030		
GCMS-TQ8040	CCMS-T0830		
GCMS-QP Serie	es GCMS-QP2010 Ultra GCMS-QP2010 SE		
GCMS-QP2010 Plus	COMS-QP2010 = GCMS-QP2010S		
GCWS-OP2010Plus	Cast-0/2010		
	For details on how to judge the type of GC/MS you are using, click <u>here</u> .	Ŧ	



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

😫 MS Navigator 💿 🖸 💌
GE ← → Anno Anno Anno Anno Anno Anno Anno An
<how help="" maintenance="" to="" use=""></how>
strow to use maintenance require
Clicking a menu in <maintenance menu=""> opens the page for that menu.</maintenance>
[(page title)] is displayed at the top of the page.
To view page content further down, use the scroll bar on the right. Citating on underlined and immediate the science area
 Circking an undernied part jumps to the related page. To return to the previous page, click [Back] at the bottom of the page, or click the browser [Back] button.
<precautions during="" maintenance=""></precautions>
1. Be sure to allow the temperature of instrument parts to fall to 50 °C or below before performing maintenance.
 Wear clean gloves when performing maintenance. Description of the second formula to be an interaction of the second with control with c
 Be sure to whe on any dirt iron the tools used for maintenance using gaize moistened with acetone. After removing parts, place them on gauze to prevent them from becoming lost or dirty.
5. When disassembling removed parts, perform the same preventative action as in 4. Before disassembling parts, be sure to fully
remember their assembled states to prevent mistakes when they are re-assembled.
<maintenance menu=""></maintenance>
E
To view a particular item or procedure, click the photo or text.
Mass Spectrometer Unit Injection Unit Column Oven
<



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 K.3 Changing Replacement Guidelines for septa and Glass Inserts" P.108.



K.2 Easy sTop TQ QP

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 depending on the settings until glass inserts and septa can be displayed.



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
MS Consumables
Detail

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 "Push the replace button" status is displayed in the [Easy sTop] window.

onitor Settings				
🙋 Line1 ลา Consuma	able			
GC Consumables Current/Rough Standar	d for Exchan	ige	MS Consumables Current/Rough Standard for E	Exchange
Septum :	45/100	times	Filament #1 : 74/1 Filament #2 : 3/1	74/1000 hr 3/1000 hr
Glass Insert :	45/500	times	Ion Source :	77/1500 hr
Septum :	4/0	times	Detector: Turbo Molecular Pump1 :	7776000 hr 1059 hr
Glass Insert :	4/0	times	Turbo Molecular Pump2 :	1059 hr
Septum :		times	Rotary Pump 1 :	1060/15000 hr
<u>G</u> lass Insert :		times	Rotary Pump 1 Oil : Rotary Pump 2 :	1060/3000 hr 0/0 hr
CRG Coolant Time		min	Rotary Pump 2 Oil :	0/0 hr
	0/0	min isy sTop]	
			Total Run :	1065 hr
				Reset Consumables
			OK Cancel	Apply Help



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	
	Push the replace button
Please click	Temperatures are low enough. the Benlace button and then replace sents or class inserts
T IEGSE CIICK	une rreplace buttori and tren replace septa or glass inserts.
_	
E	eplace 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.

Easy sTop				
Replacing				
Please click the Complete button after replacing comsumables.				
Cancel <u>H</u> elp				



Reset the usage counter for the septum and glass insert.

For instructions on how to reset usage counters, see the procedure on page *108*, starting with step 3.

K.3 Changing Replacement Guidelines for septa and Glass Inserts

For septa, replacement frequency varies depending on the syringe needle diameter. The septum can be used about 100 times with the recommended syringe, and about 30 times with a gastight syringe before replacement.

Glass insert replacement frequency varies depending on the sample. Set replacement guidelines based on the sample.



K Maintenance

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.

Modules of Analytical Line	e#1	×
SPL1 Column MS		
<u>N</u> ame :	SPUT	
Injection Unit <u>Type</u> :	SPL	
Carrier <u>G</u> as :	He	
	Injection Port Maintenance	
Heater		
<u>Z</u> one :	INJ1	
<u>M</u> aximum Temperature :	470 °C	
Flow		



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

To restore default settings, click [Default].

Injection Port Maintenance(SPL1)				
Septum Used Counts : 100	<u>D</u> efault			
Insert Used Counts : 150	J			
OK Cancel	Help			



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.



Quantitative Browser

L.1 Data Analysis using Quantitative Browser

Using this browser allows multiple samples to be quantitatively processed at one time.



No.	Item	Explanation
0	[Quantitative Result View]	Use to check the quantitative calculation results (area, concentrations, etc.) of multiple data files. Click to switch between compounds to display.
0	[Compound Table View]	Click the [Results] tab to check the quantitative values of each compound in the data file selected in [Quantitative Result View].
€	[Calibration Curve View]	Displays a calibration curve of the ID selected in [Compound Table View].
4	[Chromatogram View]	Displays chromatograms of the compounds that are in the data files selected in [Quantitative Result View] and also selected in [Compound Table View].
6	Sample Type Toolbar	Data files for the specified sample type can be displayed in [Quantitative Result View]. All: All sample types, Std: Standard samples, Unk: Unknown samples

Appendix

L.1.1 Loading Data Using Quantitative Browser



(GCMS Browser) icon on the desktop.



Click the [Quant Browser] icon on the [Browser] assistant bar.



Double-click the



Click the [Batch] tab in Data Explorer.





Drag and drop the batch file used for analysis into [Quantitative Result View].



Individual data files can be dragged and dropped to open. In addition, right-click a desired row and then click [Delete] to delete a data file.

L.1.2 Checking and Correcting Calibration Curves



L.1.3 Checking and Correcting Quantitative Results of Unknown Samples



Reference

If necessary, perform identification or peak integration with reference to "Manual Identification and Manual Peak Integration" P.57.

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	[Shift] + right-click-drag	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.

-Ĥ-Hint

The intensity axis in [Chromatogram View] can be fixed by moving the mouse pointer to the desired data file in [Quantitative Result View], right-clicking it, and then clicking [Fix the Intensity Axis to this Data].

L.2 Saving Data Files



Click 📕 (Save) on the toolbar.

The data file is saved.



Click [Save Browsing File As] on the [Layout] menu.

Enter a name and save the file. The browsing file (that stores information on the loaded data files) is saved.



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