

LabSolutions

Operators Guide

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

Introduction

Read this Instruction Manual thoroughly before using the product.

Thank you for purchasing Shimadzu analytical instrument workstation "LabSolutions" (hereafter referred to as "the software" or "LabSolutions").

This manual describes the procedures for operating this product. 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 usage location changes, ensure that this Instruction Manual is always kept together with the product.
- If this manual is lost or damaged, immediately contact your Shimadzu representative to request a replacement.
- To ensure safe operation, contact your Shimadzu representative if product installation, adjustment, or re-installation (after the product is moved) is required.

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Original version is approved in English.




Instruction Manuals

■ List of Instruction Manuals

Name	Content
Getting Started Guide	This manual follows an actual data acquisition procedure to describe basic methods of operation for first-time users. Read this manual to learn basic operations of the software.
Operators Guide	This manual describes overall operations and handy functions in more details, such as the software's system configuration, data analysis, batch processing, confirmation of data acquisition results, and report functions.
System Users Guide	This manual describes system administration and data management of the software. Refer to this manual as necessary.
Installation & Maintenance Guide	This manual describes installation and maintenance of the software.
Data Acquisition & Processing Theory Guide	This manual describes peak detection and quantitation of sample components. Refer to this manual as necessary.
Help	Clicking the on-screen [Help] button or pressing the [F1] key displays a description of on-screen parameters, answers to specific questions or solutions to various problems. Also, clicking the [Help] button on the error message window displays the details of the error or solutions to the error. Be sure to refer to Help before contacting us.

■ Indications Used in Instruction Manuals

Cautions and Notes are indicated using the following conventions, and the following symbols are used in this manual:

Indication	Meaning
 CAUTION	Indicates a potentially hazardous situation which, if not avoided, may result in minor to moderate injury or equipment damage.
 NOTE	Emphasizes additional information that is provided to ensure the proper use of this product.
 Reference	Indicates the location of related reference information.
[]	Indicates the names of buttons, menu options, setting options, windows/sub-windows, and icons that are displayed in a window. Example: Click [OK].

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Shimadzu provides the following warranty for this product.

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 (including USB dongles). 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.

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- 3) Product use in combination with hardware or software other than that designated by Shimadzu
- 4) Computer viruses leading to device failures and damage to data and software, including the product's basic software
- 5) 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
- 7) Reasons unrelated to the product itself
- 8) Product use in harsh environments, such as those subject to high temperatures or humidity levels, corrosive gases, or strong vibrations
- 9) 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/DVD-ROMs are considered consumable items.

* If there is a document such as a warranty provided with the product, or there is a separate contract agreed upon that includes warranty conditions, the provisions of those documents shall apply.

* Warranty periods for products with special specifications and systems are provided separately.

* The license cannot be reissued if you lose the USB dongle provided with the product.



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1

What is LabSolutions?

This software is a workstation for high-performance liquid chromatograph systems(hereafter referred to as "LC") or for gas chromatograph systems(hereafter referred to as "GC") .

It enables control of LC or GC from a personal computer (PC), and perform tasks such as chromatogram data acquisition, data analysis, reports generations, and data management.

This chapter introduces the main features and functions of the software.

1

1.1 Features

■ Abundant Functions with Simple Operations

Assistant Bar

Click an icon on the assistant bar to change the display to the target operation sub-window. Icons displayed on the assistant bar can be customized to support a wide variety of operations.

Data Explorer

The file content is displayed by dragging-and-dropping the file from the [Data Explorer] sub-window onto the target sub-window.

Outstanding file management functions are provided for copying, moving, and deleting files, and for browsing the history information of files.

Batch Table Wizard

Batch Tables for sequential analysis of multiple samples are easily set by following the on-screen instructions.

Compound Table Wizard

Peak integration parameters for chromatograms through to Compound Tables for quantitative calculation can be easily made by following on-screen instructions.

Data Browser

The [Data Browser] window enables import and browsing of up to 64 data files.

Quant Browser

The [Quant Browser] window enables browsing of multiple quantitative calculation results that were acquired using the same method.

■ Enhanced Identification and Quantitative Processing Functions

This software supports a variety of identification methods such as window, band, spectrum similarity, absolute retention time and relative retention time. There are 6 different quantitative calculation methods that include the external and internal standard methods, and 7 types of calibration curves such as linear and exponential.

■ Highly Flexible Report Format

The report format function offers a high degree of flexibility by allowing creation of reports such as chromatograms, calibration curves, quantitative results, summary reports, and data analysis reports.

This software has a substantial selection of pre-installed report format templates, making it easier to create the desired report format.

■ Enhanced GLP/GMP Support Functions

The software contains functions that provide sure and efficient compliance with reliability requirements mandated in various regulations such as GLP/GMP and FDA 21CFR Part 11.

FDA 21 CFR Part11 Compliance

The electronic record and electronic signature functions of this software comply with the requirements of 21 CFR Part 11.

Information such as data measurement methods, schedules, date/time, operator name, and chromatograms can all be saved at once, and human and machine readable data can be saved together as required for compliance with Part 11.



NOTE

When used in combination with the optional CLASS-Agent Manager, this software meets the Part 11 requirements for electronic records and electronic signatures for review, approval and long-term storage of data.

User Administration

The Shimadzu User Authentication Tool administers users on the Shimadzu network. Account policies such as the minimum number of characters in passwords, password update interval, and permitted number of entry attempts are set to prevent illegal accessing.

System Administration

The software is also has an audit trail function and log browser function for sure and efficient operation of the system. The audit trail function records a history of changes to instrument parameters and data processing parameters, and the log browser function allows for a quickly search of the system operation history.

■ Ensuring File Compatibility

Method files and data files from previous version workstations (LCsolution, GCsolution, CLASS-LC10, CLASS-GC10 etc.) can be loaded directly to this software. Also, files in the international standard AIA (ANDI) format are supported.

The functions have been efficiently arranged to allow the extensive range of functions to be easily put to effective use.

1.2 Basic Knowledge


The software is comprised of the following programs:

Program Name	Contents
[Realtime Analysis] program	Used to enter the data acquisition parameters and acquire the data.
[Offline Editor] program	Allows other method files and batch files to be edited during data acquisition, and can register a single or batch data acquisition to the data acquisition queue.
[Postrun Analysis] program	Analyzes the acquired data to detect the peaks of chromatogram and perform quantitative calculations on these peaks.
[Browser] program	Allows importing and browsing of up to 64 data files.
[Security Policy Settings] program [User Administration] program	Administers the system security and user accessibility to the software.

Each of these programs are opened from the [LabSolutions Main] window.

This section describes how to open the [LabSolutions Main] window and the functions contained therein.

■ Open the [LabSolutions Main] Window

The  (LabSolutions) icon is displayed on the Desktop.

- 1 Verify that the [LabSolutions Service] icon in the Systray on the Taskbar displays a green chromatogram.

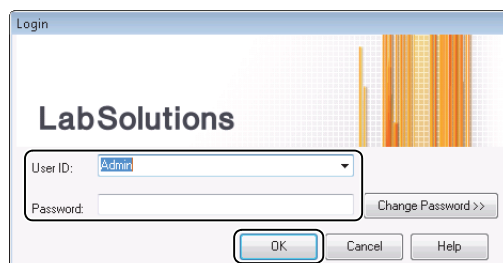


NOTE

A yellow chromatogram in the [LabSolutions Service] icon indicates that the software is still initializing. Wait for the chromatogram to turn green. A red chromatogram in the [LabSolutions Service] icon indicates that an error has occurred. Restart the PC.

- 2 Double-click the  (LabSolutions) icon on the Desktop.

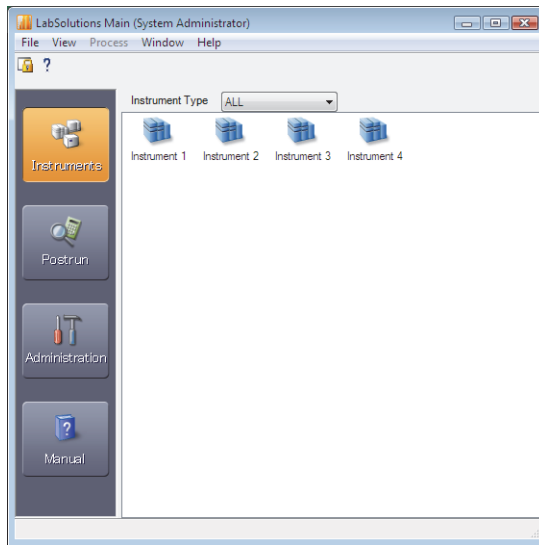
- 3 Select a registered user ID from the [User ID] list, enter the [Password] and click [OK].



NOTE


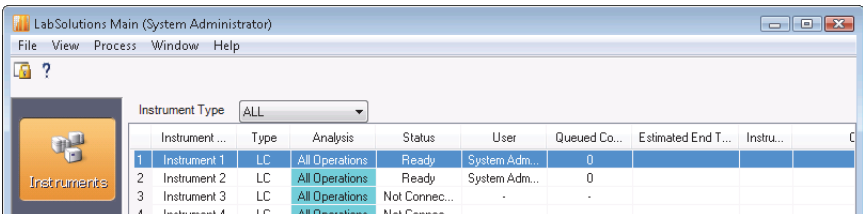
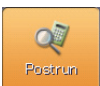

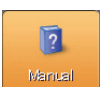
Select [Admin] in the [User ID] list for the first login to the system, and click [OK].

The [LabSolutions Main] window opens.




■ [LabSolutions Main] Window

The [LabSolutions Main] window displays an icon bar and a box for selecting a specific operation of a selected icon.

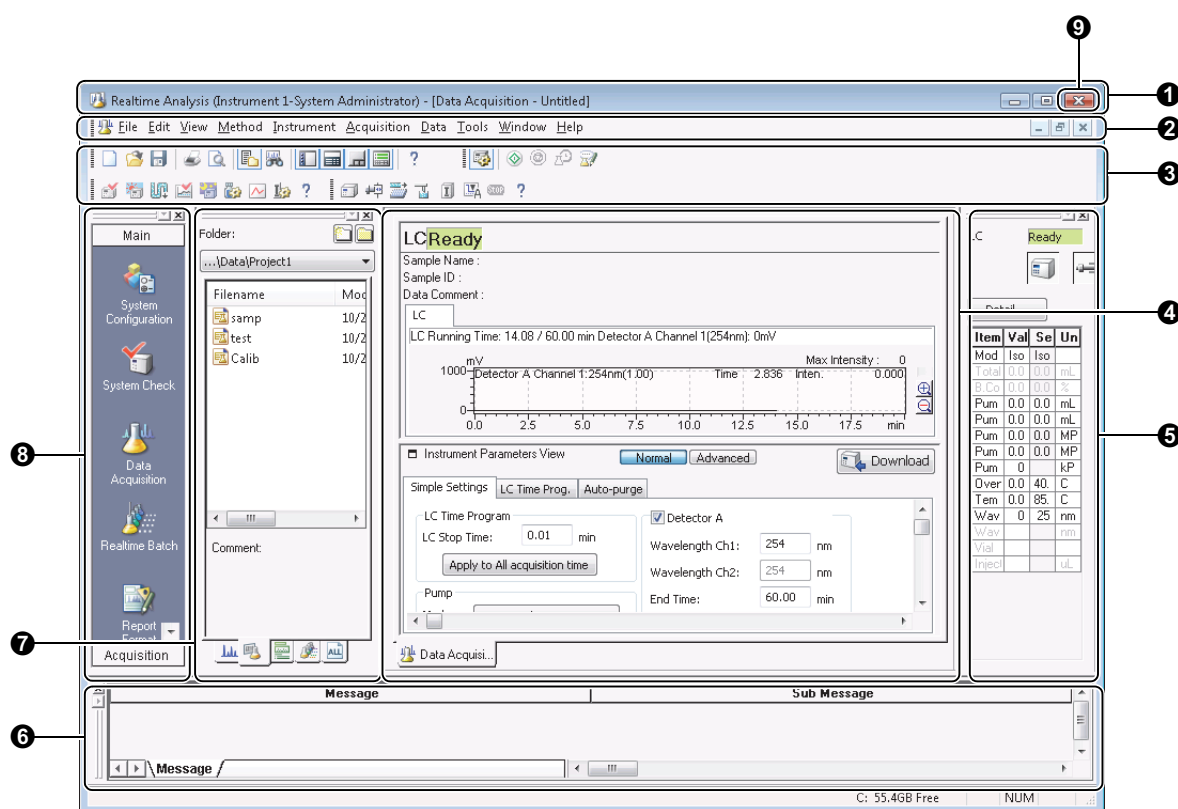
Icon Bar	Explanation
	<p>Click this icon to display icons for each of the instruments connected to the PC. Tables or icons can be displayed in the [Instruments] sub-window. Right-click on the [Instruments] sub-window, and click [Table View] from the displayed menu. The display changes to the table display.</p> <p>Double-click an instrument icon to open the [Realtime Analysis] program. The [Realtime Analysis] program is used to set the data acquisition parameters, acquire data and check the operating status of the instruments.</p> <p>[Table View]</p> 
	<p>Click this icon to open either the [Postrun Analysis] program to analyze data or the [Browser] program to display chromatograms and statistical calculation results from multiple data files.</p>
	<p>Click this icon to perform system administration functions related to the security policy, user administration, system settings, and validation.</p>
	<p>Click this icon to select a specific PDF formatted Instruction Manual or the Help files.</p>


NOTE

- Depending on the specific user's rights, the program icons in the icon bar of the [LabSolutions Main] window are sometimes not displayed or are disabled.
- Click  at the top right corner of the sub-window to close the [LabSolutions Main] window.

Basic Functions of the [Realtime Analysis] and [Postrun Analysis] Programs

This section describes the [Data Acquisition] window in the [Realtime Analysis] program.



No.	Explanation
1	The title bar displays the name of the currently running program, window name, currently loaded file name, logged in user name, and other information.
2	The menu bar displays the menus that are enabled according to the current window and rights of the logged in user.
3	The toolbar displays icons for frequently used menu items and icons for operating analytical instrument.
4	Different sub-windows such as [Data Acquisition] and [Realtime Batch] can be displayed in this section of the [Realtime Analysis] program. Sub-windows such as [Data Analysis], [PDA Data Analysis], [Calibration Curve], and [Report] are displayed in the [Postrun Analysis] program. Use the tabs under each sub-window or the icons in the assistant bar to change the displayed window.
5	The [Instrument Monitor] displays the status of the instruments and the parameter settings.
6	The [Output Window] displays a history of data acquisition operations and error messages that occur.
7	The [Data Explorer] sub-window displays the currently selected folder with the project file types (extensions) selectable from the lower tabs. The content of files is displayed by dragging-and-dropping the file in the [Data Explorer] sub-window onto the data analysis sub-window.
8	The assistant bar displays icons for the frequently used data acquisition operations. Click an icon on the assistant bar to change the data analysis sub-window. Icons displayed on the assistant bar can be customized to support a wide variety of operation flows.
9	Click  to exit the program.

1.3 File Formats

The software uses the following file formats to handle acquired data and related information:

- Method files
- Data files
- Report format files
- Batch files
- UV spectrum files
- Other files

This section describes each of the file formats.

1.3.1 Method Files

Method files store information such as instrument parameters and data processing parameters.

The file extension for method files is “.lcm” for LC, and is “.gcm” for GC.

Method files store the following information.

Stored Information	Explanation
System Configuration Information	System configuration information is saved in the method files to allow for review of the instrument parameters.
Instrument Parameters	This information includes the instrument parameters for each instrument and also the baseline evaluation results.
Data Processing Parameters	Calibration curve information, column performance parameters, QA/QC parameters, peak integration parameters, identification parameters, quantitative parameters, and Compound/Group Tables are all saved in the method file.
Sub-Window Properties	The chromatogram XY range setting, whether the status bar is displayed or hidden, etc. are also saved in the method file.

1.3.2 Data Files

The software stores the method files, batch files and report format files, chromatogram data, and quantitation results in a single data file. This is called an “All-In-One” structure and, since the data acquisition and analysis parameters are referenced from the same data file, it ensures the traceability of data.

The file extension for data files is “.lcd” for LC, and is “.gcd” for GC.



NOTE

- The report formats are also saved to the data file. Click [Data Report] on the [File] menu, then select [Print] to print the acquisition results of the currently loaded data file according to the report format stored with that data.
The report format can be edited by clicking the [Data Report] icon in the [Data Analysis] assistant bar to display the [Report] window. Click [Save Report Format File As] on the [File] menu to save the edited format for use with other data reports.
- When postrun analysis is performed on chromatogram data, the new data processing parameters are saved to the data file. [Apply to Method] on the [Data Analysis] assistant bar or [PDA Data] assistant bar must be clicked to save the parameters and allow them to be applied to other chromatogram data.



Reference

Refer to ["6.7 Save \(Export\) to Method Files" P.171](#) for more information.

1.3.3 Report Format Files

Items such as pictures or logos and placeholders for chromatograms, results and etc., are pasted into the blank format and it is saved for future printing of data acquisition results.

The file extension for report format files is “.lsr”.

If a report format file is set at the time of data acquisition or postrun analysis, the results can be immediately printed according to that format.

Reference

Refer to *"8 Report Function" P.221* for information on how to set the batch file.

1.3.4 Batch Files

Data such as sample information and quantitative calculation conditions, are saved to a batch file during sequential measurement of multiple samples.

The item displayed in the Batch Table and the overall batch processing parameters are also saved to the batch files.

The file extension for batch files is “.lcb” for LC, and is “.gcb” for GC.

Reference

Refer to *"4 Realtime Batch" P.63* for information on how to set the batch file.

1.3.5 UV Spectrum Files

The software uses the JCAMP format with the file extension of “.jcm” for the UV spectrum file.

When peak identification using the similarity of UV spectra is performed, jcm files are included in the Compound Table as standard spectrum.

The “.jcm” files can also be registered as spectra to the UV library files.

1.3.6 Other Files

The software uses the following files in addition to those described above.

File Name	Contents
UV Library Files	These files contain multiple UV spectrum data. They are used to perform library searches on the spectrum information for unknown samples. The file extension is “.lib”.
Browsing Files	These files store information such as compound information displayed in [Quantitative Results View] and the names of method and data files loaded in the [Quant Browser] window. The file extension is “.lcq”.
Layout Files	These files store information such as data file names and display layouts loaded in [Data Browser]. The file extension is “.lyt”.
System Configuration Files	These files hold the link information for the PC and analytical instruments, names of the instruments that make up the system, and information on consumables. These file names are not used for regular operations.
PDF Files	This files contain electronic versions of printed reports.

2

LC Data Acquisition

This chapter describes the basic flow of operations from entrance of the data acquisition parameters to the performance of a single run data acquisition on the LC.

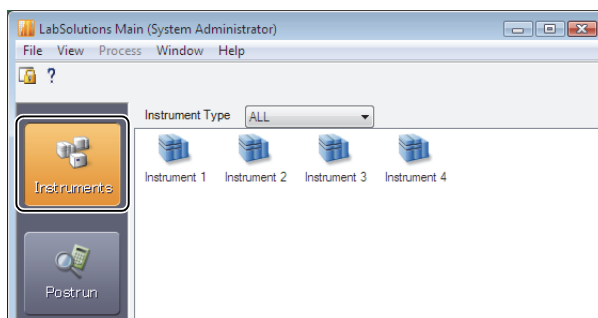
2.1 [Data Acquisition] Window

2

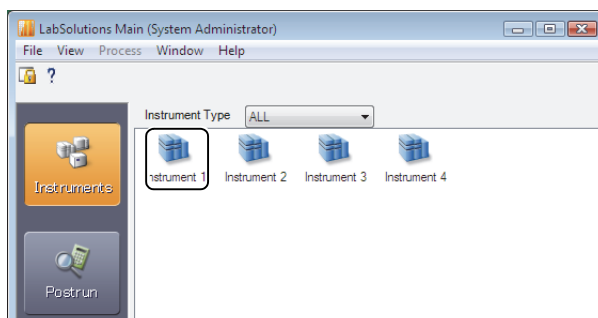
Two views of the [Data Acquisition] window are available, the [Chromatogram View] is used to display chromatograms and instrument status information and the [Instrument Parameters View] is used to display the parameters set for each instrument.

2.1.1 Open the [Data Acquisition] Window

- 1 Click the  icon.

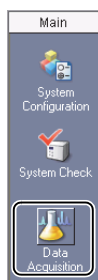


- 2 Select and double-click the instrument that will be used for data acquisition.




The [Realtime Analysis] program opens.

3 Click the  (Data Acquisition) icon on the [Main] assistant bar.

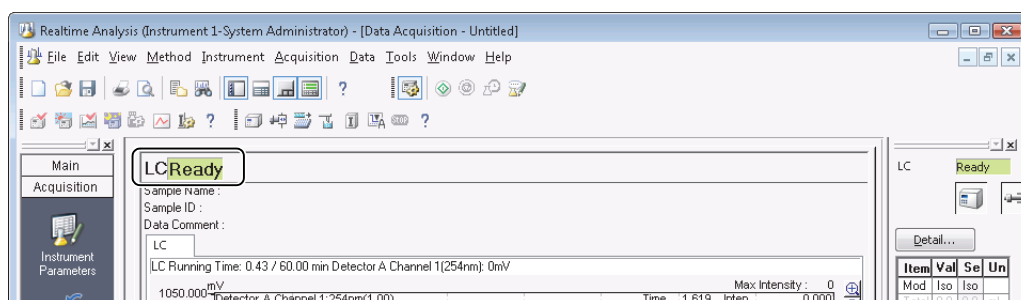


NOTE

If the  (Data Acquisition) icon is not displayed, click on the title of the assistant bar.



4 Ensure that [Ready] is displayed on the status display in the [Data Acquisition] window.

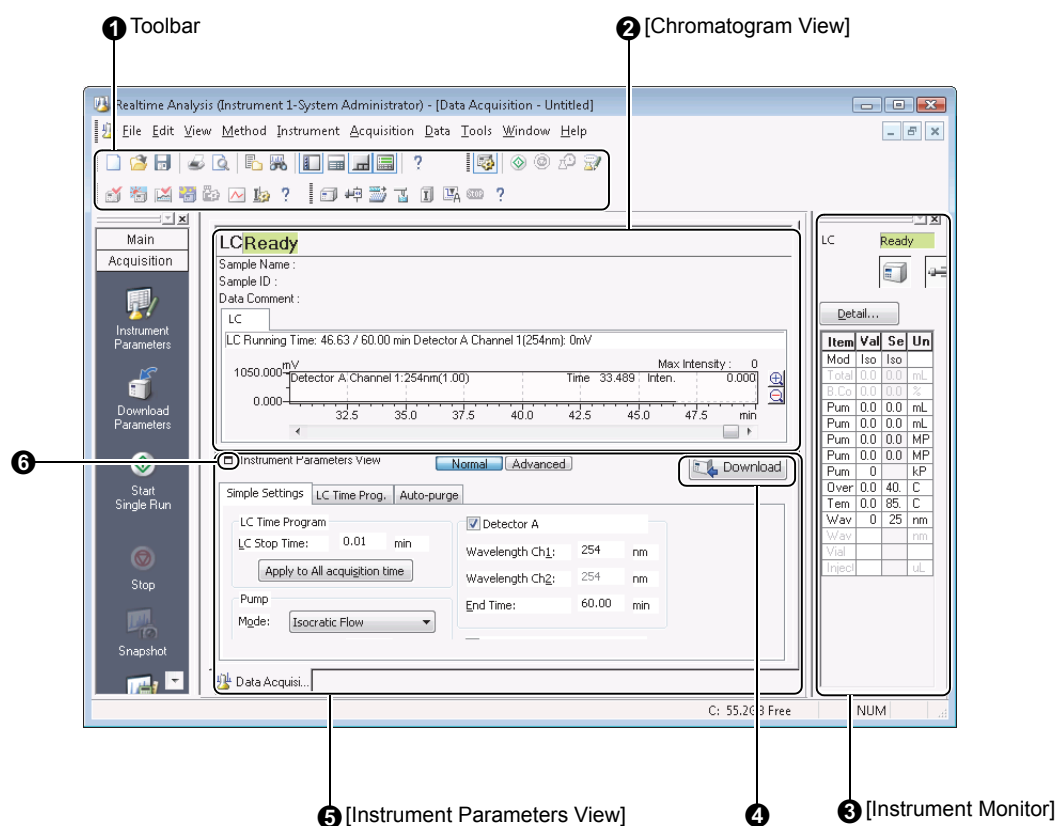


NOTE

If [Not Connected] is displayed on the status display, refer to "3.2 The Instrument Is Not Properly Recognized" in the Installation & Maintenance Guide.

2.1.2 [Data Acquisition] Window Description

This section describes how to view and use the [Data Acquisition] window.



No.	Explanation
①	Displays the [Standard] toolbar, [Data Acquisition] toolbar, [Instrument Control] toolbar, [LC Control] toolbar, and [PDA Control] toolbar.
②	Displays chromatograms and the instrument status curves. A [PDA] tab is displayed when a PDA is configured. 👉 Reference Refer to "2.3.1 Monitor the Chromatograms and Instrument Status Curves" P.15 to display the status information of instruments.
③	Displays the instrument status and parameter settings.
④	Click to transfer the data acquisition settings set in [Instrument Parameters View] to the analytical instrument. 👉 Reference Refer to "2.2.2 Analytical Instrument Startup" P.14 for details.
⑤	Displays the instrument parameters for data acquisition. In the [Normal] sub-window, the main data acquisition parameters are set on the [Simple Settings] and [LC Time Prog.] tabs. In the [Advanced] sub-window, the tab for each configured instrument module is displayed so that data acquisition parameters can be set in more detail.
⑥	Switches between the full screen and normal display.

2.2 Enter Data Acquisition Parameters

Enter the data acquisition parameters in [Instrument Parameters View].

The parameters are saved to the method file and used to perform data acquisition.

This section describes the operations in the [Instrument Parameters View].

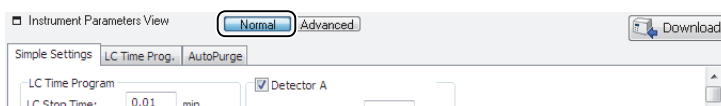
2.2.1 Set the Instrument Parameters

[Instrument Parameters View] has two sub-windows, [Normal] and [Advanced].

In the [Normal] sub-window, the main data acquisition parameters are set on the [Simple Settings] and [LC Time Prog.] tabs. In the [Advanced] sub-window, a tab for each configured instrument module is displayed so that data acquisition parameters can be set in more detail.

This section describes how to set the data acquisition parameters and create a method file.

1 Click [Normal] to open the [Normal] sub-window.



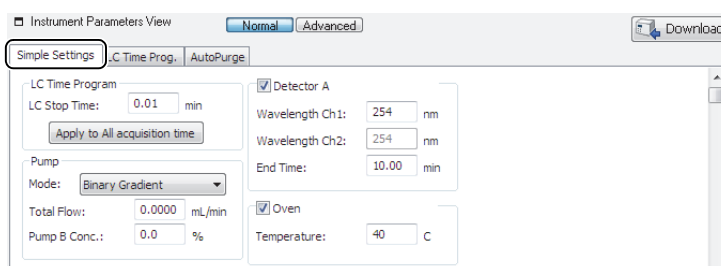
2 Click the [Simple Settings] tab and enter the data acquisition parameters.

Set the [LC Stop Time], pump flow rate and initial concentration for gradient systems, oven temperature, detector wavelength and other parameters.

- Enter the data acquisition time from one sample injection to the next sample injection at [LC Stop Time].
- Click [Apply to All acquisition time] to set the [End Time] for each detector to the same value as [LC Stop Time].
- Deselect [Oven] when the oven is not used.

NOTE

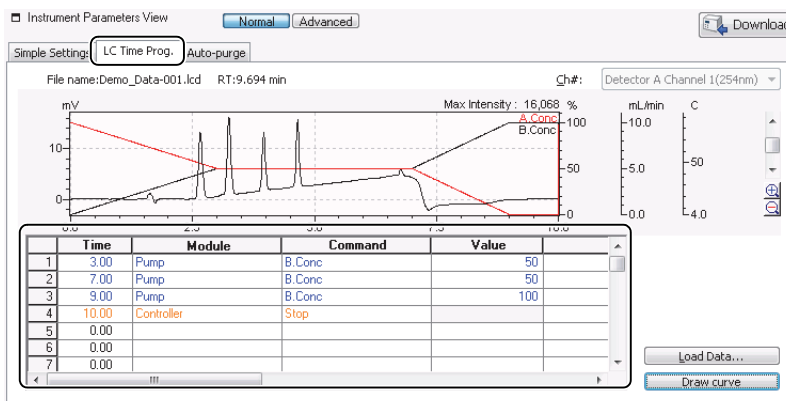
To switch the detector lamp off, make this setting on the respective detector in the [Advanced] sub-window.



3 Click the [LC Time Prog.] tab, and enter the concentration gradient conditions.

Enter [Time], [Module], [Command], and [Value] in the time program to change the concentration gradient and valve during data acquisition.

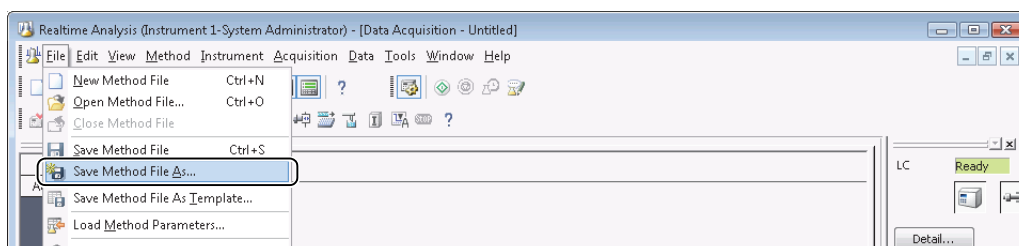
Click [Draw curve] to draw the gradient condition in the time program in a graph.



NOTE

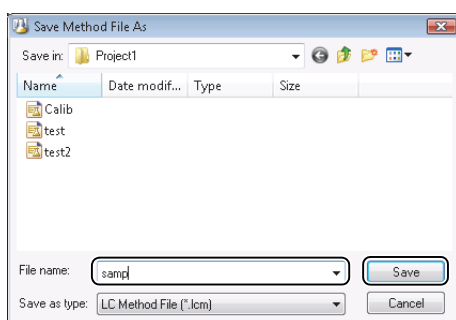
The time entered in the [Time] column of the time program corresponds to the time elapsed since the start of analysis. Enter a value of at least 0.01 min.

4 Click [Save Method File As] on the [File] menu.



The [Save Method File As] window is displayed.

5 Enter the file name, and click [Save].



A method file is created with the specified file name and the new instrument parameters are saved to the file.

NOTE


- The [Autopurge] tab is displayed when an autosampler is used. Refer to "2.3.2 Auto-Purge the Pump and Autosampler" P.19 for details.
- If a new method file is made and the rack set at [Sample Rack] on the [Autosampler] tab does not match the actual rack in use, an error message is displayed and data acquisition cannot be started. Click [Detect Rack] on the [Autosampler] tab in the [Advanced] sub-window to correct the rack selection.

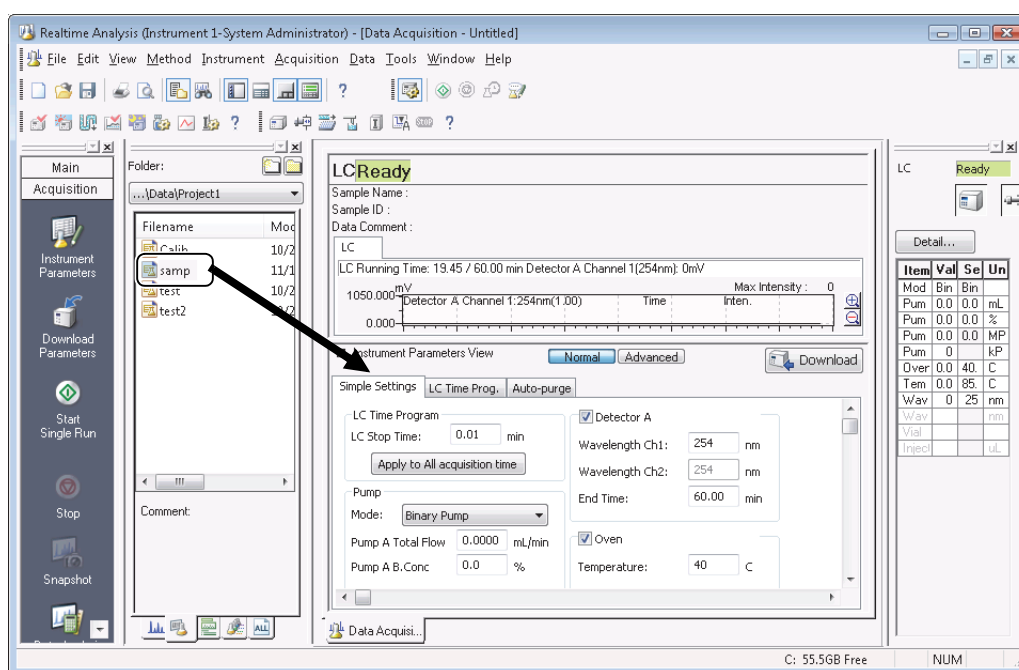
2.2.2 Analytical Instrument Startup

This section describes how to transfer (download) instrument parameters to an analytical instrument and the procedure for starting the instrument.

- 1 **Drag-and-drop the desired method file onto the [Data Acquisition] window from the [Data Explorer] sub-window.**

NOTE

If the [Data Explorer] sub-window is not displayed, click the  (Toggle Data Explorer) button on the tool bar.



The content of the method file is displayed in the [Data Acquisition] window.

- 2 **Check the instrument parameters, and click .**

The instrument parameters are transferred to the analytical instrument.

- 3 **Click the  (Instrument On/Off) button on the toolbar.**

Pump solvent delivery and oven temperature control are started.

NOTE

If the instrument is already activated when the method file is downloaded, operations are started using the downloaded instrument parameters.

2.3 Data Acquisition Preparation

This section describes the procedures to perform before starting data acquisition, such as auto-purging of the pump and autosampler, and verification of column equilibration (baseline check).

2.3.1 Monitor the Chromatograms and Instrument Status Curves

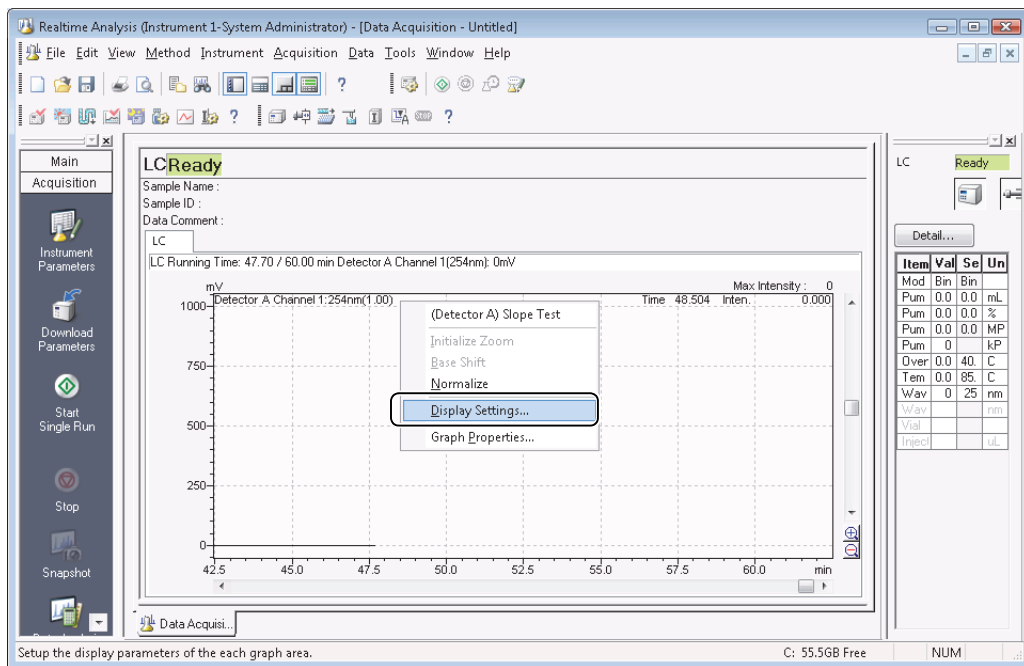
This section describes how to monitor chromatograms displayed in [Chromatogram View] and instrument status curves.

■ Chromatogram Display Settings

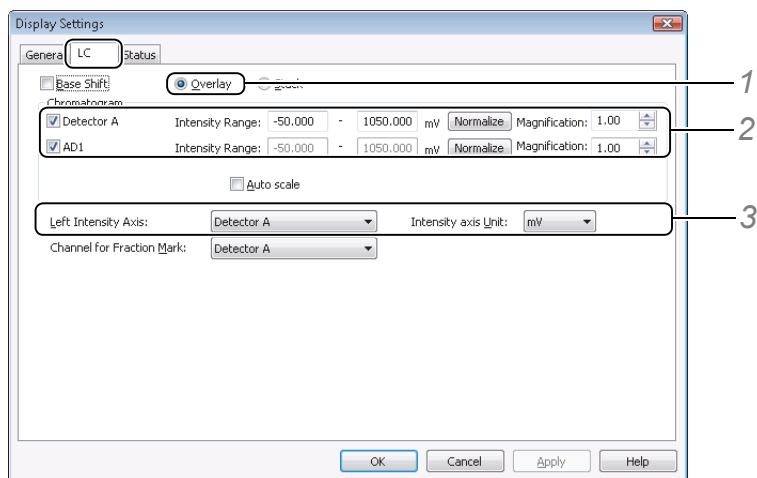
The chromatogram display scale can be changed.

This section describes how to monitor chromatograms on multiple channels.

1 Right-click on the graph in [Chromatogram View], and click [Display Settings].



2 Click the [LC] tab and enter the necessary parameters.



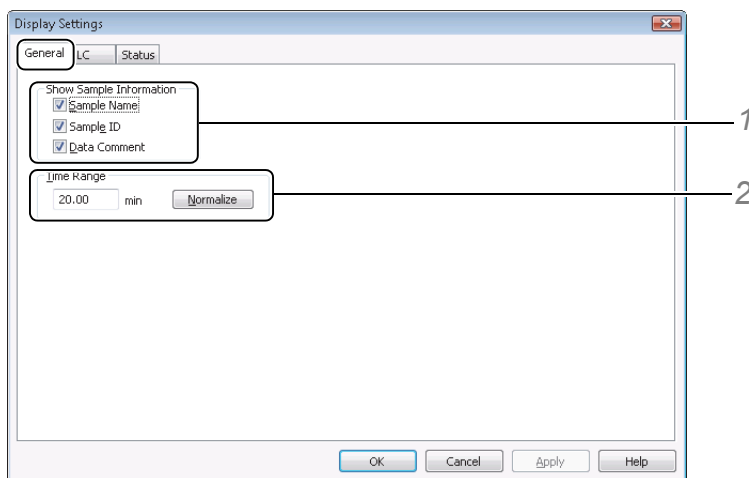
- 1 Click [Overlay] to draw chromatograms overlaid.
- 2 Enter the detector intensity range for the Y-axis.
Click [Normalize] so that the intensity range falls within the minimum and maximum values of the currently displayed chromatogram.
- 3 Select the detector (or channel in Dual Mode) and the display unit for the Y-axis.



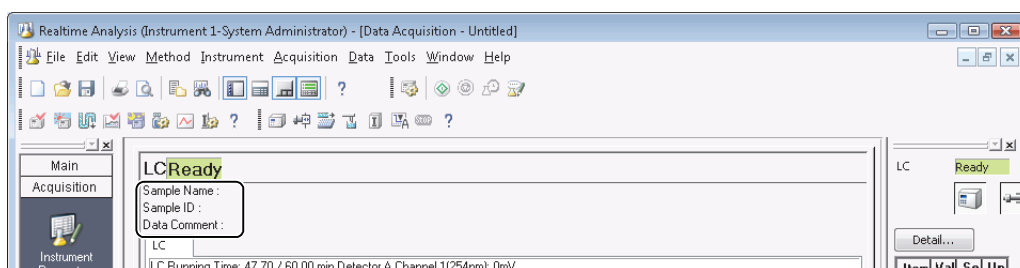
NOTE

The intensity range of each detector (or channel in Dual Mode) cannot be set in the [Overlay] mode.

3 Click the [General] tab, enter the necessary parameters, and click [OK].



- 1 Select [Sample Name], [Sample ID] and [Data Comment].
The sample information is displayed in the status display of the [Data Acquisition] window.



- 2 Enter the [Time Range] for the X axis display range.
Click [Normalize] to set the display range of the X-axis to either the [LC Stop Time] currently set in the method file or the longest detector acquisition time.

4 Click the (Save) button on the toolbar.

The time range and intensity range are saved to the method file.

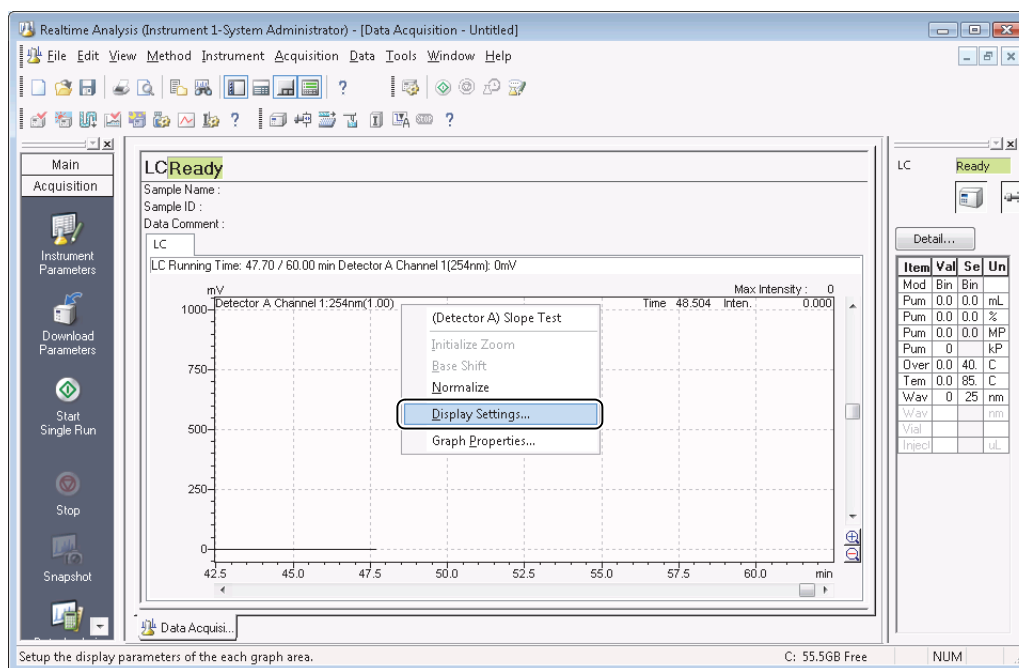
NOTE

- Settings other than the time range and intensity range are stored to memory for each user and instrument.
- The [PDA] and [UV Spectrum] tabs are displayed when a PDA detector is used.
- Click [Plot] to monitor the multi chromatograms of the PDA detector.
When the plot is started, the system status changes to [Plot].
Click [Stop] again to stop the plot.
- The reference chromatogram is drawn overlaying [Chromatogram View].
Click [Open Reference Data File] in the [File] menu to select and display the reference chromatogram.

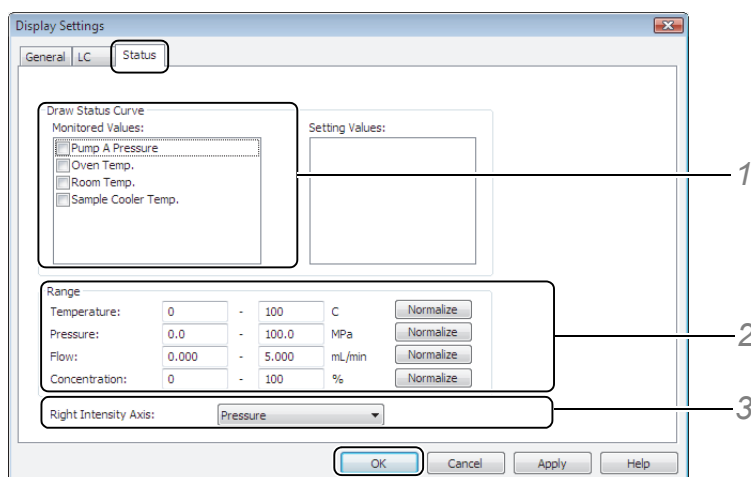
■ Display Instrument Status Curves

The instrument status curves that can be displayed on the graph in [Chromatogram View] include [Pump Press.], [Oven Temp.], [Room Temp.], and [Detector Cell Temp.].

1 Right-click on the graph in [Chromatogram View], and click [Display Settings].

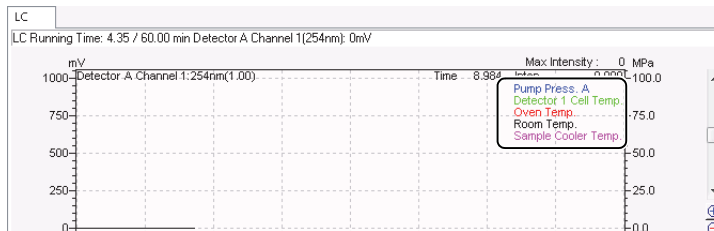


2 Click the [Status] tab, enter the necessary parameters, and click [OK].



- 1 Select the desired display items in [Draw Status Curve].
- 2 Set the display range for each status item.
- 3 Select the type of status to display on the intensity axis on the right of the graph.

The selected status is displayed on the graph.

**NOTE**

Settings are stored to memory for each user and instrument.

2

2.3.2 Auto-Purge the Pump and Autosampler

The mobile phase in the pump and the autosampler syringe rinse solution can be automatically purged.

A function is also provided to deliver solvent at a lower mobile phase flow rate after the autopurge ends until the column oven reaches its preset temperature.

Autopurge is executed in the following order: purging of pump → purging of autosampler → purging at initial concentration conditions (when pump mode is other than Isocratic) → warm up.

**NOTE**

The [Autopurge] tab is displayed when an autosampler is used.

1

Click the [Autopurge] tab in [Instrument Parameters View], and set the autopurge conditions for the pump.

1 Select the lines to be purged from the [Mobile Phase Name] list.

2 Enter a [Purge Time] for each line.

2 Set the autopurge conditions for the autosampler.

Instrument Parameters View

Simple Settings | LC Time Prog. | Auto-purge

Purge Order	Mobile Phase Name	Purge Time
1st:	Mobile Phase A	5 min
2nd:	Mobile Phase B	5 min
3rd:	None	5 min
4th:	None	25.0 min

Auto-sampler: 25.0 min

Init. Conc.-Replacement: 5 min

Warm up
 Wait time: 0 min
 Pump A Flow: 0.0000 mL/min

Activate system after auto-purge

Purged Pump
 Pump A: LC-20AB

- 1 Select [Autosampler] .
- 2 Enter the [Purge Time].

3 Set the [Warm-up] conditions.

Instrument Parameters View

Simple Settings | LC Time Prog. | Auto-purge

Purge Order	Mobile Phase Name	Purge Time
1st:	Mobile Phase A	5 min
2nd:	Mobile Phase B	5 min
3rd:	None	5 min
4th:	None	5 min

Auto-sampler: 25.0 min

Init. Conc.-Replacement: 5 min

Warm up
 Wait time: 0 min
 Pump A Flow: 0.0000 mL/min

Activate system after auto-purge

Purged Pump
 Pump A: LC-20AB


- 1 Enter the [Wait time] and [Flow].

NOTE


- [Warm up] is used to deliver solvent at a lower flow rate after purging of the autosampler ends until the oven reaches its preset temperature.
- Enter "0" min at [Wait time] to disable the [Warm up] function.

4 Click the (Save) button on the toolbar.

The settings are saved to the method file.

- 5** Click the  (Autopurge) button on the toolbar. Autopurge is started.

 **NOTE**

- Click the  (Purge autosampler) button on the toolbar. The purge is executed by [Purge Time] set on the [Autosampler] tab.
- After the autopurge ends, column equilibration can be checked using the baseline check function.

 **Reference**

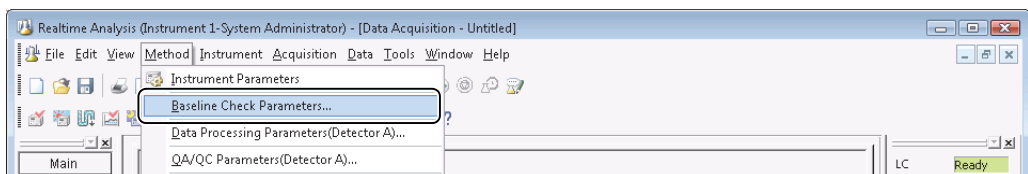
Refer to "[2.3.3 Check the Baseline](#)" P.21 for information on the baseline check procedure.

2

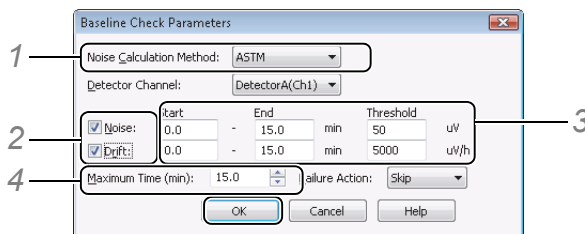
2.3.3 Check the Baseline

Use the baseline check function to determine whether the baseline noise and drift values are within the preset time and at or below the threshold for each channel.

- 1** Click [Baseline Check Parameters] from the [Method] menu in the [Data Acquisition] window.




- 2** Set the baseline check parameters, and click [OK].



- 1 Select the noise calculation method.
- 2 Select [Noise] and [Drift].
- 3 Enter the time and threshold used for checking [Noise] and [Drift].
- 4 Enter a [Maximum Time] to performing repeat the evaluation if the checks "fail".

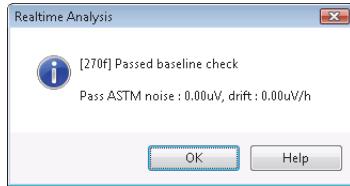
 **NOTE**

Select a [Failure Action] to be taken in the event of a baseline check failure. The [Failure Action] parameter is used when [Baseline Check] is used in the Batch Table.

- 3** Click the  (Save) button on the toolbar. The settings are saved to the method file.

4 Click on the (Baseline Check) button on the toolbar.

The baseline check is initiated, and the results of the baseline check are displayed after measurement ends.



NOTE

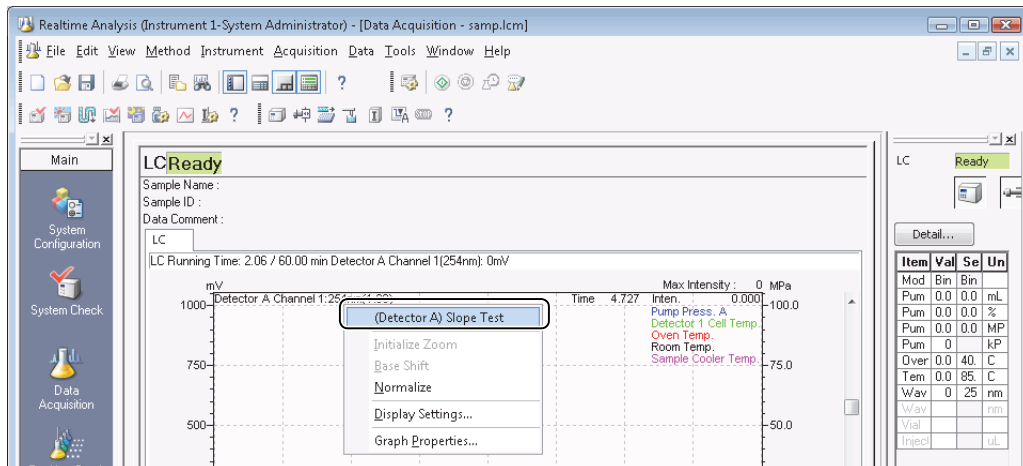
- The results of the baseline check are saved in the C:\LabSolutions\Log\Baseline folder.
- PDA baseline check cannot be performed for a channel set to [Max Plot] in the [Wavelength] column of the [Multi Chrom] tab in the [Data Processing Parameters] sub-window.

2.3.4 Calculate the Baseline Slope (Slope Test)

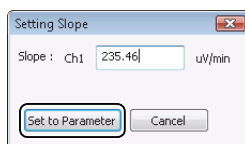
When the Slope Test is performed, the baseline of the chromatogram is measured to automatically calculate the Slope value.

The calculation results of the Slope Test can be set as the Slope value for the peak integration parameters.

1 Right-click on the graph in the [Chromatogram View], and click [Slope Test].



2 Click [Set to Parameter] to enter the on-screen value into the data processing parameters.



The data processing parameter [Slope] value is set.

NOTE

- The Slope value is generally rounded up to value that is larger than the calculated value. For example, a Slope value of “1988” is changed to “2000”.

3 Click the (Save) button on the toolbar.

The Slope value is saved to the method file.



NOTE

The Slope Test cannot be executed during data acquisition or during PDA plotting.

2.3.5 Check the Condition of Consumables (System Check)

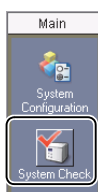
Check the system to verify that it is in good condition before starting data acquisition by checking the use frequency of the instrument consumables (i.e. the system check).



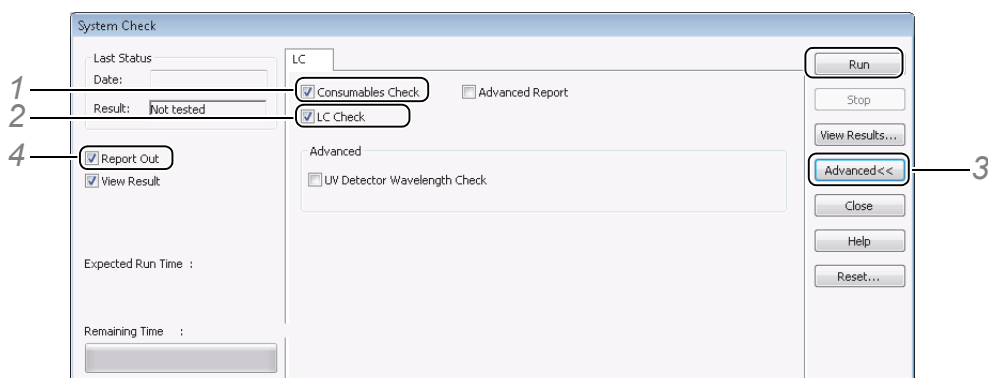
NOTE

Users are required to have the [Run System Check] rights to execute the system check.

1 Click the (System Check) icon on the [Main] assistant bar.



2 Select the items to check, and click [Run].



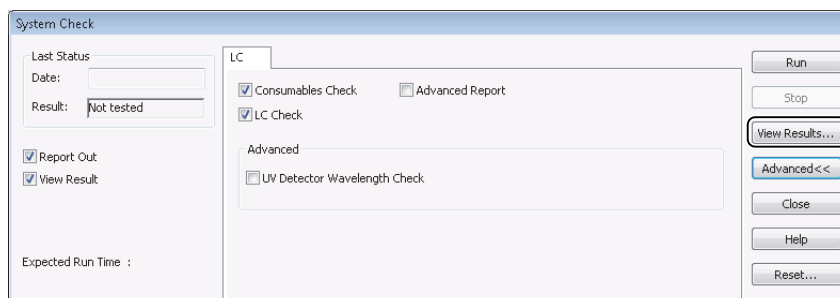
- 1 Select [Consumables Check].
- 2 Select [LC Check].
- 3 Click [Advanced], and select the items to perform the system check on.
- 4 Select [Report Out] to automatically print the system check results.



NOTE

- When using the LC-2010/LC-2010HT, logs recorded on instruments can be displayed in result reports. Up to 50 logs (30 on the CMD) can be displayed.
- When using a photodiode array detector, the [PDA] tab is displayed.
- If [Advanced Report] is selected, the system check is executed on all items.
- Click [Advanced] in the [System Check] sub-window, and select [UV Detector Wavelength Check] to simultaneously check the wavelength on the UV detector.

3 After the system check ends, click [View Results].



The [System Check Results] sub-window opens.

NOTE

- Click [Print] in the [System Check Results] sub-window to print the system check results.
- The system check results are saved to a file named according to the following rule: "SysChk#_YYYYMMDDHHMMSS.lcs" (where, "#" is the system number.)
- To check the results of previous system checks, click [Load] in the [System Check Results] sub-window, and select the desired results.
- Set [System Check] in a Batch Table, to check the use frequency of instrument consumables before starting data acquisition. Refer to ["4.2.3 Batch Table Parameters" P.78](#) for details.
- Realtime batch can be canceled according to the results of the system check by using the Batch Table action function.
- The system check is based on the consumable criteria of each instrument. Check consumable criteria in the [System Check] sub-window by clicking [System Check] in the [Properties] sub-window of each instrument.
- Click [Reset] to open the [Consumables Reset] sub-window. Reset the consumables when they have been replaced.
- Users are required to have the [Edit System Configuration] rights to set system check criteria.

2.3.6 Control Toolbar

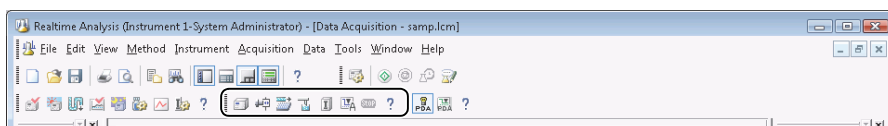
Change instrument status such as pump solvent delivery on/off, autosampler purge and rinse, heater control on/off, and detector zero correction using the [LC Control] toolbar or [PDA Control] toolbar.



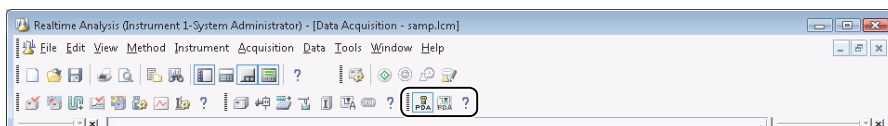
NOTE

The displayed buttons vary depending on the system configuration of the instrument.

[LC Control] toolbar



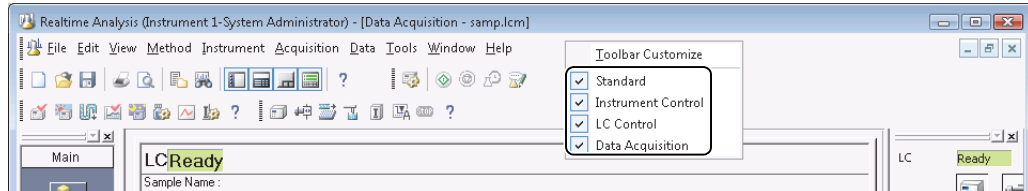
[PDA Control] toolbar



Button	Name	Explanation
	Instrument On/Off	Turns the ACTIVATE feature of the SCL-10Avp/SCL-10Asp system controller on/off. This button controls the pump and column oven for the CBM-20A/20Alite.
	Controller LCD On/Off	Turns the LCD of the SCL-10Avp/SCL-10Asp system controller on/off.
	Controller Lock/Unlock	Locks or unlocks keypad control of the SCL-10Avp/SCL-10Asp system controller. Only software control is permitted when keypad control is locked. This button is used to prevent operational errors.
	Pump On/Off	Turns the solvent delivery pump on/off.
	Purge autosampler	Executes an autosampler purge according to the [Purge Time] set on the [Autosampler] tab in [Instrument Parameters View].
	Rinse autosampler	Rinses the autosampler and sampling needle.
	Oven On/Off	Turns the column heater oven on/off.
	Zero Detector A	Returns the signal intensity of detector A to zero.
	PDA Detector Lamp On/Off	Turns the PDA detector lamp on/off.
	Zero PDA Detector	Returns the signal intensity of the PDA detector to zero.

**NOTE**

If the toolbar is hidden, use the right-click popup menu on the menu bar, and select the desired toolbar from the displayed menu.



2.3.7 Instrument Monitor

[Instrument Monitor] displays the instrument status and parameter settings. The instrument settings can be changed without changing the instrument parameters in the method file by entering a value in the [Setting] cell.

This section describes the procedure for changing the pump flow rate [PumpA. Flow].

**NOTE**

If the [Instrument Monitor] is not displayed, click the  (Toggle Instrument Monitor) button on the toolbar.

1

Click the [Pump A Total Flow] cell in the [Setting] column, and enter the new pump flow rate.

Item	Value	Setting	Units
Mode:	Binary Pump	Binary Pump	
Pump A Total Flow	0.0000	0.0000	ml/min
Pump A B Conc	0.0	0.0	%
Pump A Pressure	0.0	0.0	MPa
Pump A Degasser	0		kPa
Oven Temperature	0.0	40.0	C
Temperature Limit(Max)	0.0	85.0	C
Wavelength Ch1	0	254	nm
Wavelength Ch2			nm
Vial No (Auto-sampler)			
Injection Volume			uL

2

Press the [Enter] key.

The flow rate is changed.

**NOTE**

- Change the displayed status items in [Instrument Monitor] in the [Table Style] sub-window. Right-click on [Instrument Monitor], and select [Table Style] from the displayed menu.
- If the value in the [Setting] column is changed in [Instrument Monitor], it is not saved to method file.
Details of changes made are recorded in the operation log, and can be checked in the [Log Browser] sub-window.

2.4 Single Run

There are two ways of acquiring data, by single run (only one data acquisition), or by realtime batch (sequential analysis of multiple samples).

This section describes the procedure for a single run.

NOTE

Verify that [Ready] is displayed on the status display.


Reference

Refer to "[4 Realtime Batch](#)" P.63 for information on sequential analysis of multiple samples.

2

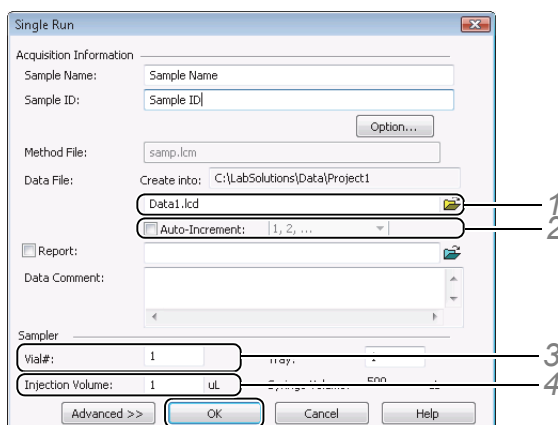
2.4.1 Execute Single Run

Execute single run from the [Data Acquisition] window.

- 1 Click the  (Start Single Run) icon on the [Acquisition] assistant bar.



- 2 Set the acquisition conditions, and click [OK].



- 1 Enter the data file name.
- 2 Select [Auto-increment], and the number type.
The data file name is automatically appended with an incremental number.
Example: "TEST-001.lcd"

NOTE

When [Auto-increment] is selected, the file is not overwritten even if the file name was previously used.

- 3 Enter the position of the sample for [Vial#].

NOTE

Enter “-1” to acquire data without injecting samples from the autosampler.

- 4 Enter the sample injection volume.

Single run is started.

During data acquisition, the [LabSolutions Service] icon in the Systray on the Taskbar flashes green.



Data acquisition ends when the data acquisition time in the method file has elapsed.

NOTE

Do not turn the PC off while the [LabSolutions Service] icon is flashing.

2.4.2 Change the End Time During Data Acquisition

The data acquisition time can be changed during data acquisition.

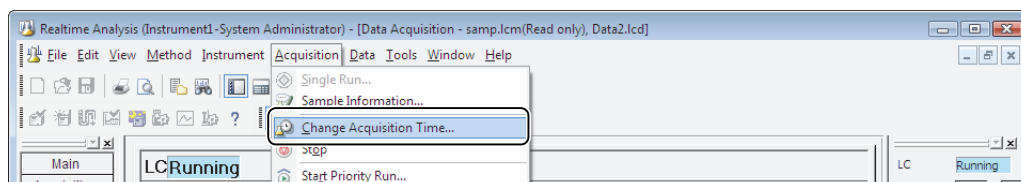
This section describes the procedure for changing the data acquisition time.

NOTE

- During data acquisition, [LC Stop Time] on the [Simple Settings] tab in [Method View] cannot be changed.
- If the acquisition time is changed using [Change Acquisition Time], a record is created in the operation log.

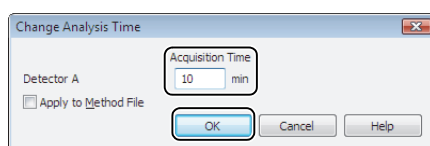
1

Click [Change Acquisition Time] on the [Acquisition] menu.



2


Enter an [Acquisition Time], and click [OK].

**NOTE**

- If multiple detectors are used, click [All Times Change] to change the data acquisition time to the longest detector acquisition time.
- If [Change to Minimum Value] is selected, click [All Times Change] to change the data acquisition time to the shortest detector acquisition time.
- Click [Apply to Method File] to apply the new acquisition time to the method file and use it for all subsequent data acquisitions.
- You cannot change the value as an analysis time that has already passed.

2.4.3 Stop Single Run

Single run can be stopped in the midway to end acquisition earlier than the preset end time.

- 1 Click the  (Stop) icon on the [Acquisition] assistant bar.
Data acquisition is stopped, and a data file is created for the data so far.

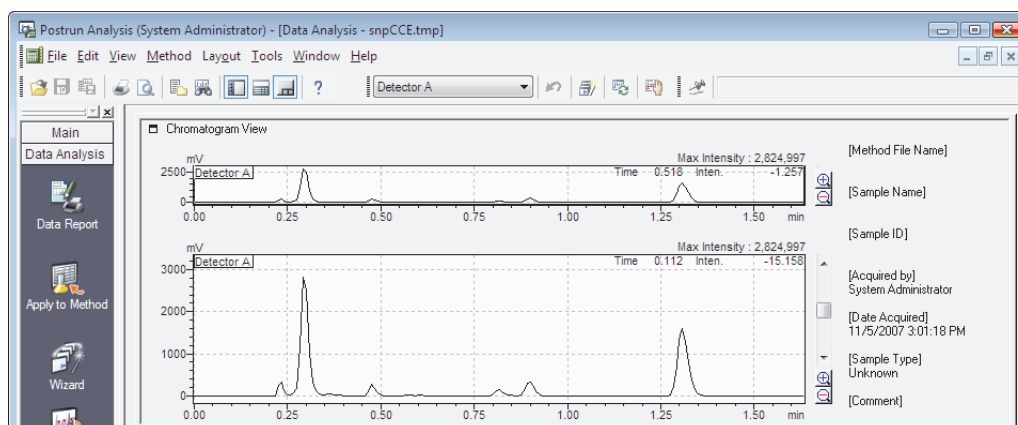
2.5 Check Analysis Results During Data Acquisition (Snapshot)

2

Execute snapshot during data acquisition to display and process the data obtained since acquisition was started.


This section describes the procedure for executing a snapshot during data acquisition.

- 1 Click the  (Snapshot) icon on the [Acquisition] assistant bar.
The data obtained so far is displayed in the [Data Analysis] window.




2.5.1 Update Snapshots

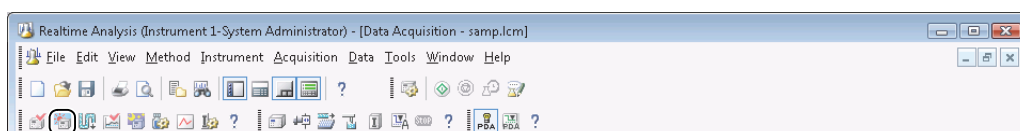
Use snapshot update to load cumulative acquired data from a continuing data acquisition after snapshot has been executed.

- 1 Click the  (Update for Snapshot) button on the toolbar in the [Data Analysis] window.
The snapshot is updated to display the latest chromatogram.

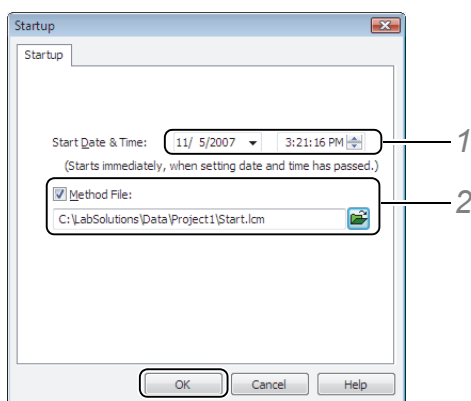
2.6 Automatic Instrument Startup


Use  (Startup) to automatically start the instrument at a specified date and time.

- 1 Click the  (Startup) button on the toolbar.



- 2 Enter the date and time to start the instrument, and click [OK].



- 1 Set the date and time to start the instrument.
- 2 Select [Method File], and enter the method file name. The method file can also be selected by clicking .



NOTE

When the method file is not specified, the analytical instruments are started up by the parameters already downloaded to the instrument (i.e. parameters used in the previous data acquisition) when a startup is performed.

The instrument starts up at the specified date and time.



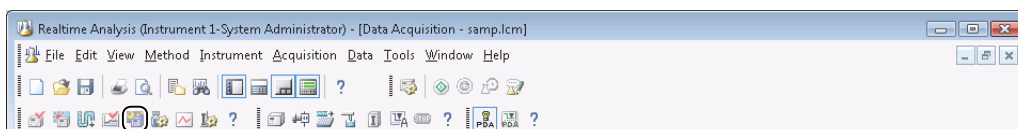
NOTE

- If startup is executed in a batch file(s) registered to the batch queue, the startup begins after processing of the previously registered batch file(s) ends.
For details on the procedure for changing the execution order of batch files registered to the batch queue, refer to ["4.5 Data Acquisition Using the Batch Queue Function" P.96.](#)
- Startup can also be set in realtime batch.
For details, refer to ["4.4.2 Start Data Acquisition at a Specified Date and Time \(Startup\)" P.87.](#)

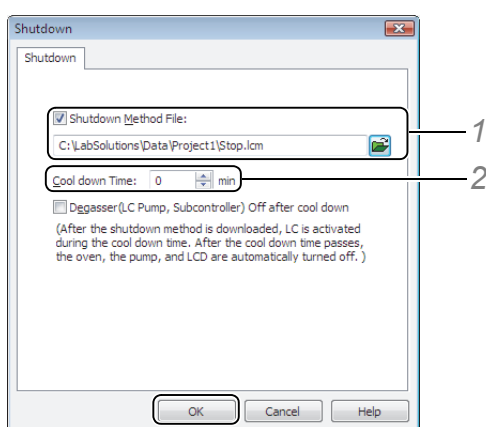
2.7 Automatic Instrument Shutdown


Use [Shutdown] to automatically shut down the instrument after data acquisition ends.

- 1 Click the  (Shutdown) button on the toolbar.



- 2 Set the date and time to shut down the instruments, and click [OK].



- 1 Select [Shutdown Method File], and enter the method file name. The method file can also be selected by clicking .



NOTE

When a method file is not specified, the analytical instruments are shut down by the parameters already downloaded to the instruments when a shutdown is performed.

- 2 Enter the time that the instrument is operated by the instrument parameters of the specified method file.

The analytical instruments shut down when the [Cool down Time] elapses.



NOTE

- If shutdown is executed in a batch file(s) registered to the batch queue, the shutdown begins after processing of the registered batch file(s) ends.
For details on the procedure for changing the execution order of batch files registered to the batch queue, refer to ["4.5 Data Acquisition Using the Batch Queue Function" P.96](#).
- Shutdown can also be set in realtime batch.
For details, refer to ["4.4.3 Shutdown Analytical Instruments After Data Acquisition \(Shutdown\)" P.88](#).

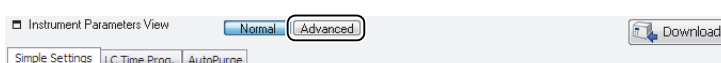
2.8 Change the Sampling Time (Period) or Frequency (Rate)

The sampling time (period) can be set matched to the peak shape of the chromatogram to acquire.

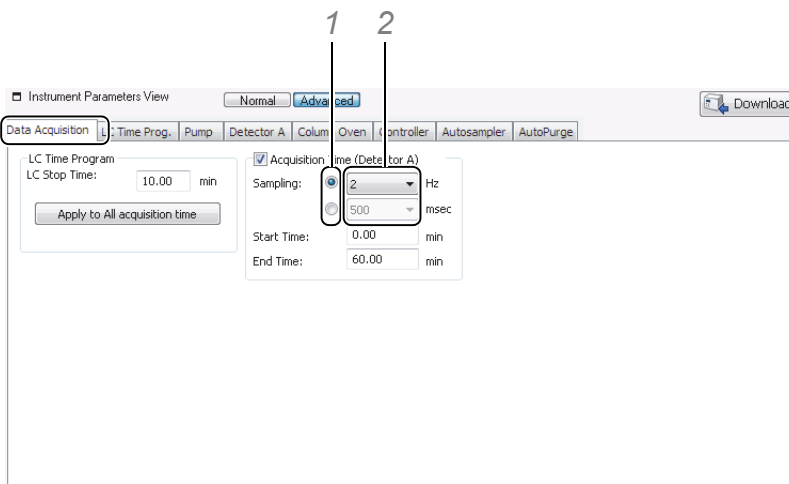
Decreasing the sampling time (i.e. increasing the sampling frequency) enables narrower sharp peaks to be detected. However, in this case, more noise might be detected, possibly preventing correct peaks from being detected.

This section describes how to set the sampling time (period).

1 Click [Advanced] in [Instrument Parameters View].



2 Click the [Data Acquisition] tab, and set the sampling time of the detector.



- 1 Select the unit to set ([Hz] or [msec]) from [Sampling].
- 2 Select the setting value from the list.

3 Click the (Save) button on the toolbar.


The settings are saved to the method file.

NOTE

- The sampling time (period) is the signal interval to record to the data file, and becomes the data points of chromatograms.
Note that data files increase in size the smaller the sampling time (i.e. larger the sampling frequency) becomes.
- The sampling time (period), and data processing parameter [Width] and detector [Response] (time constant) values also affect peak detection.

■ Setting the Data Sampling Time at [Sampling]

Set the sampling time to match the peak shape of the chromatogram.

Initial Value	Base Period of each detector set in the [System Configuration] sub-window
Setting range	Base Period 1 to 10 times of 20 msec to 1000 msec range (In Dual Mode, 1 to 10 times of 100 msec to 1000 msec range)
Recommended values	20 msec to 60 msec  NOTE Set 1 tenth of data processing parameter [Width] to be used as the upper limit (so that 10 or more data points fall within the minimum half-width value of the measured peak). For example, in cases where data processing is performed at Width = 1 (sec), set so that the sampling time is sufficiently shorter than 100 msec.

NOTE

The base period is the signal interval sent to the PC from the detector. Set the base period in the [Properties] sub-window for the detector in the [System Configuration] sub-window.

2.9 Daily Inspection of LC Hardware

Expected data acquisition results sometimes cannot be obtained even if each of the instruments on the LC system are not malfunctioning.

Trouble can be prevented by inspecting each of the instruments before starting data acquisition, while waiting for the baseline to stabilize, and after data acquisition ends. This section describes check points in daily inspection.

■ Before Starting Data Acquisition

Check Point	Remarks
Be sure to filter the mobile phase.	A suction filter in the solvent delivery pump is used to prevent inflow of dirt (solids) into the flowpath. However, since filter pores are 10 microns in diameter, particles smaller than this diameter pass through the filter, resulting in clogging or dirtying of the flowpath and column. We recommend filtering the flowpath with a membrane filter with a pore diameter of about 0.45 microns.
Return the mobile phase to room temperature before use.	If the temperature of the mobile phase is different from the room temperature, the baseline may not stabilize and may drift, air bubbles may be generated, or other troubles are likely to occur while the mobile phase is settling to room temperature. Note, that if water and organic solvents mix together, the temperature of the mixed solution sometimes changes considerably from the room temperature.
In the case of a low-pressure gradient system, fill the flowpaths with mobile phase using all 4 solutions.	Air bubbles in the gradient valve or from the solvent delivery pump up to the gradient valve may cause the retention time to fluctuate or be uneven. For this reason, fill the flowpath of each line with mobile phase.

Check Point		Remarks
Pay attention to substitution of the mobile phase	When substituting with compatible mobile phase	<p>Follow the procedure below to substitute the mobile phase:</p> <ol style="list-style-type: none"> 1. Pour the substitute mobile phase into a clean beaker (about 200 mL in size). 2. After drawing out the suction filter from the reservoir bottle, and putting it in the beaker in step (1) above, vibrate the filter section to rinse the suction filter. 3. Turn the drain valve counterclockwise to open the valve. 4. Press purge on the solvent delivery pump. (Solvent is delivered about for 3 minutes at a flow rate of 8 mL/min, though this depends on the instrument settings.) 5. Insert the suction filter into a new mobile phase reservoir bottle, and press purge on the solvent delivery pump. Next, press pump to deliver solvent and substitute the flowpath up to the column connection port. 6. Close the drain valve. 7. Connect the column, and turn the column oven on. (The oven starts to be controlled.) 8. Deliver solvent at half the data acquisition flow rate. 9. When the column oven temperature stabilizes, deliver solvent at the data acquisition flow rate.
	When substituting with incompatible mobile phase	Substitute the mobile phase with an intermediate solution (e.g. 2-propanol) that is compatible with the old and new mobile phases, and then replace the intermediate solution with the new mobile phase. Follow the procedure above.
	When substituting the buffer solution mobile phase	When using a buffer solution for one or both of the new and old mobile phases, first substitute with distilled water as the intermediate solution, and then substitute with the new mobile phase. After purging with distilled water, deliver distilled water for a while (at least 20 mins at a flow rate of 1 mL/min). During this operation, also rinse the plunger seal using the seal auto-rinsing kit. This is needed to prevent deposition of salt in the buffer solution. Note that crystals and leftover lees sometimes cannot be removed if 2-propanol or other organic solvent is passed along the flowpath before rinsing with distilled water.
Prime the suction tube with water if it is not filled with mobile phase.	<p>Prime the suction tube if it is not filled with mobile phase or if large air bubbles can be seen inside.</p> <ol style="list-style-type: none"> 1. Open the drain valve, and connect a 20 ml syringe to the drain tube ASSY outlet port. 2. Press purge. 3. Pull on the syringe with large force in a purged state. 	
Purge the instrument before using it.	<p>Air bubbles sometimes occur in the head of the solvent delivery pump when data acquisition has not been performed for some time or when the difference between day and night temperatures is large. Purging the pump removes air bubbles, preventing defective solvent delivery or other trouble.</p> <ol style="list-style-type: none"> 1. Turn the drain valve counterclockwise to open the valve. 2. Press purge on the solvent delivery pump (for 3 minutes at a flow rate of 8 mL/min). 3. Close the drain valve. 	

Check Point	Remarks
Check the rinse solution of the seal auto-rinsing kit.	When a mobile phase containing buffer solution or phosphoric acid is used, be sure to rinse the plunger seal. Use distilled water for the seal rinsing solution, and exchange the rinsing solution periodically (once every 2 or 3 days). Otherwise, germs and bacteria will breed in the distilled water. When using a solution incompatible with distilled water as the mobile phase, do not rinse seals with distilled water.
Check the autosampler rinse solution.	Use an autosampler rinse solution that is the same as the mobile phase. However, be sure to remove any salt from the rinse solution. Also, since the rinse solution contacts the mobile phase inside the high-pressure valve, select a solution that does not cause deposition of salt due to contact with liquid.
Purge the autosampler's measuring pump.	Air bubbles sometimes occur in the head of the measuring pump when data acquisition has not been performed for some time or when the difference between day and night temperatures is large. Purging the pump removes air bubbles, preventing uneven peak area values or other troubles. To purge the measuring pump, press purge . To stop the purge, press purge again.
Firmly close the autosampler door.	After closing the autosampler door, make sure that the door is firmly held against the magnets on the instrument body.
Check the column oven preset temperature.	The CTO-20A(30A) and CTO-20AC can be controlled from "room temperature +10 °C" and "room temperature -10 °C", respectively. Note, however, that when room temperature is around 26 °C, the CTO-20A cannot be controlled stably with the temperature set to 35 °C.
Check the wavelength accuracy of the UV-VIS detector.	The SPD-20A/20AV automatically checks the wavelength using the emission lines of 253.7 nm (Hg lamp) and 656.1 nm (D2 lamp) after the instrument is turned on. A warning message is displayed if the wavelengths are deviating. When "CHECK NO GOOD" is displayed, execute "WAVE ADJ" with the cell filled with water to check the wavelength again. If "CHECK NO GOOD" is displayed again, this indicates an instrument malfunction. In the case of the SPD-M20A, fill the cell with water, and check the wavelength in the [Wavelength Check] sub-window of the [PDA Utility] sub-window.

■ While Waiting for Baseline Stabilization

Check Point	Remarks
Check for liquid leaks.	Start solvent delivery, and make sure that all flowpaths, such as piping connections, are free of liquid leaks. If liquid is leaking, re-tighten the leaking spot, or replace consumables. On the 20A series, visual checks are basically not required since each instrument is provided with a liquid leak sensor.
Check the pump pressure.	Good data acquisition results cannot be obtained if the pressure of the solvent delivery pump is unstable. Pump pressure stability varies according to the pressure value and type of mobile phase. The following are reference fluctuation widths: LC-20AD, LC-20AB, LC-20ADXR, LC-30AD: within 0.2 MPa LC-20AT: within 0.3 MPa Purge the pump when pressure fluctuation is large. If this does not remedy large pressure fluctuation, probable causes are dirt in the check valve or liquid leaks from the plunger seal. For more details, refer to the Instruction Manual for the respective instrument.

Check Point	Remarks
Check the baseline.	<p>Make sure that the baseline is stable as in normal operation. The following are probable causes of the baseline not stabilizing within the preset stabilization time:</p> <ul style="list-style-type: none"> · Abnormally large noise A probable cause of this is air bubbles entering the detector cell and not being able to escape. Rinse the inside of the cell since this kind of trouble is likely to occur when it is dirty. Also, replace the lamp if lamp energy is low. · Drift or irregular waviness Rinse the line since there is the possibility that dirt in the column, piping, detector cell or mobile phase is being detected. · Relatively regular (cyclic) waviness This kind of trouble might occur when air blast from air-conditioning equipment directly strikes the detector or when air-conditioning equipment causes temperature control to fluctuate greatly, causing extreme differences in room temperature. Adjust the air-conditioning equipment so that air blast does not directly strike the detector.

■ After Data Acquisition Ends

Check Point	Remarks
Rinse the column.	When data acquisition has not been performed for some time, rinse the column, remove it from the instrument, and then put it in storage. The column rinsing method varies according to the type of column. For details, refer to the Instruction Manual for the column.
Rinse instruments.	<p>When data acquisition has not been performed for some time, rinse and remove the column according to the procedure above, and rinse the instrument flowpath. At this time, short-circuit the inlet and outlet pipes connected to the column with a coupling or other metal object, and then rinse the pipes.</p> <p>If the pipes are left connected to the column rinsed with solution containing water, mold or bacteria sometimes breeds inside the instrument flowpath. To prevent this kind of trouble, we recommend filling the instrument flowpath with 2-propanol, methanol or other kind of alcohol. Piping on both the inlet and exit ports of the suction filter and detector can be filled with solution after they are rinsed with solvent by immersing them in their reservoir bottles.</p>

Caution

Precautions When Selecting and Handling Mobile Phase Solvent

Do not use the following solvents when PEEK resin is used for piping.

Doing so might cause the intensity of the PEEK resin to drop, resulting in piping splitting and solvent spurting out.

Concentrated sulfuric acid, concentrated nitric acid, dichloroacetic acid, acetone, tetrahydrofuran (THF), dichloromethane, chloroform, and dimethyl sulfoxide (DMSO)

Note, however, that there is no problem in temporarily using a low-concentration water solution with an acetone concentration of 0.5% or less for checking low gradient performance.

**NOTE**

- Select a mobile phase solvent for the LC or equivalent, and remove any fine particles or dirt with a filter (0.45 μm or smaller) before use.
- Avoid using solvents containing halogen ions (e.g. KCl, NaCl, NH_4Cl) or solvents that generate halogen ions by reaction since halogen ions sometimes corrode the stainless steel (SUS316) pipe material. If such solvents must be used, rinse the entire flowpath sufficiently with distilled water immediately after data acquisition ends.
- When the UV detector is used at high sensitivity, use a solvent for the LC having low UV absorbance as the mobile phase solvent.
- Generation of air bubbles caused during mixing of solutions or by pressure and temperature changes, defective solvent delivery and generation of noise in the detection cell can be limited by degassing the mobile phase solvent.

3

GC Data Acquisition

This chapter describes the basic flow of operations from entrance of the data acquisition parameters to the performance of a single run data acquisition on the GC.

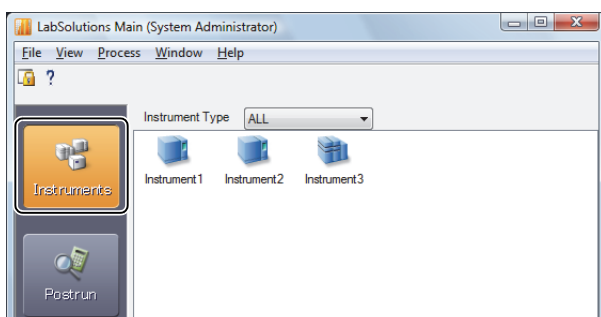
3.1 [Data Acquisition] Window

3

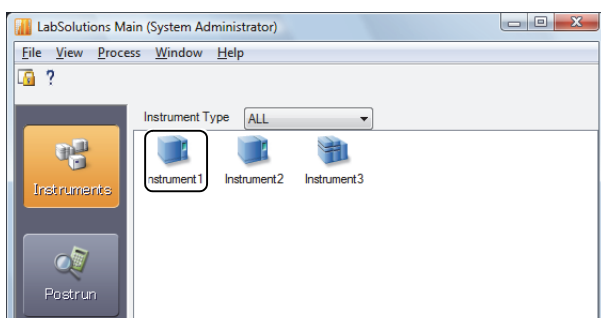
Two views of the [Data Acquisition] window are available, the [Chromatogram View] is used to display chromatograms and instrument status information and the [Instrument Parameters View] is used to display the parameters set for each instrument.

3.1.1 Open the [Data Acquisition] Window

- 1 Click the  icon.

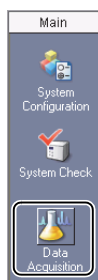


- 2 Select and double-click the instrument that will be used for data acquisition.




The [Realtime Analysis] program opens.

3 Click the  (Data Acquisition) icon on the [Main] assistant bar.

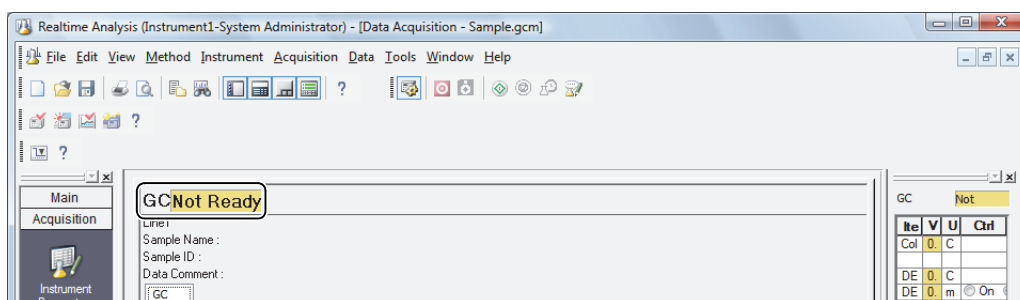


NOTE

If the  (Data Acquisition) icon is not displayed, click on the title of the assistant bar.



4 Ensure that [Ready] is displayed on the status display in the [Data Acquisition] window.

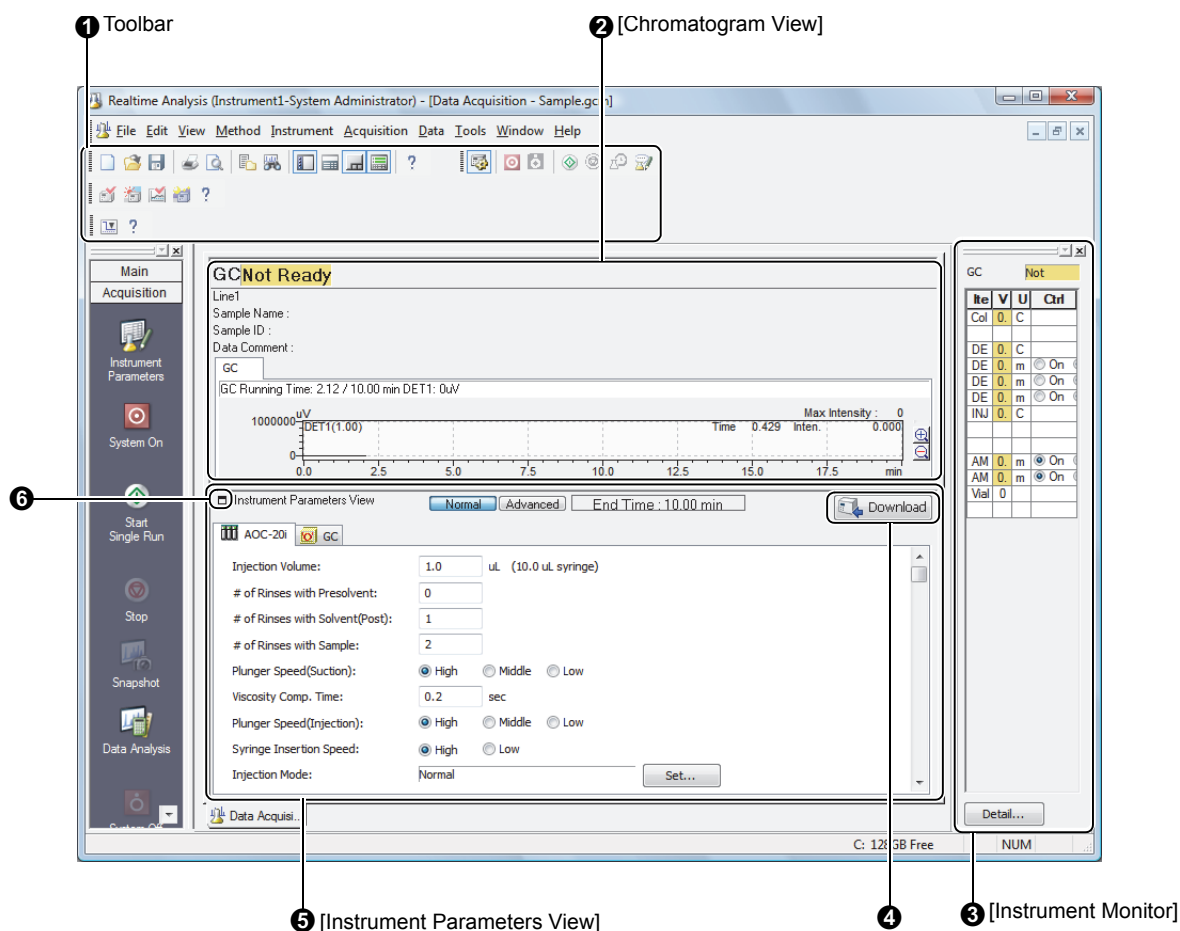



NOTE

If [Not Connected] is displayed on the status display, refer to "3.2 The Instrument Is Not Properly Recognized" in the Installation & Maintenance Guide.

3.1.2 [Data Acquisition] Window Description

This section describes how to view and use the [Data Acquisition] window.



No.	Explanation
1	Displays the [Standard] toolbar, [Data Acquisition] toolbar, [Instrument Control] toolbar, and [GC Control] toolbar.
2	Displays chromatograms and the instrument status curves. Reference Refer to " 3.3.1 Monitor the Chromatograms and Instrument Status Curves " P.45 to display the status information of instruments.
3	Displays the instrument status and parameter settings.
4	Click  to transfer the data acquisition settings set in [Instrument Parameters View] to the analytical instrument. Reference Refer to " 3.2.2 Analytical Instrument Startup " P.44 for details.
5	Displays the instrument parameters for data acquisition. In the [Normal] sub-window, the main data acquisition parameters are set on the [Autosampler] and [GC] tabs. In the [Advanced] sub-window, the tab for each configured instrument module is displayed so that data acquisition parameters can be set in more detail.
6	Switches between the full screen and normal display.

3.2 Enter Data Acquisition Parameters

Enter the data acquisition parameters in [Instrument Parameters View].

The parameters are saved to the method file and used to perform data acquisition.

This section describes the operations in the [Instrument Parameters View].

3.2.1 Set the Instrument Parameters

[Instrument Parameters View] has two sub-windows, [Normal] and [Advanced].

In the [Normal] sub-window, the main data acquisition parameters are set on the [Autosampler] and [GC] tabs. In the [Advanced] sub-window, a tab for each configured instrument module is displayed so that data acquisition parameters can be set in more detail.

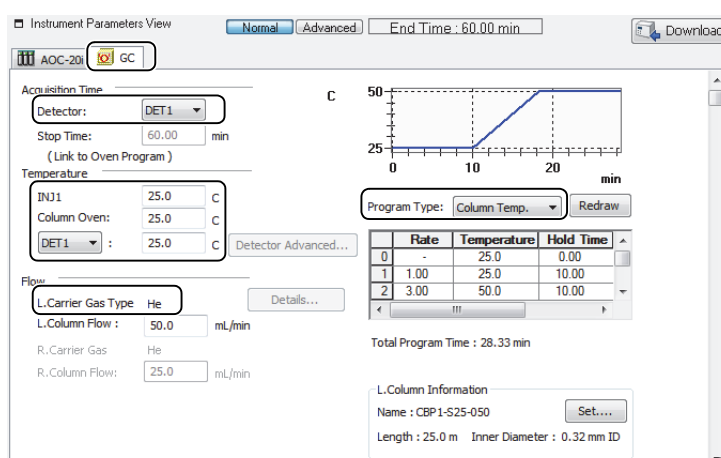
This section describes how to set the data acquisition parameters and create a method file.

1 Click [Normal] to open the [Normal] sub-window.



2 Click the [GC] tab and enter the data acquisition parameters.

Set the detector, oven temperature, carrier gas type, program type and other parameters.

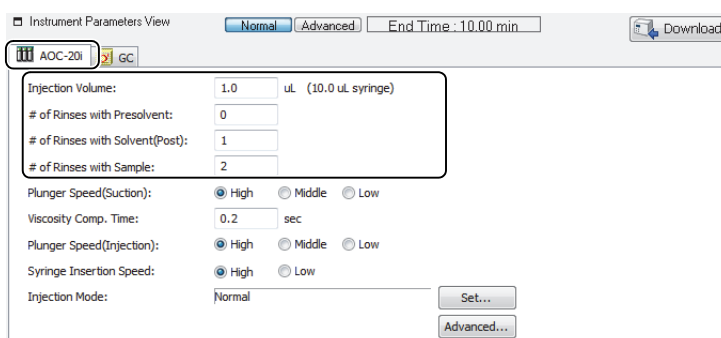


NOTE

- If [(Link to Oven Program)] is displayed, [Stop Time] cannot be set since the oven temperature program is linked to the data acquisition time. To set [Stop Time] different from [Total Program Time], right-click on the [Instrument Parameters View], and click and deselect [Link Oven Program edit and Acquisition Time] on the displayed menu.
- Click [Redraw] to draw the set program parameters in a graph.

3 Click the [Autosampler] tab, and enter the injection parameters.

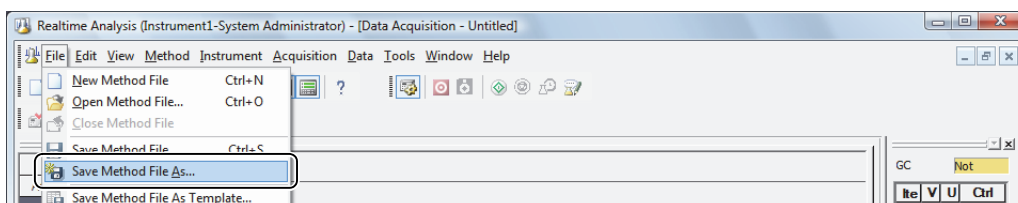
Enter the injection volume and number of rinsing.



NOTE

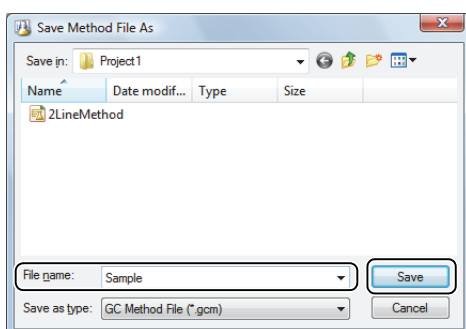
For the [Autosampler] tab, the autosampler name set in the [System Configuration] sub-window is displayed.

4 Click [Save Method File As] on the [File] menu.



The [Save Method File As] window is displayed.

5 Enter the file name, and click [Save].



A method file is created with the specified file name and the new instrument parameters are saved to the file.


3

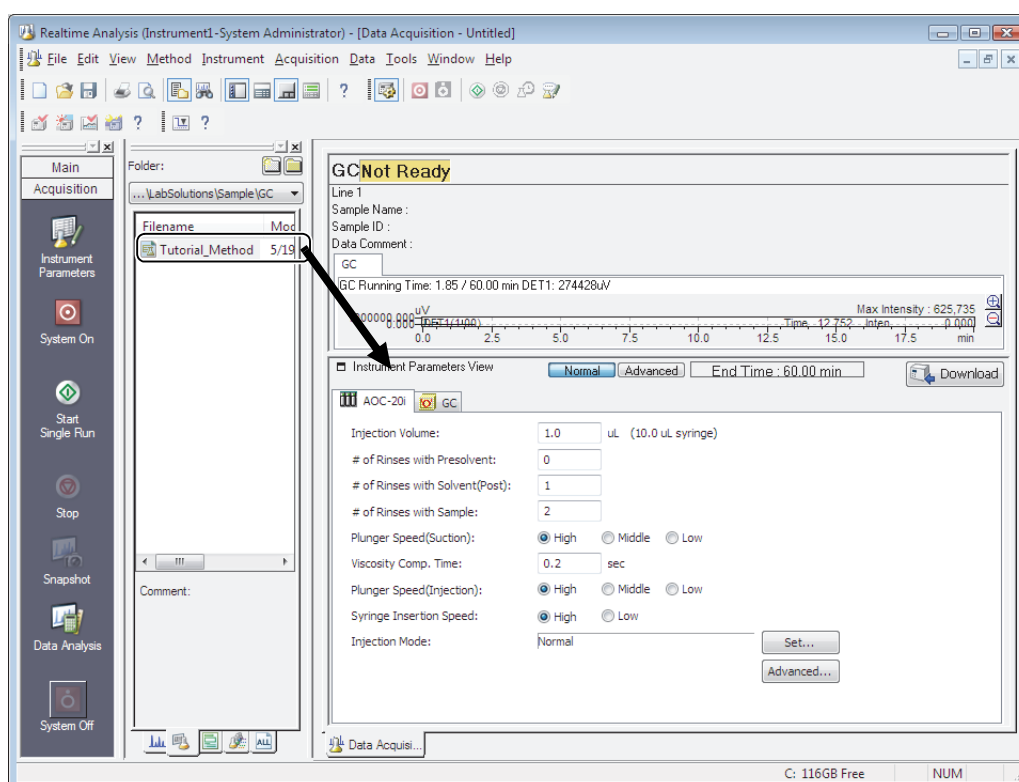
3.2.2 Analytical Instrument Startup

This section describes how to transfer (download) instrument parameters to an analytical instrument and the procedure for starting the instrument.



- 1 Drag-and-drop the desired method file onto the [Data Acquisition] window from the [Data Explorer] sub-window.**

NOTE

If the [Data Explorer] sub-window is not displayed, click the  (Toggle Data Explorer) button on the tool bar.



The content of the method file is displayed in the [Data Acquisition] window.

- 2 Check the instrument parameters, and click .**
The instrument parameters are transferred to the analytical instrument.
- 3 Click the  (GC System On) button on the toolbar.**
The carrier gas supply and oven temperature control are started.

3.3 Data Acquisition Preparation

This section describes the procedures to perform before starting data acquisition, such as baseline check.

3.3.1 Monitor the Chromatograms and Instrument Status Curves

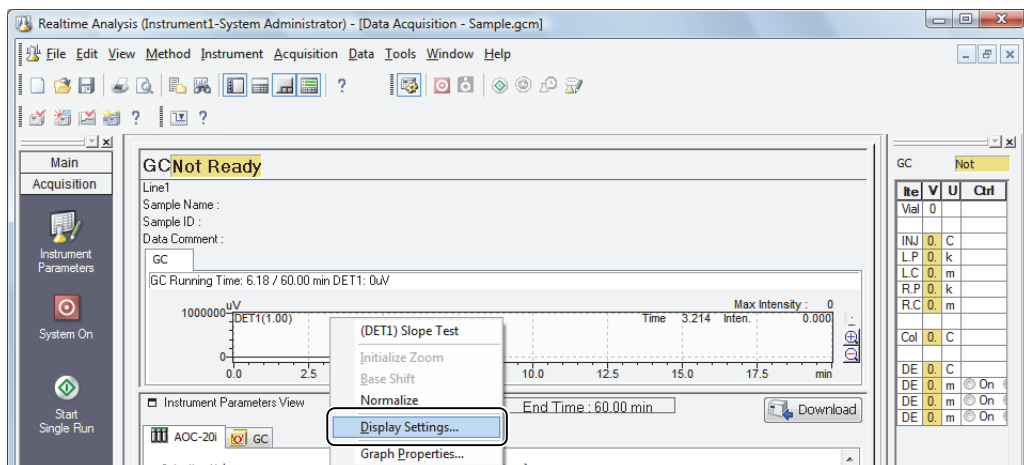
This section describes how to monitor chromatograms displayed in [Chromatogram View] and instrument status curves.

■ Chromatogram Display Settings

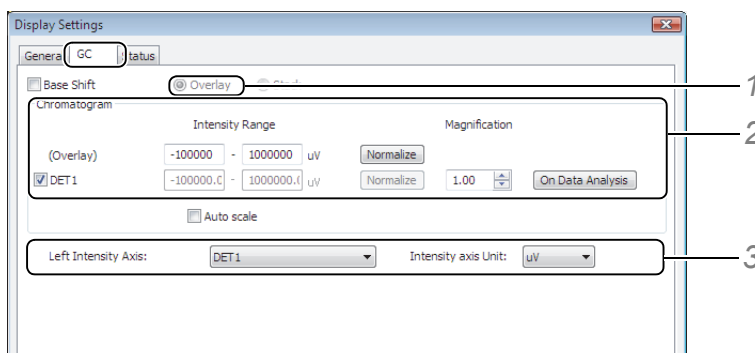
The chromatogram display scale can be changed.

This section describes how to monitor chromatograms on multiple channels.

1 Right-click on the graph in [Chromatogram View], and click [Display Settings].



2 Click the [GC] tab and enter the necessary parameters.



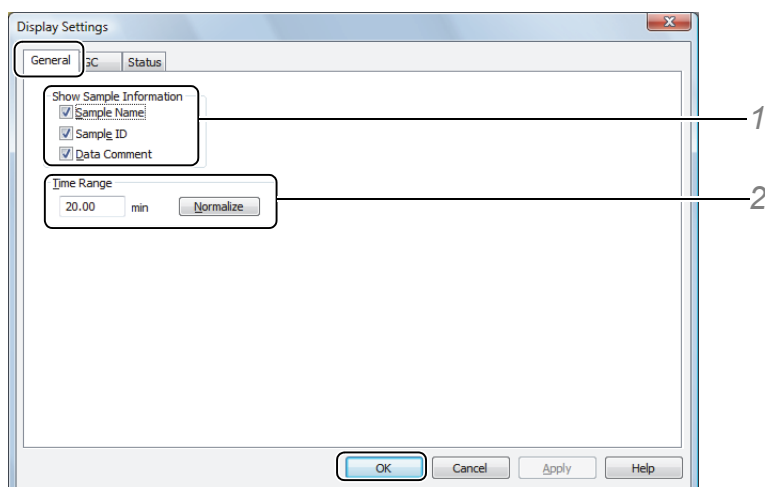
- 1 Click [Overlay] to draw chromatograms overlaid.
- 2 Enter the channel intensity range for the Y-axis.
Click [Normalize] so that the intensity range falls within the minimum and maximum values of the currently displayed chromatogram.
- 3 Select the channel and the display unit for the Y-axis.



NOTE

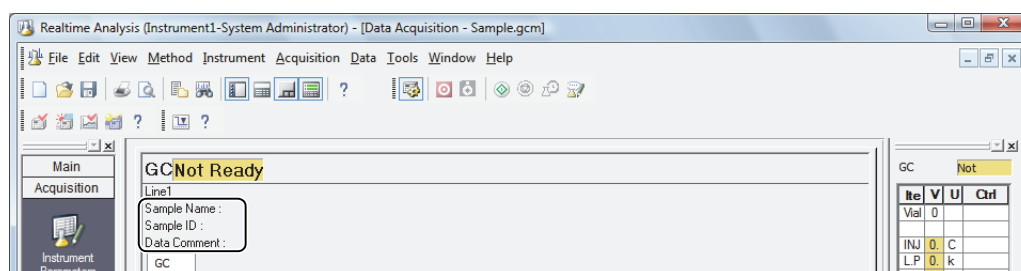
The intensity range of each channel cannot be set in the [Overlay] mode.

3 Click the [General] tab, enter the necessary parameters, and click [OK].



1 Select [Sample Name], [Sample ID] and [Data Comment].

The sample information is displayed in the status display of the [Data Acquisition] window.



2 Enter the [Time Range] for the X axis display range.

Click [Normalize] to set the display range of the X-axis to either the [Stop Time] currently set in the method file.

4 Click the (Save) button on the toolbar.

The time range and intensity range are saved to the method file.

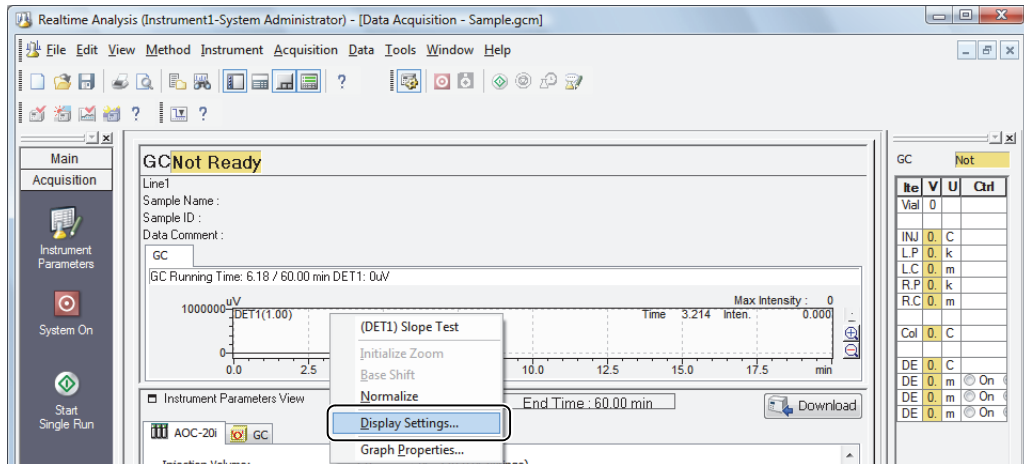
NOTE

- Settings other than the time range and intensity range are stored to memory for each user and instrument.
- The reference chromatogram is drawn overlaying [Chromatogram View].
Click [Open Reference Data File] in the [File] menu to select and display the reference chromatogram.

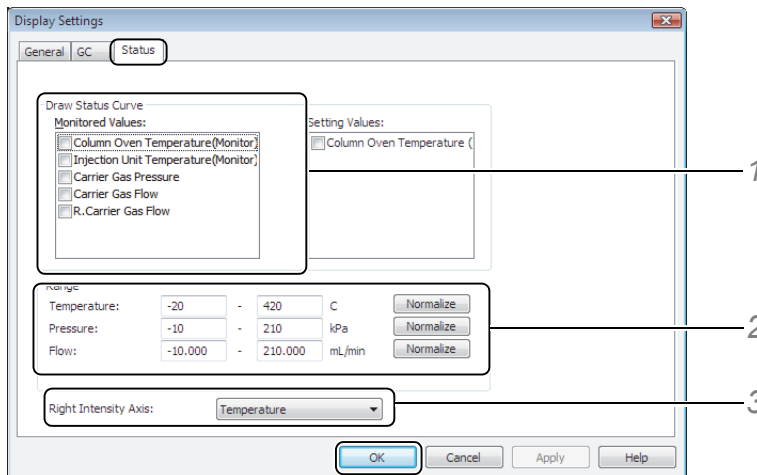
■ Display Instrument Status Curves

The instrument status curves that can be displayed on the graph in [Chromatogram View] include [Column Oven Temperature] and [Carrier Gas Pressure].

1 Right-click on the graph in [Chromatogram View], and click [Display Settings].

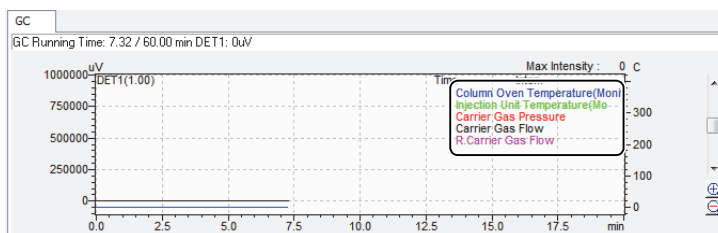


2 Click the [Status] tab, enter the necessary parameters, and click [OK].



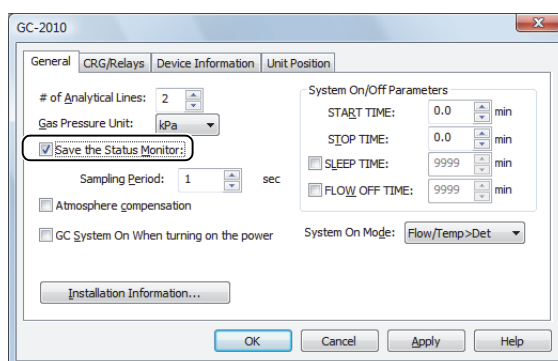
- 1 Select the desired display items in [Draw Status Curve].
- 2 Set the display range for each status item.
- 3 Select the type of status to display on the intensity axis on the right of the graph.

The selected status is displayed on the graph.



NOTE

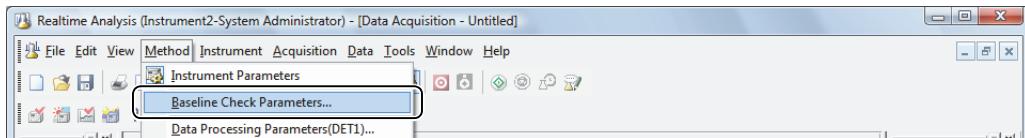
- Settings are stored to memory for each user and instrument.
- If items are not displayed at [Draw Status Curve], select [Save the Status Monitor] in the [Properties] sub-window for the GC in the [System Configuration] sub-window.



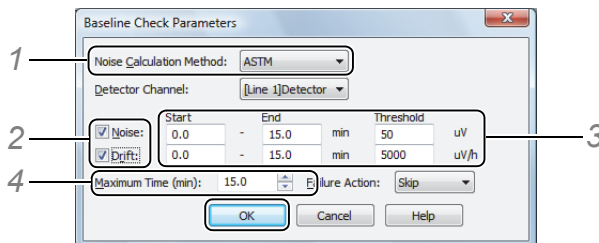
3.3.2 Check the Baseline

Use the baseline check function to determine whether the baseline noise and drift values are within the preset time and at or below the threshold for each channel.

- 1 Click **[Baseline Check Parameters]** from the **[Method]** menu in the **[Data Acquisition]** window.



- 2 Set the baseline check parameters, and click **[OK]**.



- 1 Select the noise calculation method.
- 2 Select **[Noise]** and **[Drift]**.
- 3 Enter the time and threshold used for checking **[Noise]** and **[Drift]**.
- 4 Enter a **[Maximum Time]** to performing repeat the evaluation if the checks "fail".

NOTE

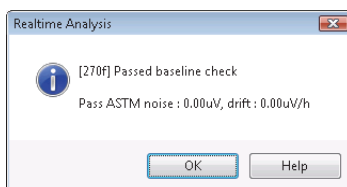
Select a **[Failure Action]** to be taken in the event of a baseline check failure. The **[Failure Action]** parameter is used when **[Baseline Check]** is used in the Batch Table.

- 3 Click the (**Save**) button on the toolbar.

The settings are saved to the method file.

- 4 Click on the (**Baseline Check**) button on the toolbar.

The baseline check is initiated, and the results of the baseline check are displayed after measurement ends.



NOTE

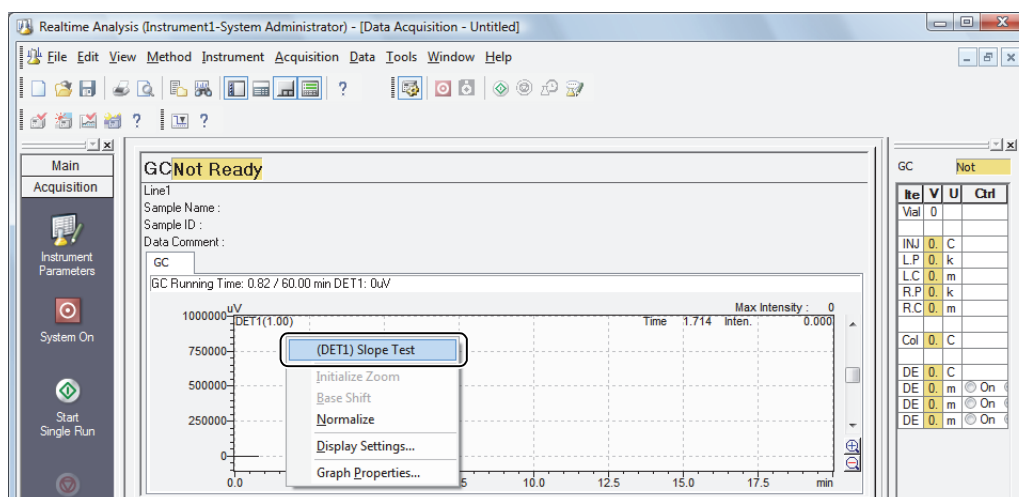
The results of the baseline check are saved in the C:\LabSolutions\Log\Baseline folder.

3.3.3 Calculate the Baseline Slope (Slope Test)

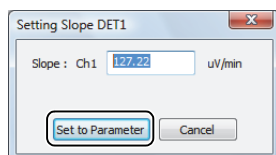
When the Slope Test is performed, the baseline of the chromatogram is measured to automatically calculate the Slope value.

The calculation results of the Slope Test can be set as the Slope value for the peak integration parameters.

- 1 Right-click on the graph in the [Chromatogram View], and click [Slope Test].



- 2 Click [Set to Parameter] to enter the on-screen value into the data processing parameters.



The data processing parameter [Slope] value is set.

NOTE

The Slope value is generally rounded up to value that is larger than the calculated value. For example, a Slope value of “1988” is changed to “2000”.


- 3 Click the  (Save) button on the toolbar.

The Slope value is saved to the method file.

NOTE

The Slope Test cannot be executed during data acquisition or during PDA plotting.

3.3.4 Detector Zero Correction

Use  (Zero Detector) on the toolbar to correct the signal intensity of the detector or CBM-102 to zero.

- 1 Click  (Zero Detector) on the toolbar.

The signal intensity of chromatograms is corrected to zero.

NOTE

The buttons displayed on the toolbar vary depending on the system configuration of the instrument.

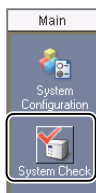
3.3.5 Check the Condition of Consumables (System Check)

Check the system to verify that it is in good condition before starting data acquisition (i.e. the system check).

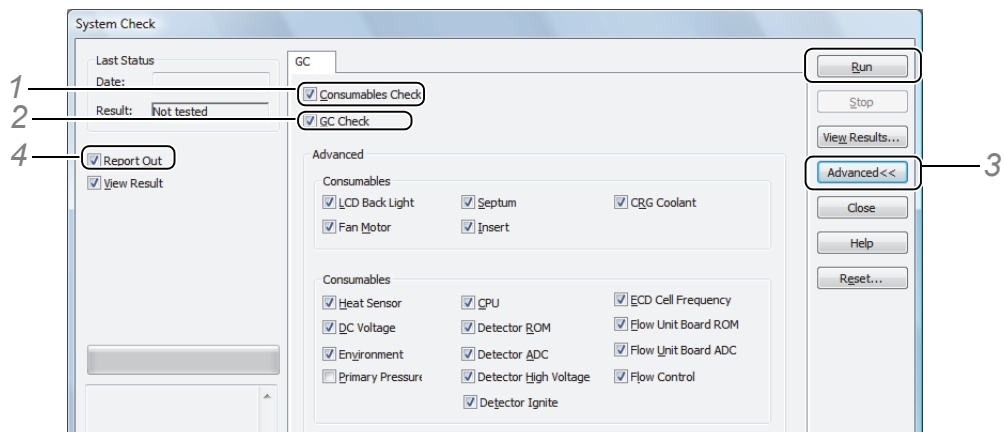
NOTE

- Users are required to have the [Run System Check] rights to execute the system check.
- For GC, the system check can be executed only if GC-2010 or GC-2014 is used.

1 Click the  (System Check) icon on the [Main] assistant bar.

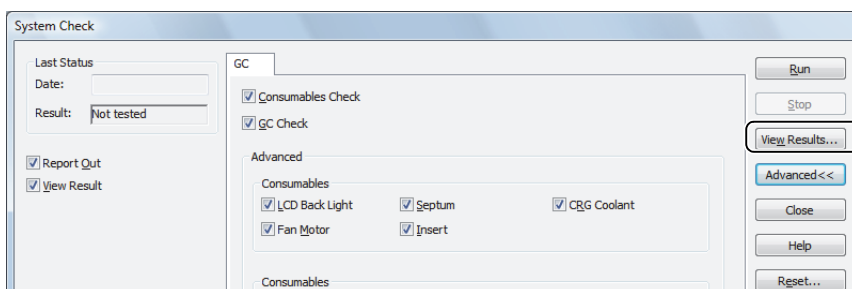


2 Select the items to check, and click [Run].



- 1 Select [Consumables Check].
- 2 Select [GC Check].
- 3 Click [Advanced], and select the items to perform the system check on.
- 4 Select [Report Out] to automatically print the system check results.

3 After the system check ends, click [View Results].



The [System Check Results] sub-window opens.

NOTE

- Click [Print] in the [System Check Results] sub-window to print the system check results.
- The system check results are saved to a file named according to the following rule: "SysChk#_YYYYMMDDHHMMSS.lcs" (where, "#" is the system number.)
- To check the results of previous system checks, click [Load] in the [System Check Results] sub-window, and select the desired results.
- Set [System Check] in a Batch Table, to check the use frequency of instrument consumables before starting data acquisition. Refer to "[4.2.3 Batch Table Parameters](#)" P.78 for details.
- Realtime batch can be canceled according to the results of the system check by using the Batch Table action function.
- The system check is based on the consumable criteria of each instrument. Check consumable criteria in the [System Check] sub-window by clicking [System Check] in the [Properties] sub-window of each instrument.
- Click [Reset] to open the [Consumables Reset] sub-window. Reset the consumables when they have been replaced.
- Users are required to have the [Edit System Configuration] rights to set system check criteria.

3.4 Single Run

There are two ways of acquiring data, by single run (only one data acquisition), or by realtime batch (sequential analysis of multiple samples).

This section describes the procedure for a single run.

NOTE


Verify that [Ready] is displayed on the status display.

Reference

Refer to "[4 Realtime Batch](#)" P.63 for information on sequential analysis of multiple samples.

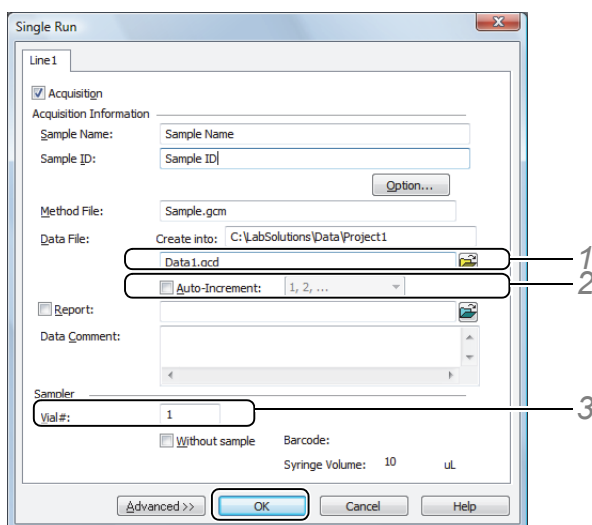
3.4.1 Execute Single Run

Execute single run from the [Data Acquisition] window.

- 1 Click the  (Start Single Run) icon on the [Acquisition] assistant bar.



2 Set the acquisition conditions, and click [OK].



- 1 Enter the data file name.
- 2 Select [Auto-increment], and the number type.
The data file name is automatically appended with an incremental number.
Example: "TEST-001.lcd", "TEST-001.gcd"



NOTE

When [Auto-increment] is selected, the file is not overwritten even if the file name was previously used.

- 3 Enter the position of the sample for [Vial#].



NOTE

- Selecting [Without sample] or entering "-1" at [Vial #] acquires data without injecting samples from the autosampler.
Data acquisition can be started without pressing the [Start] button on the GC.
- If the autosampler is TurboMatrix, data acquisition cannot be started by entering "-1" at [Vial #].

- 4 Enter the sample injection volume.

Single run is started.

During data acquisition, the [LabSolutions Service] icon in the Systray on the Taskbar flashes green.



Data acquisition ends when the data acquisition time in the method file has elapsed.



NOTE

- Do not turn the PC off while the [LabSolutions Service] icon is flashing.
- In the case of a dual-line configuration, set the data acquisition parameters on the [Line 1] and [Line 2] tabs.

3.4.2 Change the End Time During Data Acquisition

The data acquisition time can be changed during data acquisition.

This section describes the procedure for changing the data acquisition time.

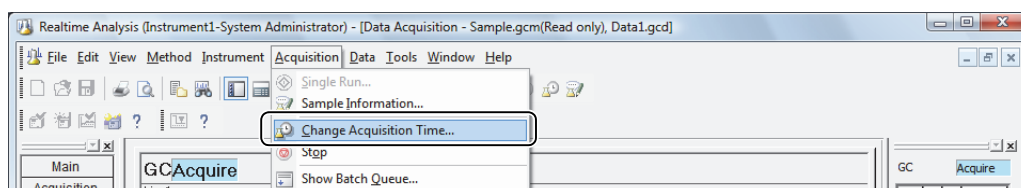


NOTE

- The end time for the detector in [Method View] is changed.
- If the acquisition time is changed using [Change Acquisition Time], a record is created in the operation log.

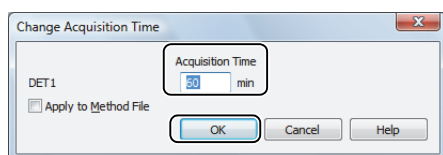
1

Click [Change Acquisition Time] on the [Acquisition] menu.



2

Enter an [Acquisition Time], and click [OK].



NOTE

- If multiple detectors are used, click [All Times Change] to changes the data acquisition time to the longest detector acquisition time.
- If [Change to Minimum Value] is selected, click [All Times Change] to change the data acquisition time to the shortest detector acquisition time.
- Click [Apply to Method File] to apply the new acquisition time to the method file and use it for all subsequent data acquisitions.
- You can not change the value as an analysis time that already passed.

3.4.3 Stop Single Run

Single run can be stopped in the midway to end acquisition earlier than the preset end time.

1


Click the  (Stop) icon on the [Acquisition] assistant bar.

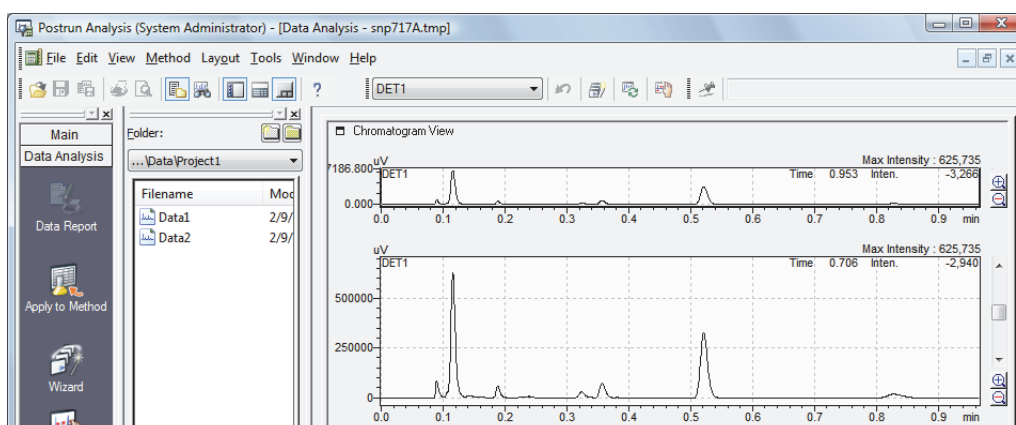
Data acquisition is stopped, and a data file is created for the data so far.

3.5 Check Analysis Results During Data Acquisition (Snapshot)

Execute snapshot during data acquisition to display and process the data obtained since acquisition was started.


This section describes the procedure for executing a snapshot during data acquisition.

- 1 Click the  (Snapshot) icon on the [Acquisition] assistant bar.
The data obtained so far is displayed in the [Data Analysis] window.




3.5.1 Update Snapshots

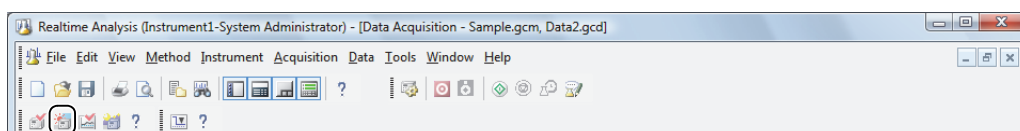
Use snapshot update to load cumulative acquired data from a continuing data acquisition after snapshot has been executed.

- 1 Click the  (Update for Snapshot) button on the toolbar in the [Data Analysis] window.
The snapshot is updated to display the latest chromatogram.

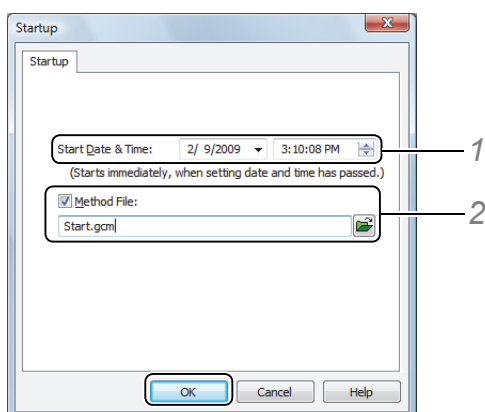
3.6 Automatic Instrument Startup


Use  (Startup) to automatically start the instrument at a specified date and time.

- 1 Click the  (Startup) button on the toolbar.



- 2 Enter the date and time to start the instrument, and click [OK].



- 1 Set the date and time to start the instrument.
- 2 Select [Method File], and enter the method file name. The method file can also be selected by clicking .



NOTE

When the method file is not specified, the analytical instrument is started up by the parameters already downloaded to the instrument (i.e. parameters used in the previous data acquisition) when a startup is performed.

The instrument starts up at the specified date and time.



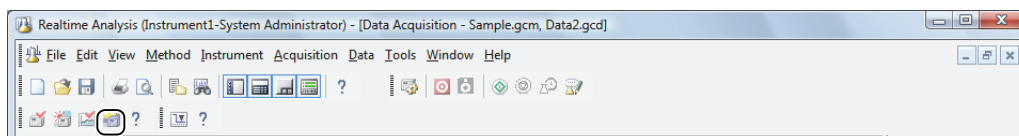
NOTE

- If startup is executed in a batch file(s) registered to the batch queue, the startup begins after processing of the previously registered batch file(s) ends.
For details on the procedure for changing the execution order of batch files registered to the batch queue, refer to ["4.5 Data Acquisition Using the Batch Queue Function" P.96.](#)
- Startup can also be set in realtime batch.
For details, refer to ["4.4.2 Start Data Acquisition at a Specified Date and Time \(Startup\)" P.87.](#)

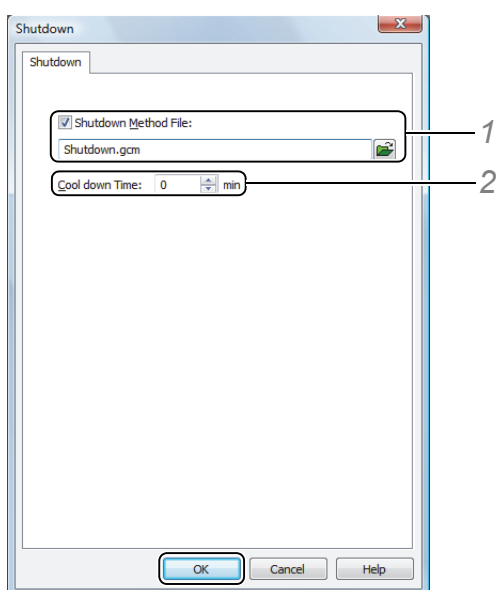
3.7 Automatic Instrument Shutdown


Use [Shutdown] to automatically shut down the instrument after data acquisition ends.

- 1 Click the  (Shutdown) button on the toolbar.



- 2 Set the date and time to shut down the instrument, and click [OK].



- 1 Select [Shutdown Method File], and enter the method file name. The method file can also be selected by clicking .

NOTE

When a method file is not specified, the analytical instrument is shut down by the parameters already downloaded to the instrument when a shutdown is performed.

- 2 Enter the time that the instrument is operated by the instrument parameters of the specified method file.

The analytical instruments shut down when the [Cool down Time] elapses.

NOTE

- If shutdown is executed in a batch file(s) registered to the batch queue, the shutdown begins after processing of the registered batch file(s) ends.
For details on the procedure for changing the execution order of batch files registered to the batch queue, refer to ["4.5 Data Acquisition Using the Batch Queue Function" P.96](#).
- Shutdown can also be set in realtime batch.
For details, refer to ["4.4.3 Shutdown Analytical Instruments After Data Acquisition \(Shutdown\)" P.88](#).
- With GC-14A/B, analytical instruments are not shutdown. The shutdown method is downloaded but the instruments continue to run even if the cool down time has elapsed.

3.8 Change the Sampling Rate

The sampling rate can be set matched to the peak shape of the chromatogram to acquire.

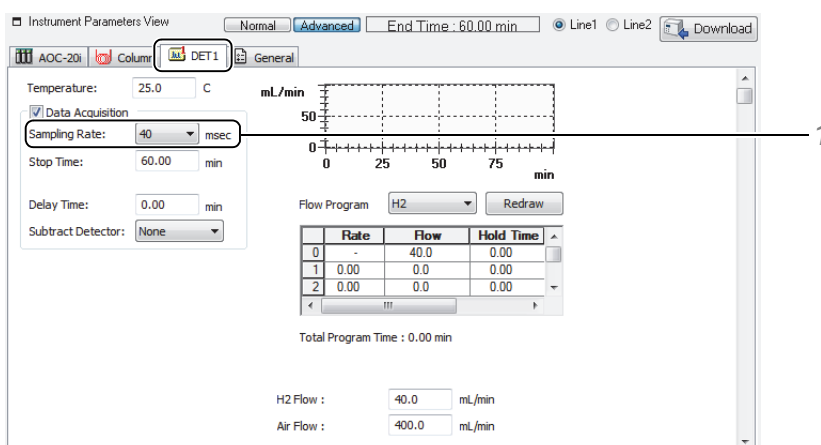
Decreasing the sampling rate enables narrower sharp peaks to be detected. However, in this case, more noise might be detected, possibly preventing correct peaks from being detected.

This section describes how to set the sampling rate.

1 Click [Advanced] in [Instrument Parameters View].



2 Click the [Detector] tab, and set the sampling interval of the detector.



1 Select the setting value from the list.

3 Click the (Save) button on the toolbar.

The settings are saved to the method file.

NOTE

- For the [Detector] tab, the detector name set in the [System Configuration] sub-window is displayed.
- The base period is the signal cycle sent to the PC from the detector. Set the base period in the [Properties] sub-window for the detector in the [System Configuration] sub-window.
- The sampling rate is the signal interval to record to the data file, and becomes the data points of chromatograms.
Note that data files increase in size the smaller the sampling rate becomes.
- The sampling rate, and data processing parameter [Width] value also affects peak detection.

■ Setting the Data Sampling Rate at [Sampling Rate]

Set the sampling rate to match the peak shape of the chromatogram.

Initial Value	Base Period of each detector set in the [System Configuration] sub-window
Setting range	Base Period 1 to 20 times of 4 msec to 80 msec range (If Base Period is 100 msec or longer: 1 to 10 times)
Recommended values	Data acquisition with a packed column: 40 msec to 160 msec Regular capillary data acquisition: 40 msec to 160 msec High-speed data acquisition with a narrow-pore column: 20 msec to 60 msec

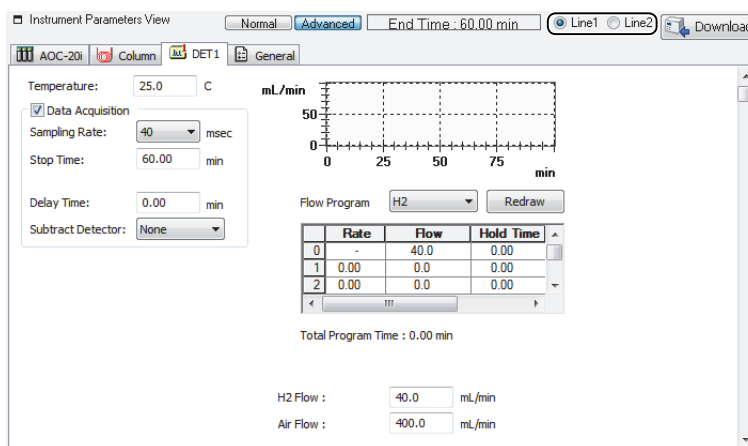
3

3.9 Set the Instrument Parameters for the Dual-Line Configuration GC

This section describes how to set the data acquisition parameters (instrument parameters) for the dual-line configuration GC.

Select [Line 1] and [Line 2] in [Instrument Parameters View], and set the parameters.

1 Click [Line 1] in [Instrument Parameters View], and set the instrument parameters to use.



Reference

Refer to ["3.2.1 Set the Instrument Parameters" P.42](#) for more details.


2 Set the parameters for [Line 2] by the same procedure.


3 Save the instrument parameters to the method file, and download it to the instrument.

Reference

Refer to ["3.2.2 Analytical Instrument Startup" P.44](#) for details on how to download the file.

3.10 Acquire Data from the [Start] Button on the GC Unit

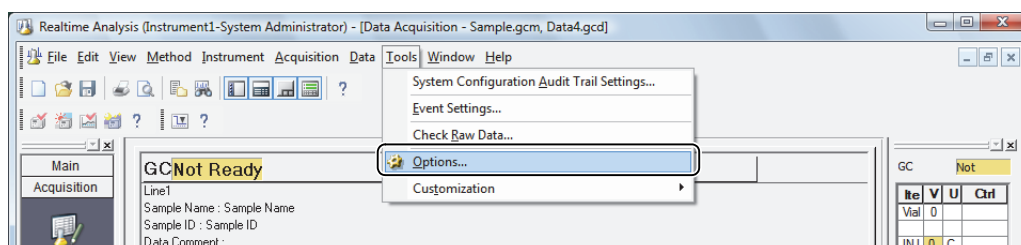
If [Acquisition Start from Instrument] is selected, data can be acquired simply by pressing the  button on the GC unit.

This section describes how to acquire data by pressing the  button on the GC unit using the pre-loaded method file.

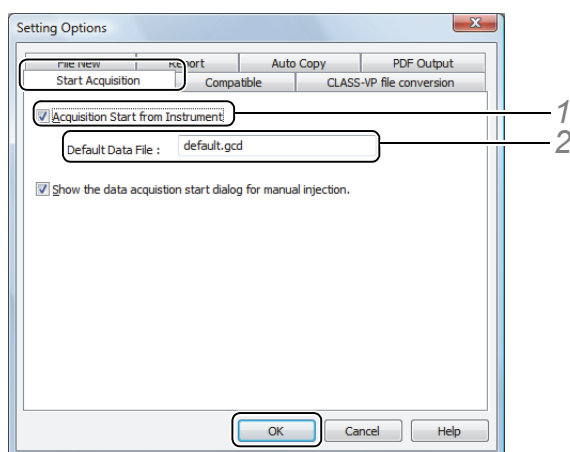
NOTE

- This function cannot be used for the system with GC-14A/B.
- If the screen is locked by the popup sub-window for setting or due to data acquisition, data acquisition cannot be started.

1 Click [Options] on the [Tool] menu.



2 Click the [Start Acquisition] tab, enter the necessary parameters, and click [OK].



- 1 Select [Acquisition Start from Instrument].
- 2 Enter the default data file name at [Default Data File].

3 Press the button on the GC unit.

Data acquisition is started.

NOTE

The acquired data is saved under the name of the file displayed at [Default Data File] in the [Setting Options] sub-window. Even if the data acquisition continues to be performed, the file is not overwritten since the data file name is automatically appended with an incremental number.

■ If Data Could Not Be Acquired Successfully

Check the following if data could not be acquired.

Download is not executed.

If the [Data Acquisition] window is started up or a method file is changed, be sure to download the file before starting data acquisition.

In the case of GC units connected via the CBM-102, data acquisition can be performed only if the method is downloaded.

Programs such as oven temperature program are not set.

Correct data acquisition can be performed only if the GC program is set.

Be sure to set the oven temperature program.

Be sure to set the hold time for isocratic analysis.

3

3.11 If Single Baseline of instrument Is Unstable

Shortly after the GC unit is started up, if the previously acquired sample remains in the injection unit or the column, the baseline may become unstable or extraneous peaks may appear.

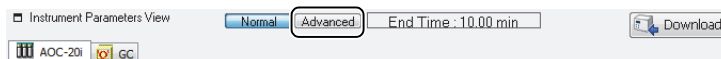
If this occurs, condition or clean up the column.

Perform the same procedure to clear the sample in the column if data acquisition fails due to a sample injection error.

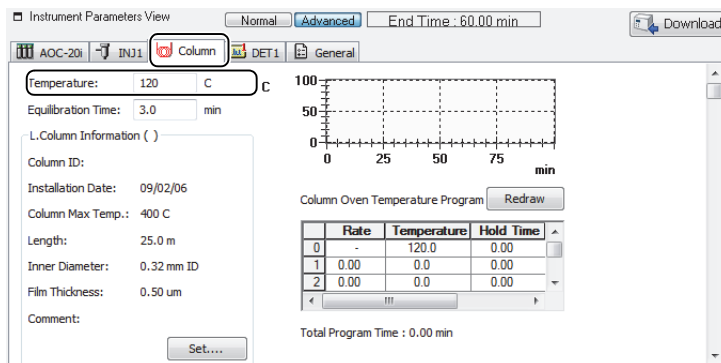
■ Change the Column Temperature for Instrument Parameters

This section describes how to change the column initial temperature from 50 °C to 120 °C and to return to 50 °C of initial temperature after conditioning and confirming that the baseline becomes stable.

1 Click [Advanced] in [Instrument Parameters View].



2 Click the [Column] tab and enter "120" at [Temperature].



3 Click .


Wait a while until the baseline becomes stable.

4 When the baseline becomes stable, enter "50" for the initial temperature at [Temperature].

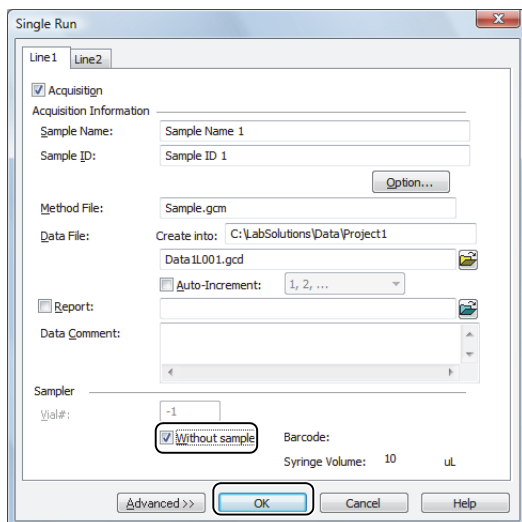
5 Click  Download.

■ Acquire Data Without Injecting Samples

Data acquisition is performed without injecting samples to check the baseline, under the same acquisition parameters as for the programmed temperature analysis, where column oven temperature is gradually raised.

1 Click the  (Start Single Run) icon on the [Acquisition] assistant bar.

2 Select [Without sample], and click [OK].



The screenshot shows the 'Single Run' dialog box with the following details:

- Line 1 | Line 2
- Acquisition
- Acquisition Information
- Sample Name: Sample Name 1
- Sample ID: Sample ID 1
- Method File: Sample.gcm
- Data File: Create into: C:\LabSolutions\Data\Project1
- Data File: Data1.L001.gcd
- Auto-Increment: 1, 2, ...
- Report:
- Data Comment:
- Sampler
- Val#: -1
- Without sample
- Barcode:
- Syringe Volume: 10 uL
- Buttons: Advanced >>, OK, Cancel, Help

NOTE

In the case of a dual-line configuration GC, make settings both on the [Line 1] and [Line 2] tabs.

■ Acquire Data With Solvent Injected (Without Injecting Samples)

In cases such as if extraneous peaks appear, data acquisition is performed with solvent rather than a sample injected to check chromatograms. Follow the same procedure as for regular data acquisition.

Reference

Refer to "3.4.1 Execute Single Run" P.52 for details on single run.

NOTE

If there is dirt in the injection unit, increase the temperature in the unit to clear the dirt. At that time, multiple injections of solvent sometimes increase the effect of clearing the dirt.

Also, replace glass insert and septum as required.

For more details, refer to the Instruction Manual for the GC unit.

4

Realtime Batch


Realtime batch is sequential data acquisition of multiple samples. Execution of realtime batch starts with the preparation of a Batch Table.

This chapter describes the procedures for automating data acquisition.

- Making Batch Tables
- Baseline check to verify the stability of the baseline
- [Startup] to begin realtime batch analysis at a specified date and time
- [Shutdown] to shutdown the instrument after realtime batch ends

4

4.1 Display Batch Tables

Click the  (Realtime Batch) icon on the [Main] assistant bar in the [Realtime Analysis] program to display the Batch Table.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Inj. Volume	Report Output	Report Format F
1					0.Unknown			1	10		

4.2 Create Batch Tables

Enter the sample information, vial #, method file name, and data file name in a Batch Table to sequentially acquire data from multiple samples.

This section describes how to create a Batch Table

4.2.1 Batch Table Wizard

Batch Tables can be made easily by using the Batch Table Wizard. This section describes how to create a Batch Table separately for LC and GC since the Batch Table Wizard varies according to the instrument in use. See "*For LC*" and "*For GC*" below.

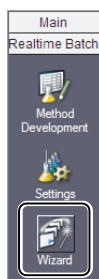


NOTE

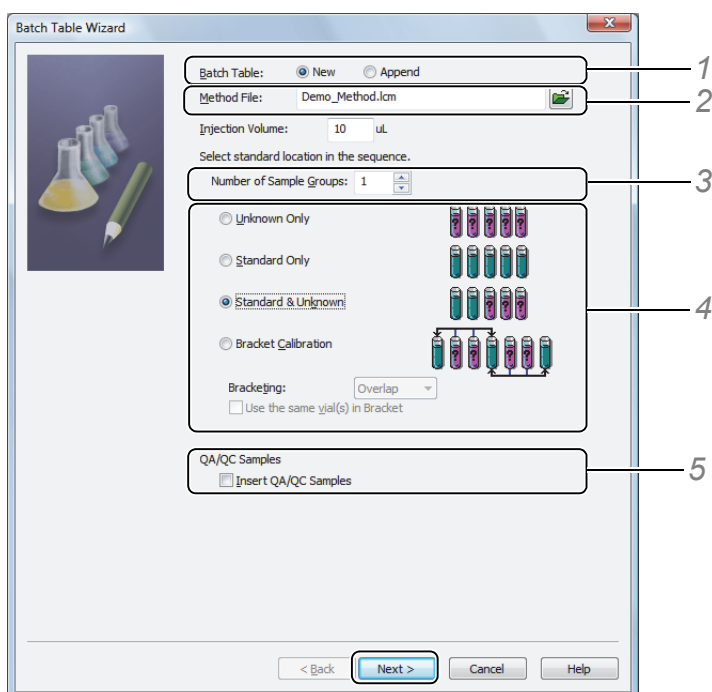
Some features of the Batch Tables cannot be set with the Batch Table Wizard. It is necessary to directly edit the Batch Table to set these functions.

■ For LC

- 1 Click the  (Wizard) icon on the [Realtime Batch] assistant bar.



- 2 Enter the parameters, and click [Next].



- 1 Click [New] at [Batch Table] to create a new Batch Table file.
Click [Add] to add a row to the currently displayed Batch Table.
- 2 Enter the [Method File].
- 3 Enter the [Injection Volume].
- 4 Enter the data acquisition pattern for the standard samples and unknown samples.
Enter a number for [Number of Sample Groups] to indicate the number of times the data acquisition pattern will be repeated.
Select [Bracket Calibration] to select the type of bracket quantitation.

Reference

For details, see ["4.4.6 Bracket Quantitation" P.92.](#)

- 5 Select [Insert QA/QC Samples] to insert a QA/QC sample.

If [Insert QA/QC Samples] is selected, the [Batch Table Wizard - QA/QC Sample] sub-window is displayed. If [Insert QA/QC Samples] is deselected, proceed to Step 4.

3 Enter the QA/QC sample information, then click [Next].

Batch Table Wizard - QA/QC Sample

QA/QC Samples

Sample Name: QA/QC sample Auto-increment

Sample ID: SST-0001 Auto-increment

Data File Name:

Create file names automatically

(Auto Filename) Auto-increment

Autosampler

Tray Definition: Rack 1.5 mL 70 vials

Tray: 1

Number of QA/QC Sample Vials: 1

Repetitions per Run: 1

Vial #: 1 - 1

Print Report

Report Format File:

< Back **Next >** Cancel Help

4 Enter the standard sample information, and click [Next].

Batch Table Wizard - Standard Sample

Standard Sample

Sample Name: Standard Sample Auto-increment

Sample ID: STD-0001 Auto-increment

Data File Name:

Create file names automatically

(Auto Filename) Auto-increment

Number of Calibration Levels: 3

Number of Standard Sample Vials per Level: 1

Repetitions per Run: 1

Autosampler

Tray Definition: Rack 1.5 mL 70 vials

Tray: 1

Vial #: 2 - 4

Clear all calibrations at the beginning

Use the same standard sample vial for all groups

Print Report

Report Format File: CalibrationCurveReport_1.lsr

Data Comment:

< Back **Next >** Cancel Help

- 1 Enter [Sample Name] and [Sample ID] for the standard sample.
If [Auto-increment] is selected, the [Sample Name] and [Sample ID] are automatically appended with an incremental number.
- 2 Enter a [Data File Name].
Select [Create file names automatically] to automatically generate a data file name.

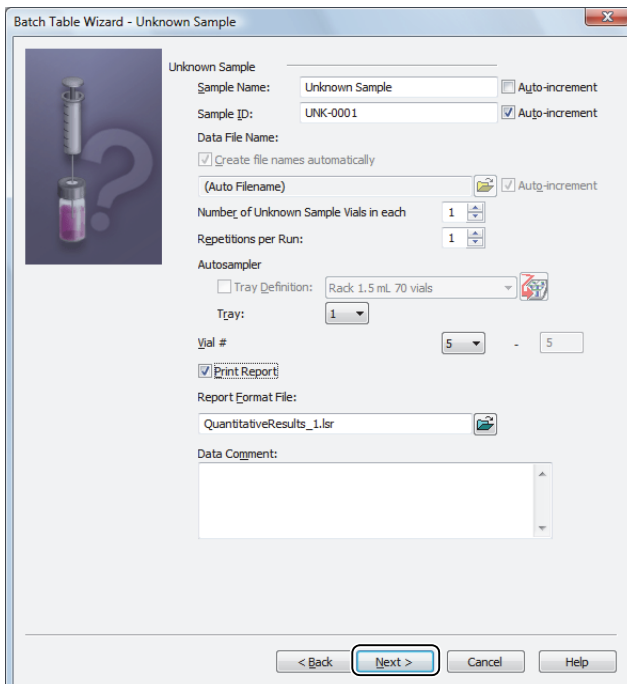
Reference

For details, see *"Set the Data File Name" P.104.*

- 3 Set the [Number of Calibration Levels] (number of calibration points), [Repetitions per Run] (number of injections) and select [Clear all calibrations at the beginning] to initialize the calibration curve.
The final vial No. of the standard sample you have set is displayed at [Vial#] in the Batch Table.
- 4 Select [Print Report] and set [Report Format File] to create reports.

5

Enter the unknown sample information, as with the standard sample, and click [Next].



Batch Table Wizard - Unknown Sample

Unknown Sample

Sample Name: Unknown Sample Auto-increment

Sample ID: UNK-0001 Auto-increment

Data File Name:

Create file names automatically

(Auto Filename) Auto-increment

Number of Unknown Sample Vials in each: 1

Repetitions per Run: 1

Autosampler

Tray Definition: Rack 1.5 mL 70 vials

Tray: 1

Vial #: 5 - 5

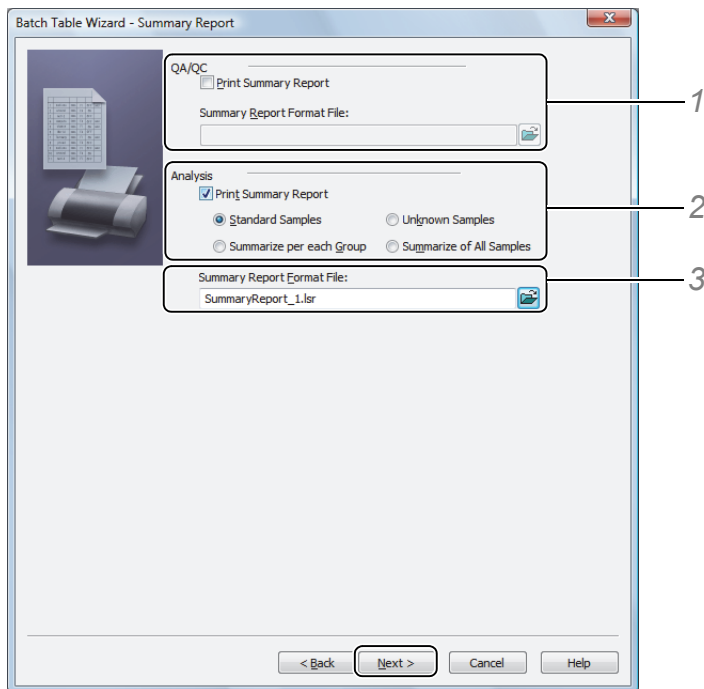
Print Report

Report Format File: QuantitativeResults_1.lsr

Data Comment:

< Back Next > Cancel Help

6 Set the summary report output parameters, and click [Next].



- 1 Select [Print Summary Report] for [QA/QC], and select a [Summary Report Format File].



NOTE

[QA/QC] is not displayed if [Insert QA/QC Samples] is deselected in the [Batch Table Wizard] sub-window.

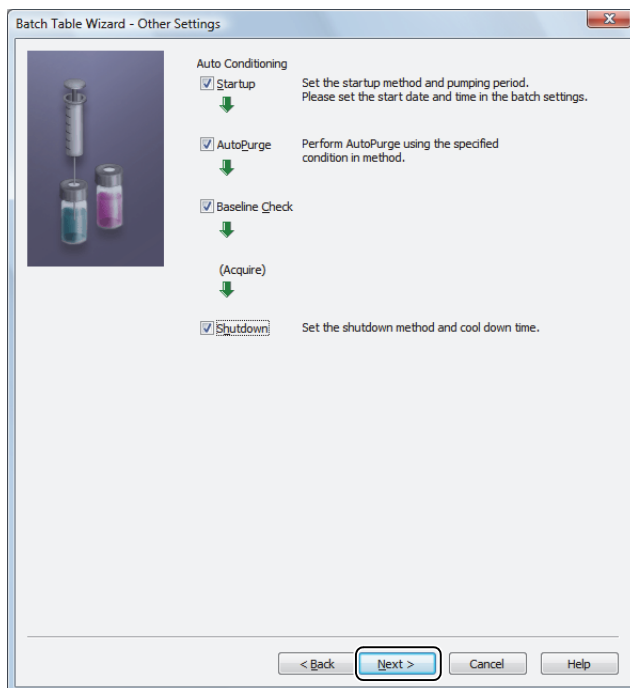
- 2 Select [Print Summary Report] for [Analysis], and select the type of sample summary that will be reported.
- 3 Select the [Summary Report Format File].

7

Select the items to be executed, and click [Next].

If [Startup] or [Shutdown] are selected, a setting sub-windows for each item is displayed. (Steps 8 or 9)

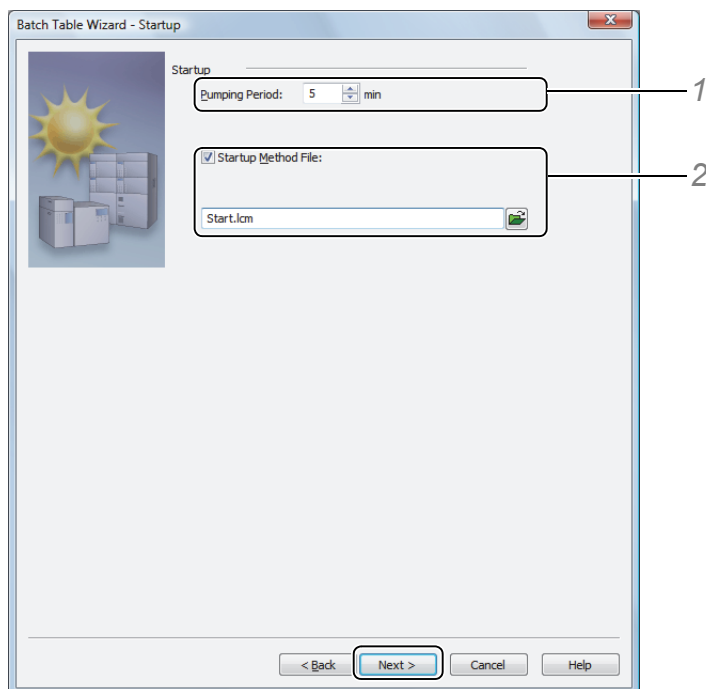
If all of these items are deselected, proceed to Step 10.



8 Select the startup settings, and click [Next].

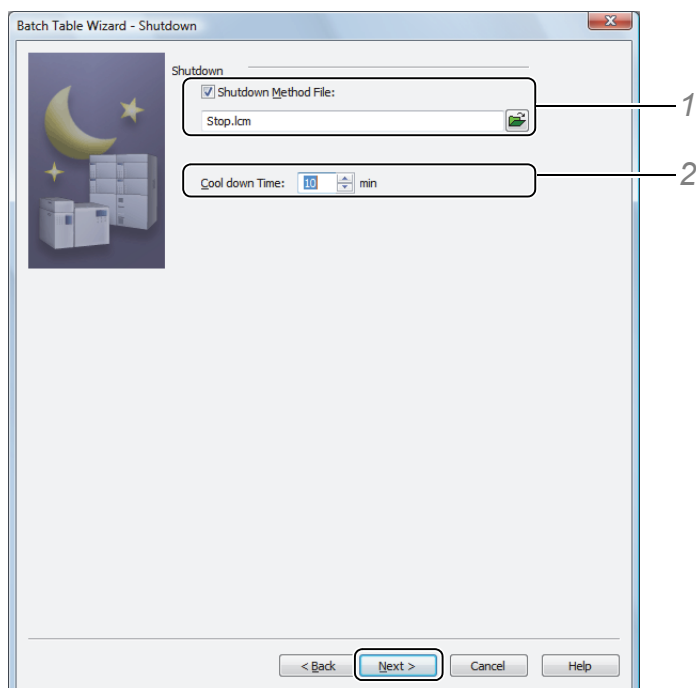
NOTE

The startup start date and time cannot be set in the Batch Table Wizard. Refer to ["4.4.2 Start Data Acquisition at a Specified Date and Time \(Startup\)" P.87](#) to enter a specified date and time.



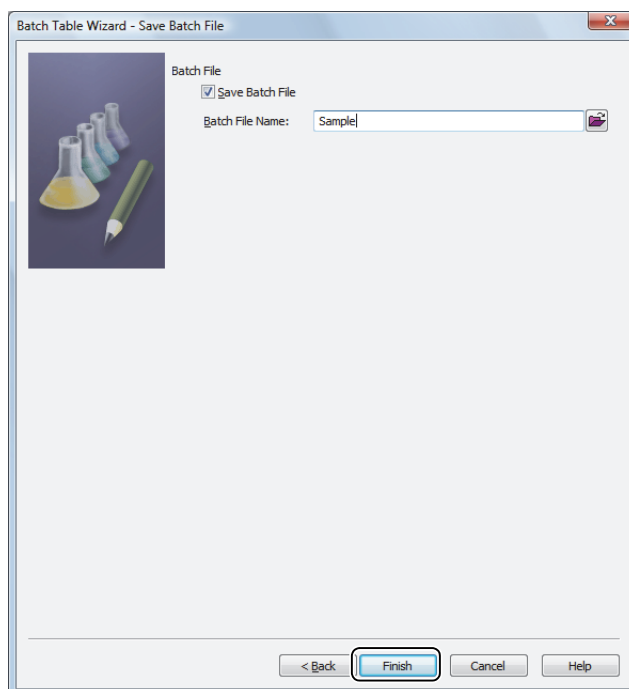
- 1 Enter an instrument startup time at [Pumping Period].
- 2 Select [Startup Method File], and enter the method file.

9 Select the shutdown settings, and click [Next].



- 1 Select [Shutdown Method File], and enter the method file.
- 2 Enter an instrument shutdown time at [Cool down Time].

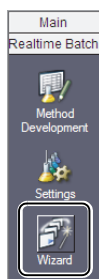
10 Enter a batch file name, and click [Finish].



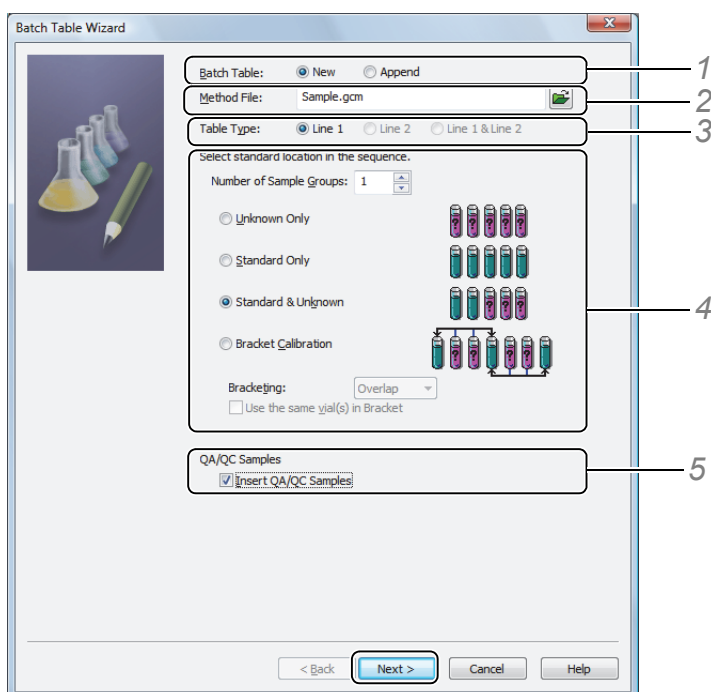
This completes Batch Table setup using the Batch Table Wizard. The batch file is created using the specified file name. This Batch Table is displayed in the Batch Table sub-window. Check the contents of the Batch Table.

■ For GC

- 1 Click the  (Wizard) icon on the [Realtime Batch] assistant bar.



- 2 Enter the parameters, and click [Next].



- 1 Click [New] at [Batch Table] to create a new Batch Table file.
Click [Add] to add a row to the currently displayed Batch Table.
- 2 Enter the [Method File].
- 3 Select the [Table Type].
In the case of dual-line configuration, select [Line 1 & Line 2].
- 4 Enter the data acquisition pattern for the standard samples and unknown samples.
Enter a number for [Number of Sample Groups] to indicate the number of times the data acquisition pattern will be repeated.
Select [Bracket Calibration] to select the type of bracket quantitation.

Reference

For details, see ["4.4.6 Bracket Quantitation" P.92](#).

- 5 Select [Insert QA/QC Samples] to insert a QA/QC sample.

**NOTE**

Refer to "4.4.8 Set the Injection Volume and Multi-Injection Counts for the GC" P.95 to set the injection volume for each sample using the same method file.

If [Insert QA/QC Samples] is selected, the [Batch Table Wizard - QA/QC Sample] sub-window is displayed. If [Insert QA/QC Samples] is deselected, proceed to Step 4.

3

Enter the QA/QC sample information, then click [Next].

Batch Table Wizard - Line1 QA/QC Sample

QA/QC Samples

Sample Name: QA/QC sample Auto-increment

Sample ID: SST-0001 Auto-increment

Data File Name:

Create file names automatically:

(Auto Filename) Auto-increment

Number of QA/QC Sample Vials: 1

Repetitions per Run: 1

Vial #: 1 - 1

Print Report

Report Format File:

< Back **Next >** Cancel Help

4

4

Enter the standard sample information, and click [Next].

Batch Table Wizard - Line1 Standard Sample

Standard Sample

Sample Name: Standard Sample Auto-increment

Sample ID: STD-0001 Auto-increment

Data File Name:

Create file names automatically

(Auto Filename) Auto-increment

Number of Calibration Levels: 1

Number of Standard Sample Vials per Level: 1

Repetitions per Run: 1

Vial #: 2 - 2

Clear all calibrations at the beginning

Use the same standard sample vial for all groups

Print Report

Report Format File:

CalibrationCurveReport_1.lsr

Data Comment:

< Back **Next >** Cancel Help

- 1 Enter [Sample Name] and [Sample ID] for the standard sample.
If [Auto-increment] is selected, the [Sample Name] and [Sample ID] are automatically appended with an incremental number.
- 2 Enter a [Data File Name].
Select [Create file names automatically] to automatically generate a data file name.

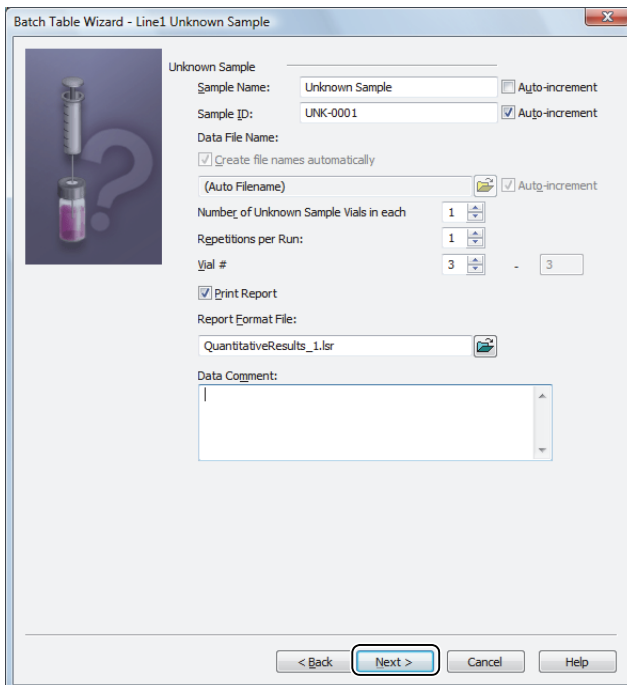
Reference

For details, see "[Set the Data File Name](#)" P.104.

- 3 Set the [Number of Calibration Levels] (number of calibration points), [Repetitions per Run] (number of injections) and select [Clear all calibrations at the beginning] to initialize the calibration curve.
The final vial No. of the standard sample you have set is displayed at [Vial#] in the Batch Table.
- 4 Select [Print Report] and set [Report Format File] to create reports.

5

Enter the unknown sample information, as with the standard sample, and click [Next].



Batch Table Wizard - Line1 Unknown Sample

Unknown Sample

Sample Name: Unknown Sample Auto-increment

Sample ID: UNK-0001 Auto-increment

Data File Name:

Create file names automatically

(Auto Filename) Auto-increment

Number of Unknown Sample Vials in each: 1

Repetitions per Run: 1

Vial #: 3 - 3

Print Report

Report Format File: QuantitativeResults_1.lsr

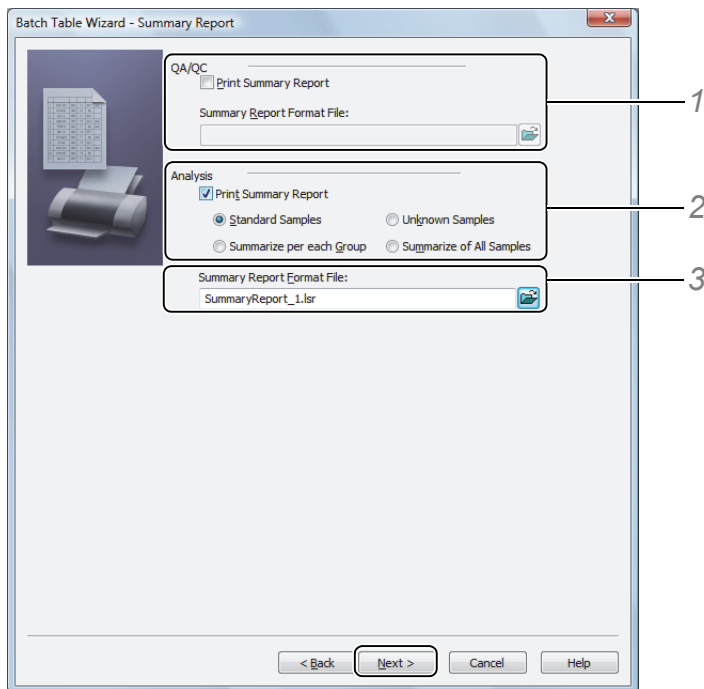
Data Comment:

< Back **Next >** Cancel Help

NOTE

If [Line 1 & Line 2] is selected at Step 2, the setting sub-windows for standard sample and unknown sample for Line 2 are displayed consecutively. Set each item in the same way as for Line 1.

6 Set the summary report output parameters, and click [Next].



- 1 Select [Print Summary Report] for [QA/QC], and select a [Summary Report Format File].



NOTE

[QA/QC] is not displayed if [Insert QA/QC Samples] is deselected in the [Batch Table Wizard] sub-window.

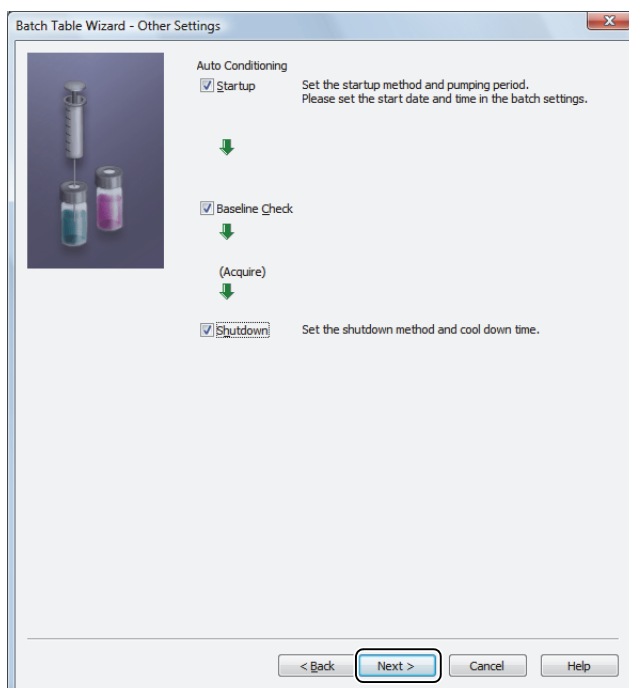
- 2 Select [Print Summary Report] for [Analysis], and select the type of sample summary that will be reported.
- 3 Select the [Summary Report Format File].

7

Select the items to be executed, and click [Next].

If [Startup] or [Shutdown] are selected, a setting sub-windows for each item is displayed. (Steps 8 or 9)

If all of these items are deselected, proceed to Step 10.



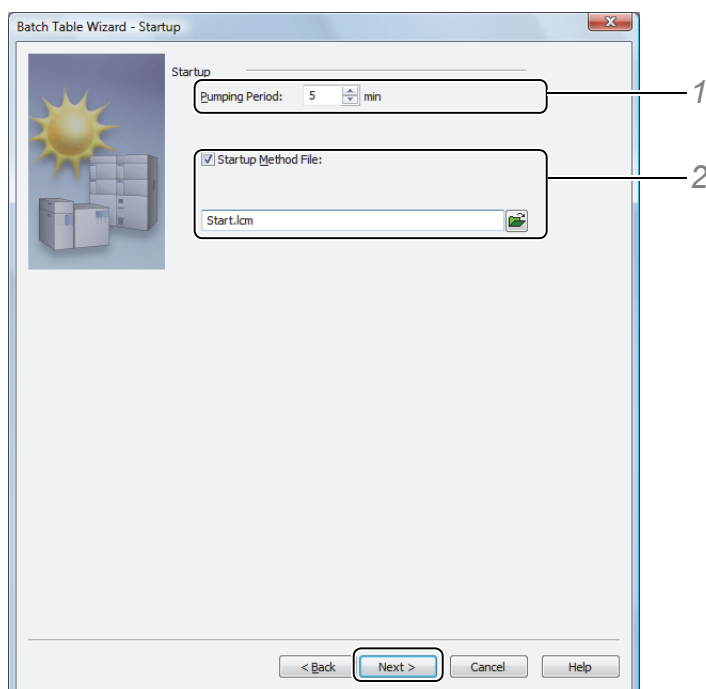
8

Select the startup settings, and click [Next].



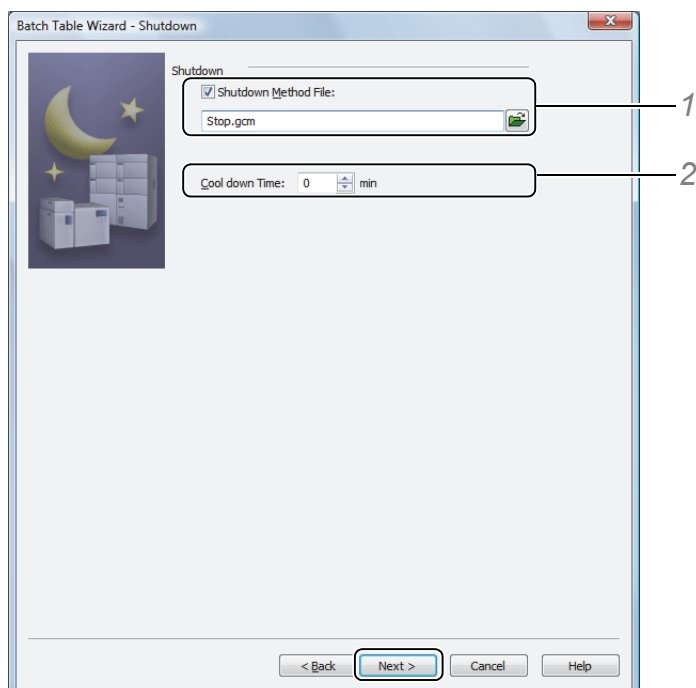
NOTE

The startup start date and time cannot be set in the Batch Table Wizard. Refer to ["4.4.2 Start Data Acquisition at a Specified Date and Time \(Startup\)" P.87](#) to enter a specified date and time.



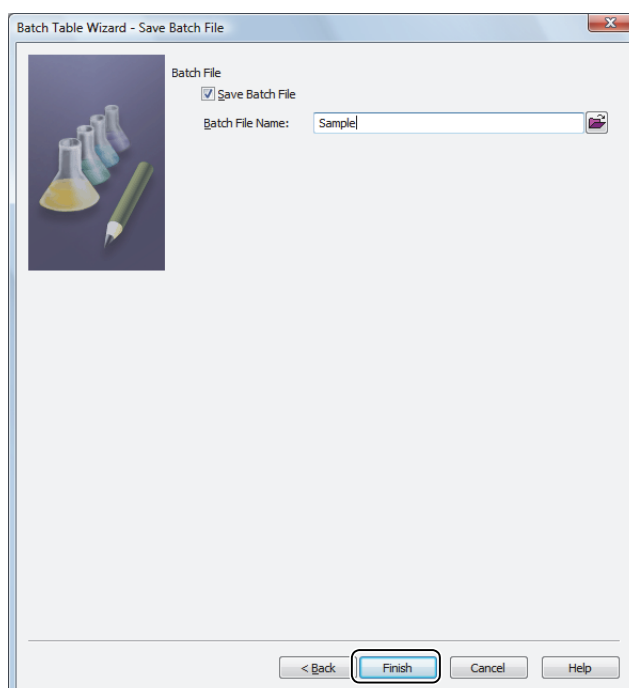
- 1 Enter an instrument startup time at [Pumping Period].
- 2 Select [Startup Method File], and enter the method file.

9 Select the shutdown settings, and click [Next].



- 1 Select [Shutdown Method File], and enter the method file.
- 2 Enter an instrument shutdown time at [Cool down Time].

10 Enter a batch file name, and click [Finish].



This completes Batch Table setup using the Batch Table Wizard. The batch file is created using the specified file name. This Batch Table is displayed in the Batch Table sub-window. Check the contents of the Batch Table.

4.2.2 Edit Batch Tables

This section describes 2 functions, [Fill Series] and [Fill Down], that are often used for direct Batch Table editing.

■ Append Table Settings with an Incremental Number

The [Vial#], [Sample Name], [Sample ID], and [Data File] entries in the Batch Table are appended with an incremental number.

This section describes how to add an incremental extension to the [Vial#].

1 Enter the [Vial#] for the top row.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Inj. Volume	Report Output
1			Standard Sample	STD-0001	1:Standard(I)	SampleMethod.lcm	(Auto Filename)	1	1	
2			Standard Sample	STD-0002	1:Standard	SampleMethod.lcm	(Auto Filename)	2	1	
3			Standard Sample	STD-0003	1:Standard	SampleMethod.lcm	(Auto Filename)	3	1	
4			Standard Sample	STD-0004	1:Standard	SampleMethod.lcm	(Auto Filename)	4	1	
5			Standard Sample	STD-0005	1:Standard	SampleMethod.lcm	(Auto Filename)	5	1	
6			Unknown Sample	UNK-0001	0:Unknown	SampleMethod.lcm	(Auto Filename)	0	1	

2 Right-click the top [Vial#] cell, and click [Fill Series] from the displayed menu.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Inj. Volume	Report Output
1				STD-0001	1:Standard(I)	SampleMethod.lcm	(Auto Filename)	1	1	
2				STD-0002	1:Standard	SampleMethod.lcm	(Auto Filename)	2	1	
3				STD-0003	1:Standard	SampleMethod.lcm	(Auto Filename)	3	1	
4				STD-0004	1:Standard	SampleMethod.lcm	(Auto Filename)	4	1	
5				STD-0005	1:Standard	SampleMethod.lcm	(Auto Filename)	5	1	
6				UNK-0001	0:Unknown	SampleMethod.lcm	(Auto Filename)	0	1	

NOTE

If [Vial#] is blank, the [Vial#] sub-window opens. If a value is entered in the [Vial#] cell that value is used incrementally fill the [Vial#] cells in the rest of the table.

3 If the [Vial#] sub-window is displayed, enter the [Row#], [Vial#], [Repetitions], and select [Auto-increment], then click [OK].

The [Vial#] column is incrementally filled.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Inj. Volume	Report Output
1	1		Standard Sample	STD-0001	1:Standard(I)	SampleMethod.lcm	(Auto Filename)	1	1	
2	2		Standard Sample	STD-0002	1:Standard	SampleMethod.lcm	(Auto Filename)	2	1	
3	3		Standard Sample	STD-0003	1:Standard	SampleMethod.lcm	(Auto Filename)	3	1	
4	4		Standard Sample	STD-0004	1:Standard	SampleMethod.lcm	(Auto Filename)	4	1	
5	5		Standard Sample	STD-0005	1:Standard	SampleMethod.lcm	(Auto Filename)	5	1	
6	6		Unknown Sample	UNK-0001	0:Unknown	SampleMethod.lcm	(Auto Filename)	0	1	

[Fill Series]

[Fill Series] functions according to how the cell is selected and the value entered in the cell.

- If the end of the character string is not a number (ex: "standard sample")
A 3-digit number is appended starting with the row following the selected cell.
"standard sample", "standard sample 001", "standard sample 002", and so forth.
- If the end of the character string is a number (ex: "STD01")
The cells are filled with STD01, STD02, STD03 and so forth.
- If only 1 cell is selected (ex: "ABC")
The cells following the selected cell become ABC001, ABC002, ABC003 and so forth.

- If multiple cells are selected (ex: “STD1”, “AAA” and “STD5” are selected in this order)
The selected cells are changed to STD1, STD2, and STD3.
- If a blank cell is selected (ex: a cell in the [Sample Name] column)
The [Sample Name] sub-window opens. Enter the sample name parameters, and click [OK].

Sample Name dialog box showing Row#: 1, Sample Name field, Auto-increment checkbox, and Repeats: 1.

■ Copy Settings

The individual columns of the Batch Table can be copied.

This section describes how to copy and fill the [Sample Name] column.

4

1 Enter a [Sample Name] in the top row.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Inj. Volume	Report Output
1	1	1	STD	STD-0001	1:Standard(I)	SampleMethod.lcm	(Auto Filename)	1	1	
2	2	1	Standard Sample	STD-0002	1:Standard	SampleMethod.lcm	(Auto Filename)	2	1	
3	3	1	Standard Sample	STD-0003	1:Standard	SampleMethod.lcm	(Auto Filename)	3	1	
4	4	1	Standard Sample	STD-0004	1:Standard	SampleMethod.lcm	(Auto Filename)	4	1	
5	5	1	Standard Sample	STD-0005	1:Standard	SampleMethod.lcm	(Auto Filename)	5	1	
6	6	1	Unknown Sample	UNK-0001	0:Unknown	SampleMethod.lcm	(Auto Filename)	0	1	

2 Right-click the top cell of the [Sample Name] column that is to be copied, and click [Fill Down].

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Inj. Volume	Report Output
1	1	1	STD	Fill Series		SampleMethod.lcm	(Auto Filename)	1	1	
2	2	1	Standard Sam	Fill Down		SampleMethod.lcm	(Auto Filename)	2	1	
3	3	1	Standard Sam			SampleMethod.lcm	(Auto Filename)	3	1	
4	4	1	Standard Sam	Cut		SampleMethod.lcm	(Auto Filename)	4	1	
5	5	1	Standard Sam	Copy		SampleMethod.lcm	(Auto Filename)	5	1	
6	6	1	Unknown Sam	Paste		SampleMethod.lcm	(Auto Filename)	0	1	

The contents of the top cell is copied to the subsequent cells of the [Sample Name] column.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Inj. Volume	Report Output
1	1	1	STD	STD-0001	1:Standard(I)	SampleMethod.lcm	(Auto Filename)	1	1	
2	2	1	STD	STD-0002	1:Standard	SampleMethod.lcm	(Auto Filename)	2	1	
3	3	1	STD	STD-0003	1:Standard	SampleMethod.lcm	(Auto Filename)	3	1	
4	4	1	STD	STD-0004	1:Standard	SampleMethod.lcm	(Auto Filename)	4	1	
5	5	1	STD	STD-0005	1:Standard	SampleMethod.lcm	(Auto Filename)	5	1	
6	6	1	STD	UNK-0001	0:Unknown	SampleMethod.lcm	(Auto Filename)	0	1	

[Fill Down]



[Fill Down] functions according to how the cell is selected.

- If only 1 cell is selected (ex: “STD”)
All selected cells following the selected cell become STD.
- If multiple cells are selected (ex: “STD1”, “AAA” and “STD5” are selected in this order)
All cells become the same STD1 as the initial cell.
- If a blank cell is selected (ex: a cell in the [Sample Name] column)
The [Sample Name] sub-window opens. Enter the [Sample Name] parameters, and click [OK].

Sample Name dialog box showing Row#: 1, Sample Name field, Auto-increment checkbox, and Repeats: 1.

4.2.3 Batch Table Parameters

In addition to sample information and sample type, method file, data file, and report output settings, the following Batch Table parameters can also be set.

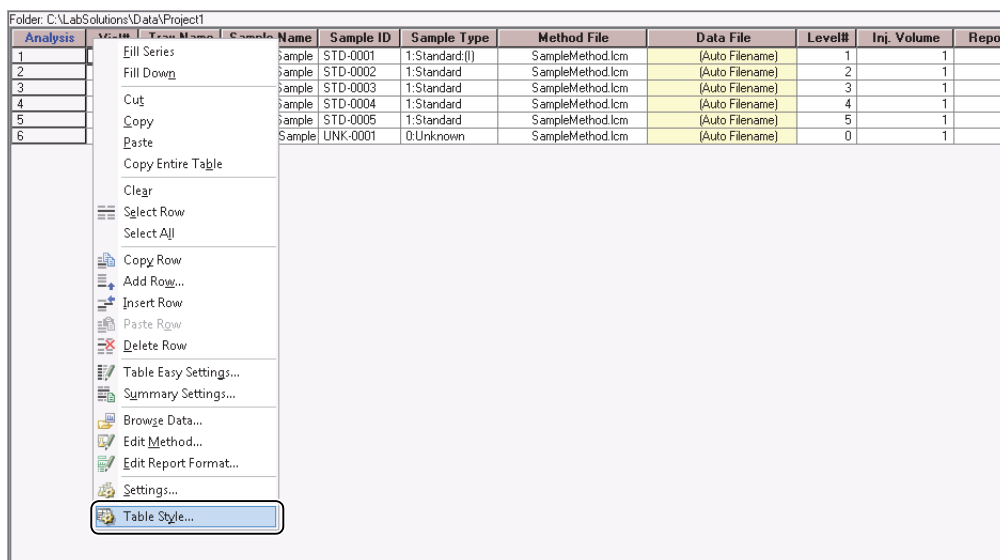
Parameter	Contents
Run mode	Determines whether there is a standby period before data acquisition, and whether to execute data acquisition and data processing on each row of the Batch Table.
Background compensation	Performs compensation using the blank (solvent only) chromatogram to subtract baseline drift or solvent peaks.  Reference For details, refer to "4.4.5 Background Data File" P.91 .
System check	Performs a system check before data acquisition, enter the system check parameter in the top row of the Batch Table. Click the [System Check] cell, and enter the system check parameters in the [System Check] sub-window.
System suitability	Checks the suitability of the system based on the analysis results of known multiple samples. The results can be displayed or output in text format.
Custom parameters	Calculation formulas can be set for totaling the peak area of related substances in analysis data and for compensating quantitative values. The results are output to a Quantitative Results Table or reports.  Reference For details, refer to "4.4.7 Custom Calculation Function" P.93 .
Action	The batch processing can be controlled according to pass/fail of the check conditions in each row of the Batch Table.
Options 1 to 10	Up to ten additional information columns can be added to the Batch Table. Once you enter [Option Title] in <Settings> - [Option Items] Tab, this additional sample information is saved in the same data as [Sample Name] and [Sample ID].

Hide or Display Batch Table Items

Use the [Table Style] sub-window to hide or display columns in the Batch Table.

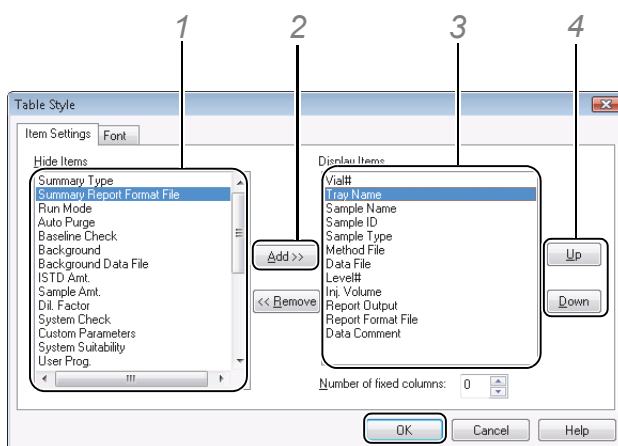
This section describes how to add or delete displayed items to the Batch Table.

1 Right-click on the Batch Table, and select [Table Style].



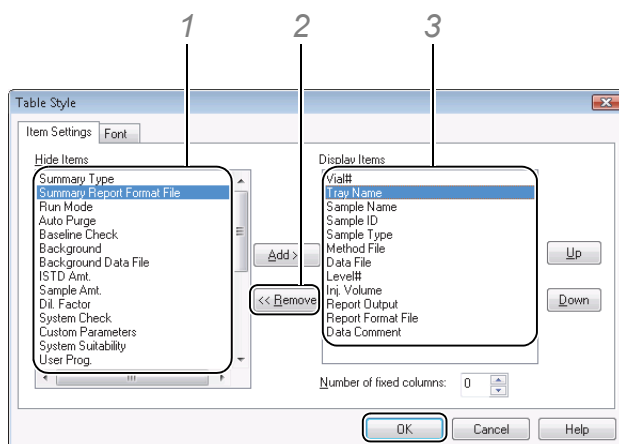
2 Select the desired items, and click [OK].

Display Hidden Batch Table Items



- 1 Select the items to display from the [Hide Items] list.
- 2 Click [Add].
The selected items are added to the end of the [Display Items] list.
- 3 Select an item to change the display order.
- 4 Click [Up] or [Down].
The top item in the [Display Items] list is displayed in the first (left) Batch Table column.

Hide Items in the Batch Table



- 1 Select the items to hide from the [Display Items] list.
- 2 Click [Remove].
The selected items move to the [Hide Items] list.

NOTE

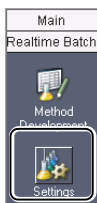
Realtime batch is executed based on settings in the Batch Table even if the items are hidden. For example, if a summary report output and summary report format file are entered, the summary report is output after realtime batch ends even if these items are hidden in the Batch Table.

4.2.4 Before Editing Batch Tables in Dual-Line Configuration

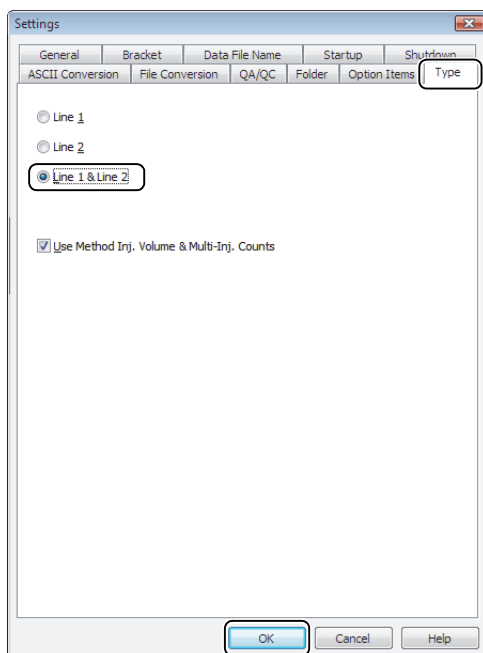
In the case of dual-line configuration GC, realtime batch analysis can be performed in dual-line configuration. To perform realtime batch analysis in dual-line configuration, a Batch Table must be switched to the Batch Table for dual lines before editing the Batch Table.

This section describes how to switch to the Batch Table for dual lines. Referring to ["4.2.1 Batch Table Wizard"](#) or ["4.2.2 Edit Batch Tables"](#), create a Batch Table using the Batch Table for the dual lines.

- 1 Click the  (Settings) icon on the [Realtime Batch] assistant bar.



2 Click the [Type] tab, select [Line1 & Line2], and click [OK].



NOTE

Selecting [Line 2] configures batch processing to be executed only for [Line 2].

If [Line 1 & Line 2] is selected, the lines are displayed in the Batch Table by a row number and a line number such as "1-1" or "1-2", and the Batch Table edition or realtime batch analysis is executed by two rows at a time.

Analysis	Vial#	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Report Output	Report Format File	Data C
1-1				0:Unknown			0	<input type="checkbox"/>		
1-2				0:Unknown			0	<input type="checkbox"/>		



NOTE

Editing the Batch Table items in the second row for Line 2 is restricted as follows.

- The [Sample Type], [Method File], [Level#], [Baseline Check], [System Check], [User Prog.], and [Action] items are in common with the Line 1 and cannot be edited for Line 2.
- In [Run Mode], there are common items set for both Line 1 and Line 2 and items set for each Line. Therefore, in the [Run Mode] sub-window for setting the cell content, common items are set on Line 1 and only [Data Acquisition] and [Data Analysis] at [Process] can be set on Line 2.

4.3 Data Acquisition Using Batch Tables

Perform data acquisition using the Batch Table created in ["4.2 Create Batch Tables"](#).

This section describes partial execution of a Batch Table, how to stop realtime batch, and how to pause realtime batch to edit the Batch Table.

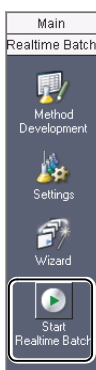
4.3.1 Partial Execution of a Batch Table

This section describes how to perform data analysis on only part of the Batch Table (1 to 3 rows).

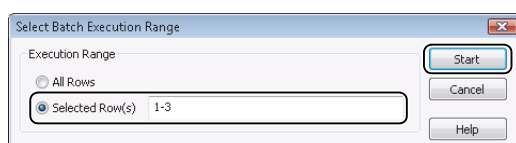
1 Select the row numbers to be analyzed.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Inj. Volume	Report Output
1	1	1	Standard Sample	STD-0001	1:Standard()	SampleMethod.lcm	(Auto Filename)	1	1	
2	2	1	Standard Sample	STD-0002	1:Standard	SampleMethod.lcm	(Auto Filename)	2	1	
3	3	1	Standard Sample	STD-0003	1:Standard	SampleMethod.lcm	(Auto Filename)	3	1	
4	4	1	Unknown Sample	UNK-0001	0:Unknown	SampleMethod.lcm	(Auto Filename)	0	1	
5	5	1	Unknown Sample	UNK-0002	0:Unknown	SampleMethod.lcm	(Auto Filename)	0	1	
6	6	1	Unknown Sample	UNK-0003	0:Unknown	SampleMethod.lcm	(Auto Filename)	0	1	

2 Click the (Start Realtime Batch) icon on the [Realtime Batch] assistant bar.



3 Check [Selected Row(s)], and click [Start].



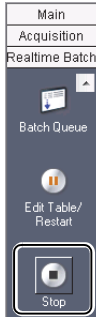
A screen for confirming partial execution opens.

4 In this screen, click [OK].

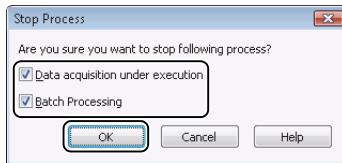
Batch processing of the selected rows is executed.

4.3.2 Stop Realtime Batch

- 1** Click the  (Stop) icon on the [Realtime Batch] assistant bar.



- 2** Select the processes to stop, and click [OK].



Batch processing is stopped.

NOTE

- If only [Data acquisition under execution] is selected, the current data acquisition is stopped and processing moves to the next row of the Batch Table, and data acquisition is started on that row.
- If only [Batch Processing] is selected, processing for the entire Batch Table stops after the current data acquisition ends.
- If both [Data acquisition under execution] and [Batch Processing] are selected, Batch Table processing stops in the middle of the current acquisition.
- When data acquisition is resumed in the row after the stop of batch processing, some information such as, pass/fail information for the QA/QC function, may be cleared.

4.3.3 Pause Realtime Batch to Edit the Batch Table

Realtime batch can be paused and the non-acquired rows of the Batch Table can be edited (add, insert, delete).

This section describes how to delete a non-acquired row of the Batch Table.



NOTE

- This operation cannot be performed on rows that have already been acquired.
- If the TurboMatrixHS is used for GC, realtime batch analysis cannot be paused.

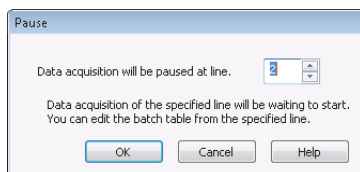
1

During realtime batch, click the  (Edit Table/Restart) icon on the [Realtime Batch] assistant bar.



2

Set the row where realtime batch is to be paused, and click [OK].

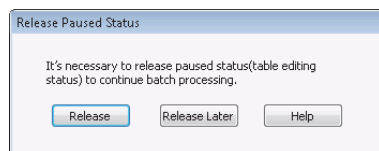


Data acquisition goes into the standby state at the selected row, and batch processing is paused.



NOTE

Data acquisition continues until the row selected in the [Pause] sub-windows reached. The [Release Paused Status] sub-window opens when the pause is executed.



- 3** Select the row to be deleted on the Batch Table, right-click on the selected row, and click [Delete Row].

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1	1	1	Standard Sample	STD-0001	1:Standard(I)	SampleMethod.lcm	(Auto Filename)	1
2 >>	2	1	Standard Sample	STD-0002	1:Standard	SampleMethod.lcm	roject1\Sample_004.lcd	2
3	3	1	Standard Sample	STD-0003	1:Standard	SampleMethod.lcm	Sample_005.lcd	3
4			Unknown Sample	UNK-0001	0:Unknown	SampleMethod.lcm	Sample_006.lcd	1
5			Unknown Sample	UNK-0002	0:Unknown	SampleMethod.lcm	Sample_007.lcd	0
6			Unknown Sample	UNK-0003	0:Unknown	SampleMethod.lcm	Sample_008.lcd	0


Context menu options: Fill Series, Fill Down, Cut, Copy, Paste, Copy Entire Table, Clear, Select Row, Select All, Copy Row, Add Row..., Insert Row, Paste Row, Delete Row, Table Easy Settings...

The selected row is deleted.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1	1	1	Standard Sample	STD-0001	1:Standard(I)	SampleMethod.lcm	(Auto Filename)	1
2 >>	2	1	Standard Sample	STD-0002	1:Standard	SampleMethod.lcm	roject1\Sample_004.lcd	2
3	3	1	Standard Sample	STD-0003	1:Standard	SampleMethod.lcm	Sample_005.lcd	3
4	5	1	Unknown Sample	UNK-0002	0:Unknown	SampleMethod.lcm	Sample_007.lcd	0
5	6	1	Unknown Sample	UNK-0003	0:Unknown	SampleMethod.lcm	Sample_008.lcd	0

- 4** Click the  (Save) button on the toolbar.

The method file is overwritten and saved.

- 5** Click the  (Edit Table/Restart) icon on the [Realtime Batch] assistant bar.

Batch processing is resumed from the paused row.

4

4.4 Automation of Data Acquisition Operations

Using the Batch Table to automate data acquisition allows for the automation of baseline check, system check, startup and shutdown as well as mobile phase substitution (autopurge).

This section describes how to automate data acquisition, output of summary reports, background compensation, bracket quantitation, and the custom calculation function.



NOTE

Use the Batch Table [Action] function to control batch processing actions.

4.4.1 Check Baseline Stability Before Data Acquisition (Baseline Check)

This section describes how to check the baseline before starting data acquisition. Set the baseline check thresholds and other items in the baseline check parameter of the method file.



Reference

See ["2.3.3 Check the Baseline" P.21](#) for LC, or ["2.3.3 Check the Baseline" P.21](#) for GC, for details on setting the baseline check parameter of the method file.

1

Select [Baseline Check] in the row where baseline check is to be performed.




Reference

If [Baseline Check] is not displayed in the Batch Table, refer to ["Hide or Display Batch Table Items" P.79](#).

Analysis	Level#	Inj. Volume	Report Output	Report Format File	Data Comment	Baseline Check
1	1	1	<input type="checkbox"/>			<input checked="" type="checkbox"/>
2	2	1	<input type="checkbox"/>			<input checked="" type="checkbox"/>
3	3	1	<input type="checkbox"/>			<input checked="" type="checkbox"/>
4	1	1	<input type="checkbox"/>			<input type="checkbox"/>
5	1	1	<input type="checkbox"/>			<input type="checkbox"/>

2

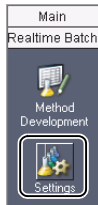
Click the  (Save) button on the toolbar.

The baseline check settings are saved to the batch file.

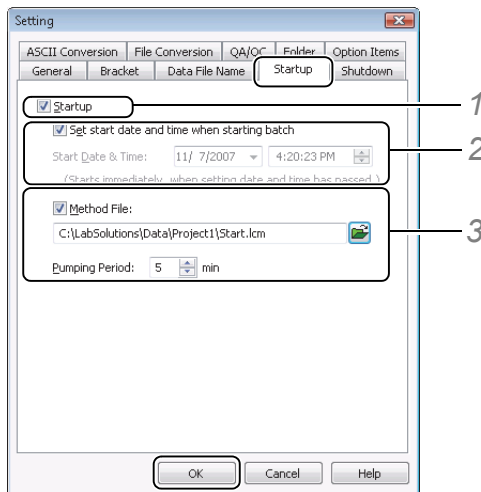
4.4.2 Start Data Acquisition at a Specified Date and Time (Startup)


Use realtime batch Startup to automatically start realtime batch at a preset date and time. This section describes how to use Startup.


- 1 Click the  (Settings) icon on the [Realtime Batch] assistant bar.



- 2 Click the [Startup] tab, enter the conditions for automatically starting the analytical instruments, and click [OK].



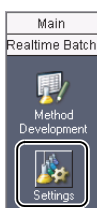
- 1 Select [Startup].
- 2 When [Set start date and time when starting batch] is selected, the sub-window for entering the start date and time is displayed.
The analytical instruments are started at the specified [Start Date & Time].
- 3 Select [Method File], and enter the name of the method file that contains the parameters for analytical instruments startup.
 - Click  to change the referenced file.
 - Enter a time in [Pumping Period] for the analytical instruments to operate at the initial conditions before batch processing begins.
 - If a method file is not specified, the analytical instruments are started up by the parameters downloaded to the instruments when the startup is performed.

- 3 Click the  (Save) button on the toolbar.
The startup settings are saved to the batch file.

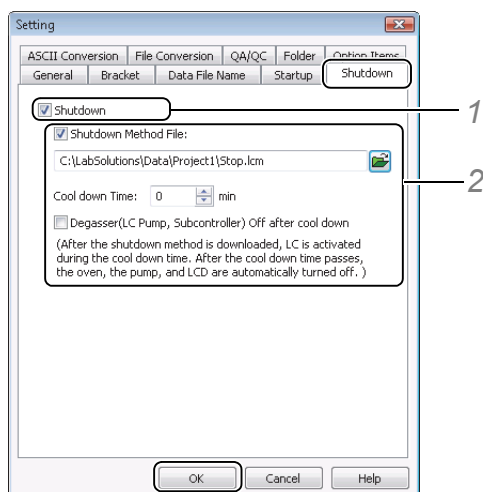
4.4.3 Shutdown Analytical Instruments After Data Acquisition (Shutdown)


Use realtime batch Shutdown to automatically shut down the analytical instruments after realtime batch ends. This section describes how to use Shutdown.


- 1 Click the  (Settings) icon on the [Realtime Batch] assistant bar.



- 2 Click the [Shutdown] tab, enter the conditions for automatic shutdown of the analytical instruments, and click [OK].

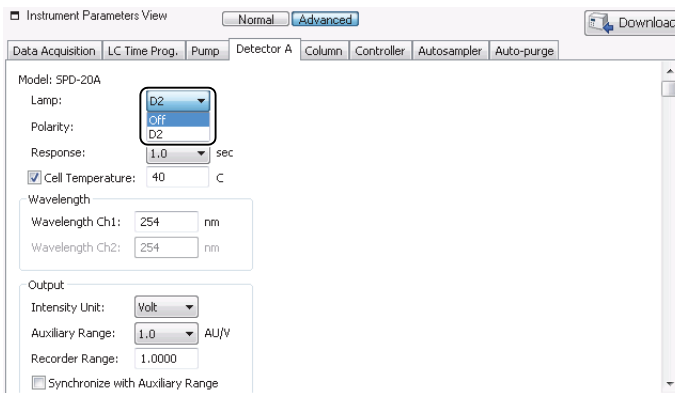


- 1 Select [Shutdown].
- 2 Select [Shutdown Method File], and enter the name of the method file that contains the parameters for shutdown of the analytical instruments.
 - Click  to change the referenced file.
 - Enter a time in [Cool Down Time] for the instruments to run after analysis and before shutdown.
 - If a method file is not specified, the analytical instruments are shut down by the parameters downloaded to the instruments when a shutdown is performed.

- 3 Click the  (Save) button on the toolbar.
The shutdown settings are saved to the batch file.

■ Turn the Detector Lamp Off

When creating a shutdown method file, select [Off] in the [Lamp] parameter.



4

4.4.4 Print a Summary Report

A summary report summarizes the chromatograms and the statistical calculation results from multiple data. This section describes how to set a summary report.

1 Drag and select the rows in the Batch Table to be included in the summary report.

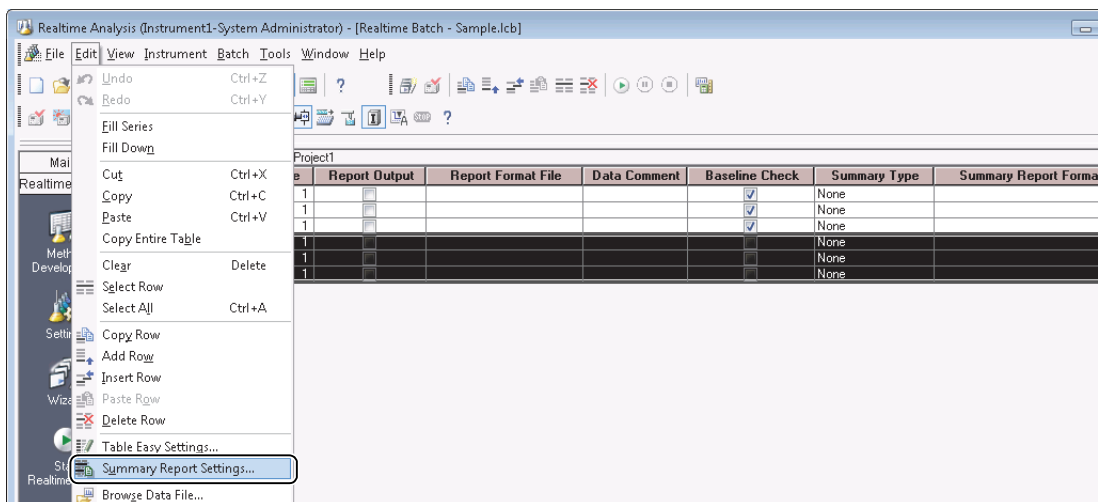
Analysis	Inj. Volume	Report Output	Report Format File	Data Comment	Baseline Check	Summary Type	Summary Report Format File
1	1	<input type="checkbox"/>			<input checked="" type="checkbox"/>	None	
2	1	<input type="checkbox"/>			<input checked="" type="checkbox"/>	None	
3	1	<input type="checkbox"/>			<input checked="" type="checkbox"/>	None	
4	1	<input type="checkbox"/>			<input checked="" type="checkbox"/>	None	




NOTE

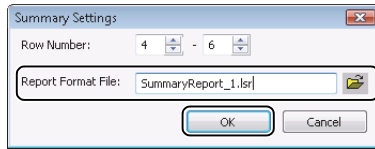
If the [Summary Type] and [Summary Report Format File] items are not displayed in the Batch Table, refer *"Hide or Display Batch Table Items"* P.79.

2 Right-click on the selected rows, and click [Summary Report Settings].



3 Select a [Report Format File], and click [OK].

- Click  to change the referenced file.
- The selected start row and end row numbers are displayed at [Row Number]. Change the numbers to change the rows to be printed in the summary report.



Reference

See "[8.4 Create a Report Format File](#)" P.232 for details on the report format.

4 Click the (Save) button on the toolbar.

The summary report settings are saved to the batch file.

4.4.5 Background Data File

Background data refers to a chromatogram obtained by performing the gradient analysis (LC) or programmed temperature analysis (GC) without injecting a sample. Use the background data file to compensate for baseline drift in the acquired sample data.


This section describes how to acquire background data and perform background compensation in the same realtime batch.

Analysis	Sample Name	Sample ID	Sample Type	Method File	Data File	Background	Background Data File	Level#	Inj.
1	Baseline		0:Unknown	SampleMethod.lcm	Baseline.lcd			0	
2	Standard Sample	STD-0001	1:Standard()	SampleMethod.lcm	Data1.lcd	<input checked="" type="checkbox"/>	Baseline.lcd	1	
3	Standard Sample	STD-0002	1:Standard()	SampleMethod.lcm	Data2.lcd	<input checked="" type="checkbox"/>	Baseline.lcd	2	
4	Unknown Sample	UNK-0001	0:Unknown	SampleMethod.lcm	Data3.lcd	<input checked="" type="checkbox"/>	Baseline.lcd	0	
5	Unknown Sample	UNK-0002	0:Unknown	SampleMethod.lcm	Data4.lcd	<input checked="" type="checkbox"/>	Baseline.lcd	0	
6	Unknown Sample	UNK-0003	0:Unknown	SampleMethod.lcm	Data5.lcd	<input checked="" type="checkbox"/>	Baseline.lcd	0	

- 1 Select the row where background data will be acquired.



NOTE

- Ensure that the background data row is above the sample rows.
- If [Auto Filename] is selected for the [Data File] column, click the  (Settings) icon on the [Realtime Batch] assistant bar, and select [Create filenames automatically with] on the [Data File Name] tab.

Analysis	Sample Name	Sample ID	Sample Type	Method File	Data File	Background	Background Data File	Le
1	Baseline		0:Unknown	SampleMethod.lcm	(Auto Filename)	<input checked="" type="checkbox"/>		
2	Standard Sample	STD-0001	1:Standard()	SampleMethod.lcm	(Auto Filename)	<input checked="" type="checkbox"/>	Baseline.lcd	
3	Standard Sample	STD-0002	1:Standard()	SampleMethod.lcm	(Auto Filename)	<input checked="" type="checkbox"/>	Baseline.lcd	


- 2 Select [Background] for the rows where background compensation will be applied.
- 3 Enter a [Background Data File] for each of the rows where [Background] is selected.



Reference

If [Background] and [Background File] are not displayed in the Batch Table, refer to ["Hide or Display Batch Table Items" P.79](#).

5

Click the  (Save) button on the toolbar.

The background compensation settings are saved to the batch file.

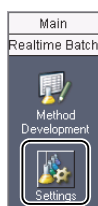
4.4.6 Bracket Quantitation

When sequential data acquisition is performed on multiple samples, the detector sensitivity may change over time and sometimes affect the initial and final data acquisition results. To correct this situation, the quantitative value for unknown samples can be obtained by bracketing the unknown sample with standard samples, and creating a calibration curve from the standard sample data acquired before and after the unknown sample.

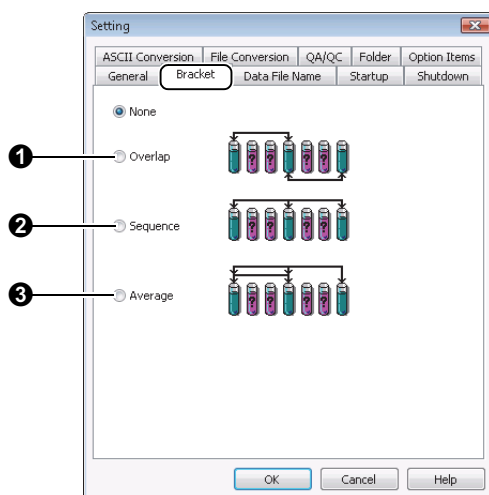
Three different types of bracket calibration curves are available, [Overlap], [Sequence] and [Average]. Select the appropriate type according to how the standard sample calibration points are set.

This section describes how to select bracket quantitation.


- 1 Click the  (Settings) icon on the [Realtime Batch] assistant bar.



- 2 Click the [Bracket] tab, select the bracket quantitation type, and click [OK].



No.	Parameter	Explanation
1	Overlap	Quantitates the unknown sample using the calibration curve made from the results of the standard samples acquired before and after the unknown sample.
2	Sequence	Quantitates the unknown sample using the calibration curve made from the results of all standard samples regardless of the position of the bracketed unknown sample.
3	Average	Quantitates the unknown sample using the calibration curve made by averaging the results of all standard samples before the unknown sample and the results of the standard sample directly after the unknown sample.

- 3 Click the  (Save) button on the toolbar.
The bracket quantitation settings are saved to the batch file.

4.4.7 Custom Calculation Function

The custom calculation function allows for automation of operations, such as totaling of the peak area and quantitative value compensation.

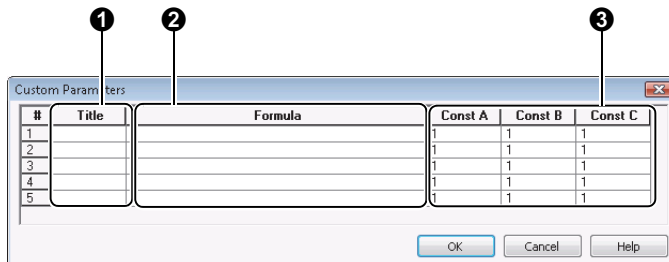
This section describes how to set custom parameters.

- 1 Click the [Custom Parameters] cell in the Batch Table where custom calculations are necessary.

Reference

If the [Custom Parameters] column is not displayed in the Batch Table, refer to ["Hide or Display Batch Table Items" P.79.](#)

- 2 Enter [Title], [Formula] and constants to display in the Compound Result Table, and click [OK].



No.	Parameter	Explanation
1	Title	Enter a title to displayed in the Compound Result Table.
2	Formula	Enter a formula using numeric values, macro variables and operators (+, -, *, /, e). <ul style="list-style-type: none"> Macro variables <ul style="list-style-type: none"> Retention time (RetTime), area (Area), height (Height), concentration (Conc) For a specific peak <ul style="list-style-type: none"> RetTime [1] (retention time of peak with compound ID "1") To specifying peaks between data <ul style="list-style-type: none"> RetTime [1] (3) (retention time of peak with compound ID "1" of data at 3 rows above the preset row)
3	Const A to C	Up to any three constants can be specified in each calculation formula.

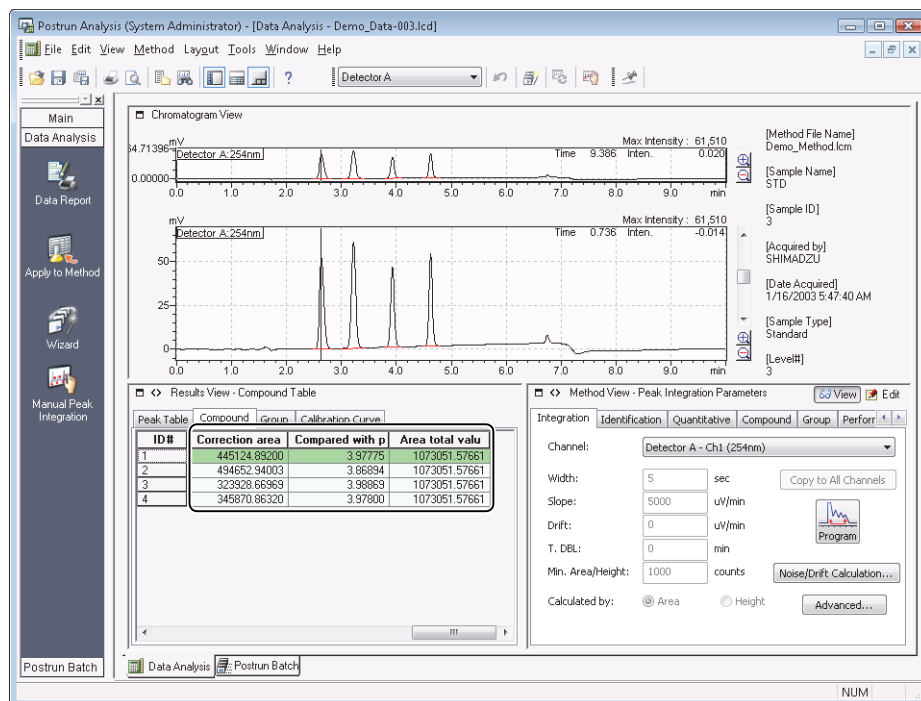
3 Click the (Save) button on the toolbar.

The custom parameter settings are saved to the batch file.



NOTE

Execute batch processing to check the calculation results, and then check the results on the [Compound] tab in [Results View]. If custom parameters are not displayed, display them using the [Table Style] sub-window.



Custom Parameter Example

#	Title	Formula	Const A	Const B	Const C
1	Correction ar	Area*A	1.5	1	1
2	Compared	Area[0]/Area[3]	1	1	1
3	Area total val	Area[1]+Area[2]+Area[3]+Area[4]	1	1	1
4			1	1	1
5			1	1	1

The 1st row is an example of a compensated area calculation. In this example, each peak area of the unknown sample is multiplied by the compensation factor to obtain the compensated area.

The 2nd row is an example of a calculation between samples. In this example, calculation uses the peak area of an unknown sample and the peak area of a standard sample that was acquired three samples before the unknown sample.

The 3rd row is an example of calculation between peaks. In this example, the total value of 4 peak values is calculated.

4.4.8 Set the Injection Volume and Multi-Injection Counts for the GC

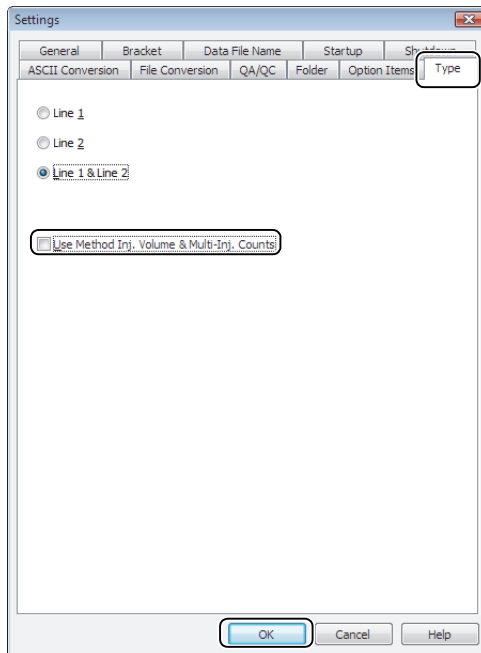
With the GC unit, the injection volume and Multi-injection counts are set for each sample in the Batch Table to perform data acquisition using the same method file.

This section describes how to set the sample injection volume or multi-injection counts in the Batch Table.

- 1 Click the  (Settings) icon on the [Realtime Batch] assistant bar.



- 2 Click the [Type] tab, deselect [Use Method Inj. Volume & Multi-Inj. Counts], and click [OK].



NOTE

In the case of a dual-line configuration GC, select the line to use in the Batch Table.

- 3 Set [Inj. Volume] and [Multi Injection] in the Batch Table.

Reference

If [Inj. Volume] and [Multi Injection] are not displayed in the Batch Table, refer to ["Hide or Display Batch Table Items" P.79](#) at ["4.2.3 Batch Table Parameters"](#).

- 4 Click  (Save) on the toolbar.

[Inj. Volume] and [Multi Injection] settings are saved to the batch file.

NOTE

Items in the [Setting] sub-window are stored to memory for each batch file.

4.5 Data Acquisition Using the Batch Queue Function

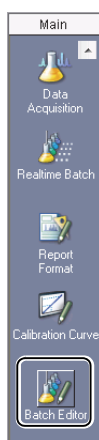
This software allows you to perform continuous data acquisition using different batch files. Batch files used for continuous data acquisition are registered to a memory area called the “batch queue”.

In the batch queue, registered batch files are displayed as a list, and are executed in order by realtime batch from the top of the queue.


The order of registered batch files can be changed and registered batch files can be deleted from the list.

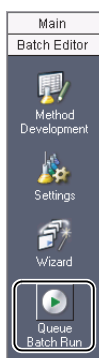
4.5.1 Register Batch Files to the Batch Queue

- 1 Click the  (Batch Editor) icon on the [Main] assistant bar.



- 2 Open the batch file in the [Batch Editor] window.

- 3 Click the  (Queue Batch Run) icon on the [Batch Editor] assistant bar.

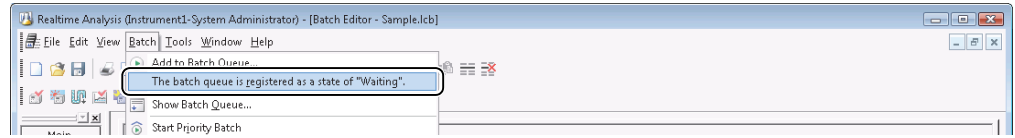


The batch file is added to the batch queue.



NOTE

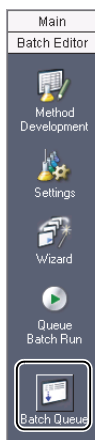
- The information for batch files that are registered to the batch queue is retained even if the [Realtime Analysis] program is exited.
- The status of a batch file registered to the batch queue can be set to “Waiting” (pause) before realtime batch analysis begins on that batch file. Select [The batch queue is registered as a state of “Waiting”] on the [Batch] menu, select the rows of the batch queue to set to the “Waiting” status,

and click [Start] to save the batch queue settings.

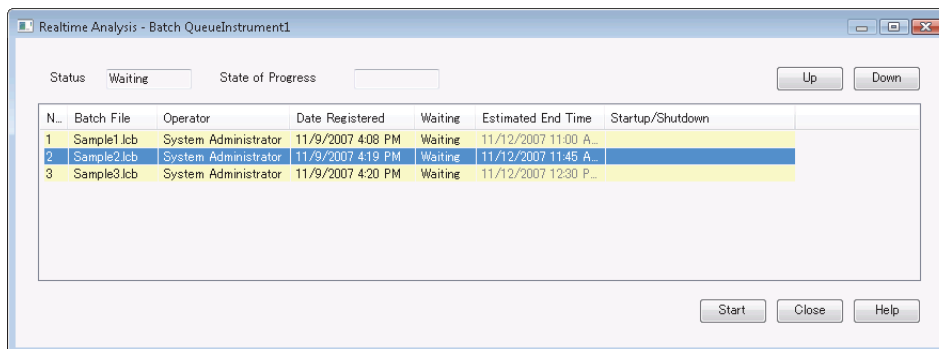


4.5.2 Change the Batch Queue Order or Delete Batch Files

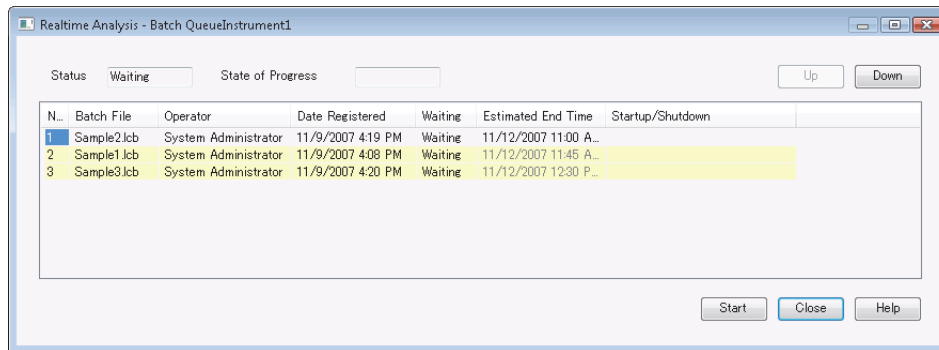
- 1 Click the  (Batch Editor) icon on the [Main] assistant bar.
- 2 Click the  (Batch Queue) icon on the [Batch Editor] assistant bar.



- 3 To change the order of batch files in the batch queue, select the desired row, and click [Up] or [Down].

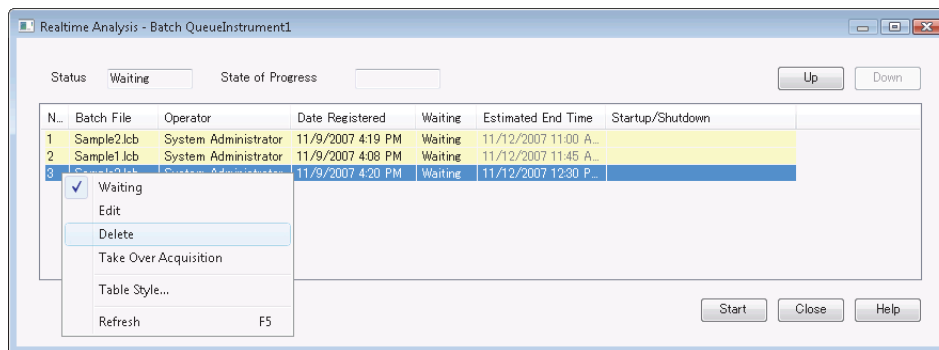


The order of batch files in the batch queue is changed.

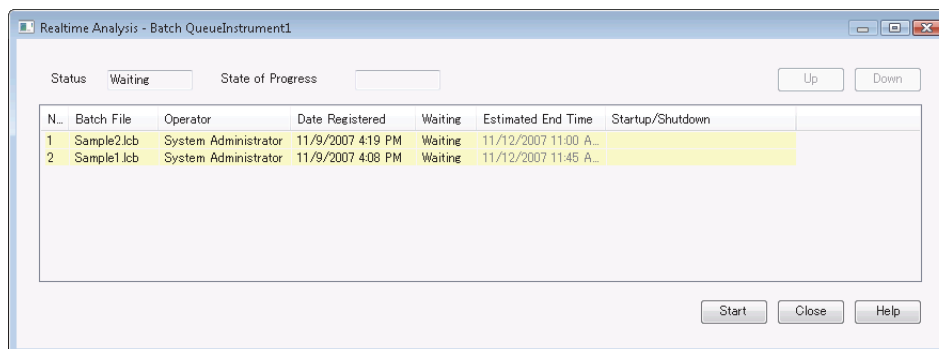


4

To delete a registered batch file from the batch queue, right-click on the desired row, and click [Delete].



The selected row is deleted from the batch queue.




5

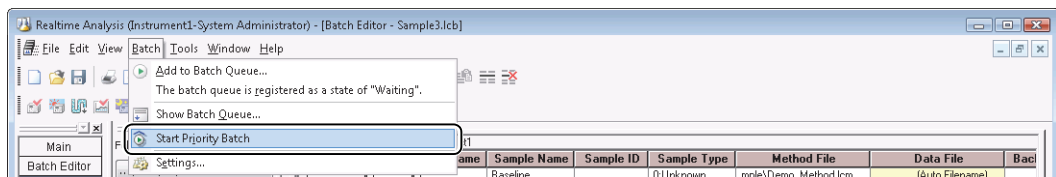
Click [Start].

Realtime batch is started in the new batch file order.

4.5.3 Priority Batch

The currently acquiring batch file can be paused to give priority to another batch file that must be measured immediately in realtime batch. This is called "priority batch".

- 1 Click the  (Batch Editor) icon on the [Main] assistant bar.
- 2 Display the batch file to give priority to in realtime batch.
- 3 Click [Start Priority Batch] on the [Batch] menu.

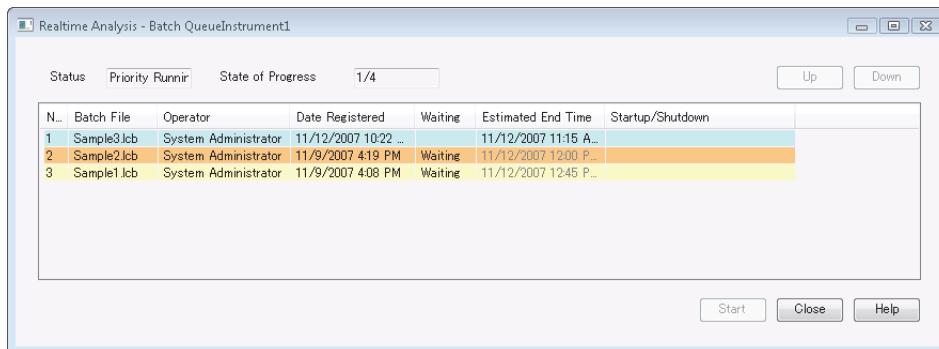


The priority batch is started.

NOTE

- Priority batch is started after the current data acquisition ends.
- Priority batch cannot be set to batch files set with bracket quantitation, summary report, QA/QC, and batch action.

The following shows an example of how the [Batch Queue] sub-window changes when priority batch is set for batch file Sample3.lcb.





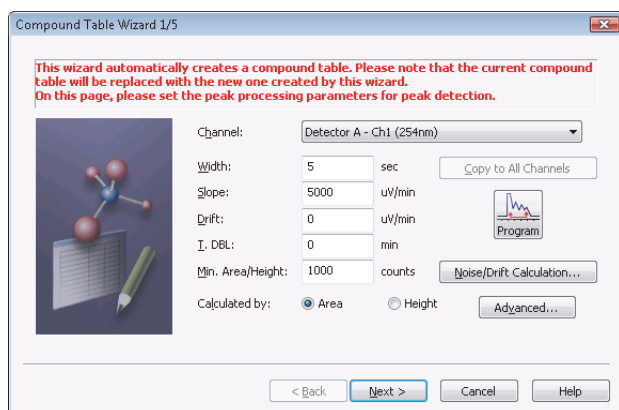
4.6 Create a Calibration Curve to Quantitate an Unknown Sample



If data processing parameters have already been determined for a target compound, they may be extracted from a method so that a calibration curve can automatically be established during acquisition of standard samples and used for quantitation of unknown samples.

This section describes how to set data processing parameters and Batch Table items to perform quantitative calculations.

4.6.1 Edit the Data Processing Parameters

- 1 Click the  (Data Analysis) icon on the [Acquisition] assistant bar.
- 2 Drag-and-drop the data file onto the [Data Analysis] window from the [Data Explorer] sub-window.
Select a data file with data acquisition conditions (instrument parameters) that match those for the target component to be analyzed.
- 3 Click the  (Wizard) icon on the [Data Analysis] assistant bar.
- 4 Refer to "[6.5.1 Compound Table Wizard](#)" to set the data processing parameters using the Compound Table Wizard.



- 5 Click  (View Mode) in [Method View].
The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the analysis results in [Chromatogram View] and [Results View].
- 6 Click the  (Apply to Method) icon on the [Data Analysis] assistant bar.
The parameters are exported to the method file.

Reference

For details, see "[6.7 Save \(Export\) to Method Files](#)" P.171.

4.6.2 Edit Batch Tables

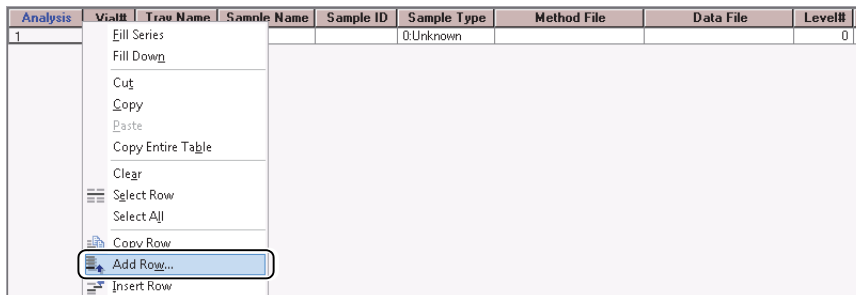
This section describes how to set the [Method File], [Sample Type], [Level#], [Data File], [Sample Amt.], [Dil. Factor.], and [ISTD Amt.] items required for quantitative calculation.

NOTE

See "4.2 Create Batch Tables" P.63 for details on other items.

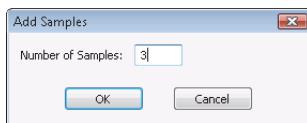
■ Add Rows to Batch Tables

- 1 Right-click on the Batch Table, and select [Add Row] from the displayed menu.



Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1					0:Unknown			0

- 2 Enter the number of samples, and click [OK].



Add Samples

Number of Samples:

OK Cancel

Rows are added to the Batch Table.

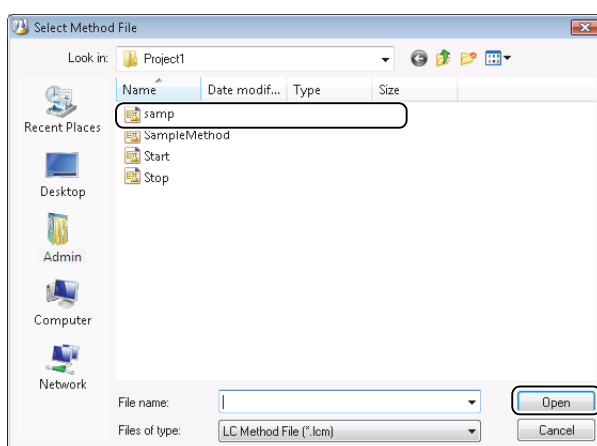
Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1					0:Unknown			0
2					0:Unknown			0
3					0:Unknown			0
4					0:Unknown			0

■ Set the Method File

1 Click the [Method File] cell on the Batch Table.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1					0:Unknown			0
2					0:Unknown			0
3					0:Unknown			0
4					0:Unknown			0

2 Select the method file, and click [Open].



The method file is set.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1					0:Unknown	SampleMethod.lcm		0
2					0:Unknown			0
3					0:Unknown			0

3 Set other [Method File] cells in the same way.

👉 Reference

Refer to *"Copy Settings" P.77* to copy and paste the same method file name to multiple rows.

■ Set the Sample Type

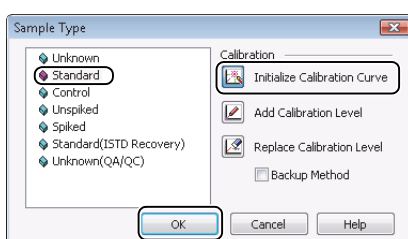
Set the type of sample to measure.

In the case of a standard sample, set the first standard sample to [Initialize Calibration Curve] and the next standard sample to [Add Calibration Level]. The default setting [0: Unknown] is used for unknown samples.

1 Click the [Sample Type] cell of the first standard sample.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1					0:Unknown	SampleMethod.lcm		0
2					0:Unknown	SampleMethod.lcm		0
3					0:Unknown	SampleMethod.lcm		0
4					0:Unknown	SampleMethod.lcm		0

2 Click [Standard], select [Initialize Calibration Curve] and click [OK].

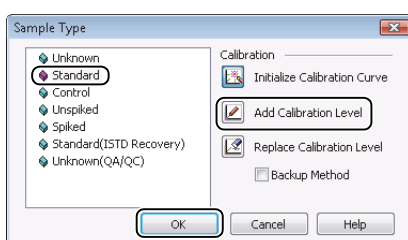


The initial cell for the sample type is displayed as [1: Standard (I)].

3 Click the [Sample Type] cell of the next standard sample.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1					1:Standard(I)	SampleMethod.lcm		1
2					0:Unknown	SampleMethod.lcm		0
3					0:Unknown	SampleMethod.lcm		0
4					0:Unknown	SampleMethod.lcm		0

4 Click [Standard], select [Add Calibration Level] and click [OK].



The [Sample Type] cell is displayed as [1: Standard].

Repeat steps 3 and 4 for multiple standard samples.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1					1:Standard(I)	SampleMethod.lcm		1
2					1:Standard	SampleMethod.lcm		1
3					0:Unknown	SampleMethod.lcm		0
4					0:Unknown	SampleMethod.lcm		0

■ Set the Level#

Set the standard sample [Level#] according to the concentration value in the Compound Table of the method file. The calibration points are created from the level number of the Compound Table and the area and height values of the preset standard sample.



NOTE

[Level#] values are not used for unknown samples, even if they are set.

1

Click the [Level#] cell for the standard sample.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1					1:Standard ()	SampleMethod.lcm		1
2					1:Standard	SampleMethod.lcm		1
3					0:Unknown	SampleMethod.lcm		0
4					0:Unknown	SampleMethod.lcm		0

2

Enter the level number.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#
1					1:Standard ()	SampleMethod.lcm		1
2					1:Standard	SampleMethod.lcm		2
3					0:Unknown	SampleMethod.lcm		0
4					0:Unknown	SampleMethod.lcm		0

The level number is changed.

3

Set the [Level#] cell for other standard samples.

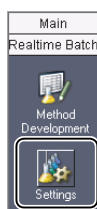
■ Set the Data File Name

Either directly enter a file name in the [Data File] cell, or automatically create the data file.

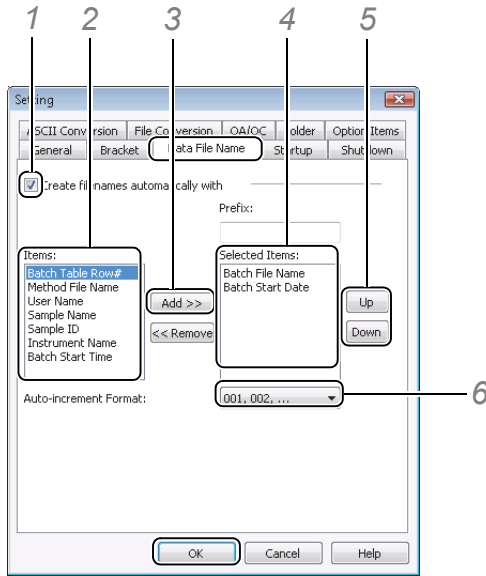
This section describes how to automatically create a data file name.

1

Click the  (Settings) icon on the [Realtime Batch] assistant bar.



2 Click the [Data File Name] tab, set each item, and click [OK].



4

- 1 Select [Create filenames automatically with].
- 2 Select the items for the file name to automatically create from the [Items] list. Enter a character string in the [Prefix] box to create a data file name with a fixed character string.
- 3 Click [Add].
Items are added onto the end of [Selected Items], and the file name is created using the currently displayed items.
- 4 Select an item in the [Selected Items] list to change the display order.
- 5 Change the display order by clicking [Up] or [Down].



NOTE

Automatically created file names use an _ (underscore) to join together items in order starting with the top item in the [Selected Items] box.
For example, when a file name is automatically created using Batch File Name (AAA), Batch Start Date (2008/04/01):
the file name is “AAA_20080401”.

- 6 Select a numeric format to automatically append the file name with an incremental number at [Auto-increment Format].

The data file name in the Batch Table is displayed as [Auto Filename].

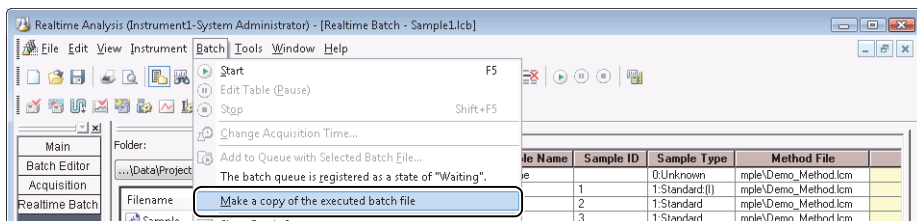
Analysis	Sample Name	Sample ID	Sample Type	Method File	Data File	Background	Background Data File	Level#	Inj.
1	Baseline		0:Unknown	SampleMethod.lcm	(Auto Filename)	<input type="checkbox"/>		0	
2	Standard Sample	STD-0001	1:Standard(I)	SampleMethod.lcm	(Auto Filename)	<input checked="" type="checkbox"/>	Baseline.lcd	1	
3	Standard Sample	STD-0002	1:Standard	SampleMethod.lcm	(Auto Filename)	<input checked="" type="checkbox"/>	Baseline.lcd	2	
4	Unknown Sample	UNK-0001	0:Unknown	SampleMethod.lcm	(Auto Filename)	<input checked="" type="checkbox"/>	Baseline.lcd	0	
5	Unknown Sample	UNK-0002	0:Unknown	SampleMethod.lcm	(Auto Filename)	<input checked="" type="checkbox"/>	Baseline.lcd	0	
6	Unknown Sample	UNK-0003	0:Unknown	SampleMethod.lcm	(Auto Filename)	<input checked="" type="checkbox"/>	Baseline.lcd	0	



NOTE

Postrun batch reprocessing cannot be executed when a field is set to [Auto-increment Format] because a specific filename and path are required. Therefore, it is recommended to copy the batch after realtime acquisition ends. When a batch is copied, the data file name generated at the time of data acquisition is transferred to the appropriate cell of the copied batch allowing postrun batch processing to be executed.

To copy a batch, select the following menu item.



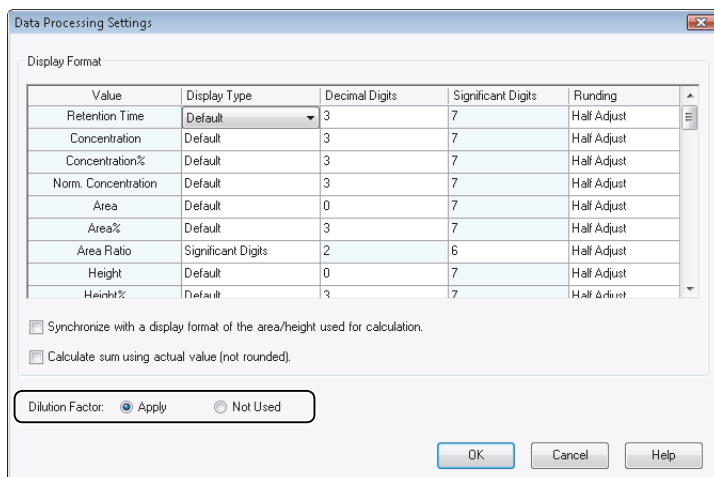
■ Set the Sample Amount, Dilution Factor, and ISTD Amount.

Enter values in each cell of the Batch Table to set the [Sample Amt.] (weight) and dilution factor for an unknown sample, and ISTD amount (for internal standard method) to spike the unknown sample.

This section describes how to set the ISTD amount.

NOTE

- Enter the ISTD amount for sample types other than the standard sample when the quantitative calculation method is internal standard method.
- Enter the concentration of the ISTD for the number of internal standard substances set in the Compound Table.
- Set [Dilution Factor] to either [Apply] or [Not Used] in the [Data Processing Setting] sub-window in the [System Settings] sub-window.



Reference

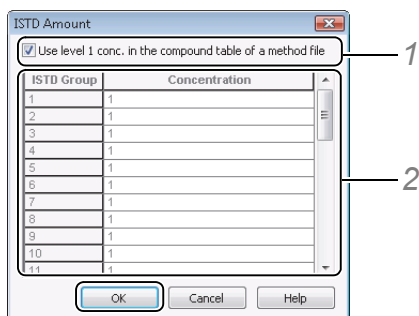
If [Sample Amt.], [Dil. Factor] and [ISTD Amt.] are not displayed in the Batch Table, refer to ["Hide or Display Batch Table Items" P.79](#).

1

Click the [ISTD Amt.] cell for the unknown sample.

Analysis	Vial#	Tray Name	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	ISTD Amt.	Inj. Volume
1					1:Standard(I)	SampleMethod.lcm		1	(Level) Con	10
2					1:Standard	SampleMethod.lcm		2	(Level) Con	10
3					0:Unknown	SampleMethod.lcm		1	(Level) Con	10
4					0:Unknown	SampleMethod.lcm		1	(Level) Con	10

2 Enter the concentration for each internal standard substance, and click [OK].



- 1 Deselect [Use level 1 conc. in the compound table of a method file].
If [Use level 1 conc. in the compound table of a method file] is selected, the level 1 concentrations of the compounds specified as the internal standard substances in the method file are used. Select this checkbox when a standard sample and unknown sample are spiked with the same amount of internal standard substances.
- 2 Enter the concentrations of the internal standard substances in each group.

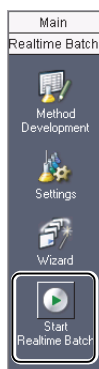
4

3 Enter the [ISTD Amt.] cell for other unknown samples.

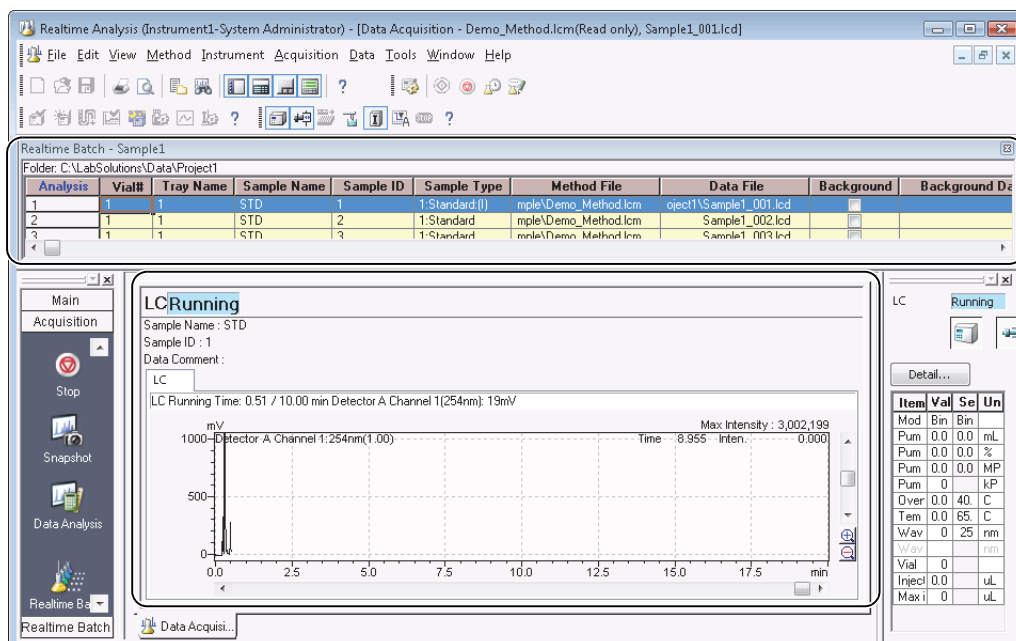
4.6.3 Data Acquisition Using Batch Tables

Perform data acquisition using a preset batch file.

- 1 Click the  (Start Realtime Batch) icon on the [Realtime Batch] assistant bar.



When data acquisition is started, the [Realtime Batch] and [Data Acquisition] windows change as follows.



During data acquisition, the [LabSolutions Service] icon in the Systray on the Taskbar flashes green.



NOTE

Do not turn the PC off while the [LabSolutions Service] icon is flashing.

Reference


See "4.3.2 Stop Realtime Batch" P.83 for details on how to stop or pause realtime batch.

■ When an Autosampler Is Not Used

For LC

When a manual injector on the LC is connected to the Manual Inject (start) terminals of the system controller, initiate acquisition by rotating the manual injector to the inject position.

For GC

If the connection is configured to initiate data acquisition by the START input signal of the GC, inject the sample, and then press the  button on the GC. For more details, refer to the Instruction Manual for the GC unit.

In all other cases, click [Start] in the [Start Data Acquisition] sub-window and press the [start / stop] button on the CBM-102.

4.6.4 Check the Quantitation Results

Check the quantitation results for the unknown sample in the [Data Analysis] window.

- 1 Click the  (Data Analysis) icon on the [Realtime Batch] assistant bar.

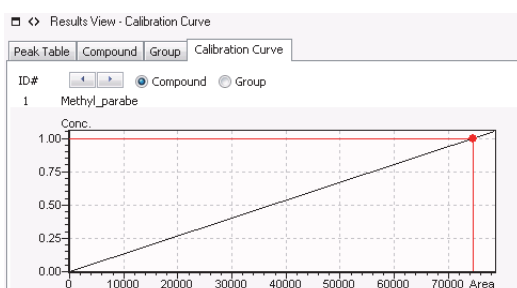


The [Postrun Analysis] program is displayed, and the data file for the selected row on the Batch Table is loaded.

- 2 Click the [Compound] and [Calibration Curve] tabs in [Results View], and check the quantitation results.

Results View - Compound Table

Peak Table	Compound	Group	Calibration Curve		
ID#	Name	Ret. Time	Conc.	Unit	Chann
1	Methyl_paraben	2.636	1.000	mg/L	Detector A
2	Ethyl_paraben	3.216	1.000	mg/L	Detector A
3	Propyl_paraben	3.926	1.000	mg/L	Detector A
4	Butyl_paraben	4.619	1.000	mg/L	Detector A



4.7 Acquisition Cycle Time Optimization

The total time for the batch analysis can be reduced by using the acquisition cycle time optimization function that overlaps autosampler pretreatment for next sample during current data acquisition.




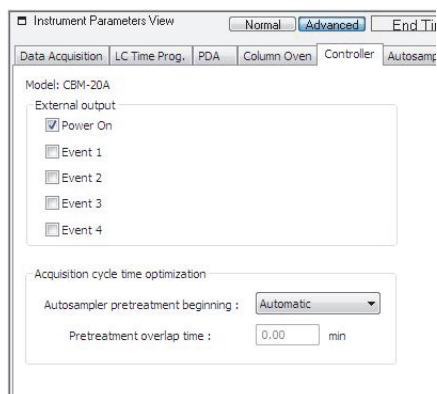
NOTE

This function can be performed when using CBM-20A/20Alite(Ver.2.0 or later) as a LC System Controller. (It is available for any autosampler controlled by CBM-20A/20Alite.)

Both method file and batch file should be set to use the acquisition cycle time optimization function. This section describes how to set these parameters.

4.7.1 Set the Instrument Parameters

- 1 Click the  (Data Acquisition) icon on the [Main] assistant bar in the [Realtime Analysis] program.
- 2 Click [Advanced] on the [Instrument Parameters View] to open the [Advanced] sub-window.
- 3 Click the [Controller] tab, and select [Automatic] for the [Autosampler pretreatment beginning].




Reference

Refer to Help for details.

- 4 Click [Save Method File As] on the [File] menu to save the method file.

4.7.2 Create Bath Tables

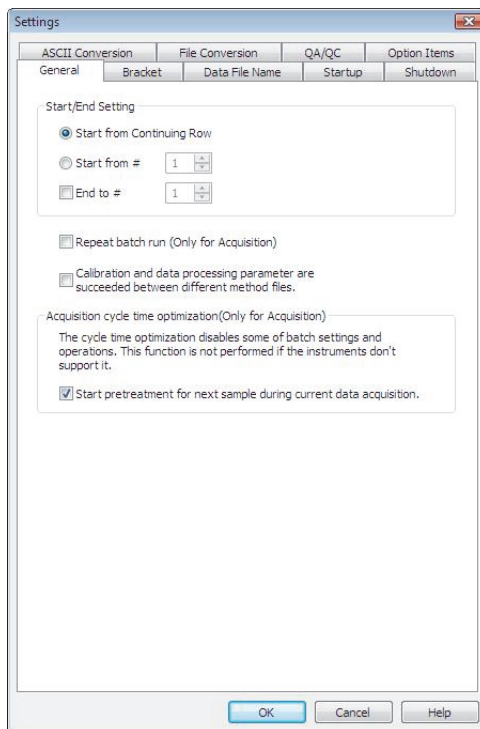
- 1 Click the  (Realtime Batch) icon on the [Main] assistant bar.
- 2 Open the batch file in the [Realtime Batch] window.
- 3 Enter the method file saved above to all rows of [Method File] column.

NOTE

- By entering the method file to the top row and then selecting [Fill Down] from right-click menu on the cell, it can be set to all rows.
- The overlap injection can not be performed when the method file name is different between lines.

- 4 Click the  (Settings) icon on the [Realtime Batch] assistant bar.

- 5 Select a [Start pretreatment for next sample during current data acquisition] checkbox in the [General] tab.



Reference

Refer to Help for details.

- 6 Save the batch file and execute the batch analysis.

5

Calibration Curves

This chapter describes how to make calibration curves and check calibration curve information.

There are two ways to make a calibration curve:

- Automatic creation by batch processing
- Manual creation in the [Calibration Curve] window

This section describes how to make calibration curves automatically by postrun batch processing at "[5.1 Calibration Curves by Postrun Batch](#)" and manually in the [Calibration Curve] window at "[5.2 \[Calibration Curve\] Window](#)".

Reference

See "[4.6 Create a Calibration Curve to Quantitate an Unknown Sample](#)" P.100 for details on automatically making calibration curves using realtime batch.

5

5.1 Calibration Curves by Postrun Batch

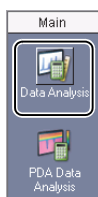
Use postrun batch to automatically make a calibration curve using the data file of a standard sample that has already been acquired.


This section describes how to set data processing parameters and Batch Table items to make calibration curves.

5.1.1 Edit the Data Processing Parameters

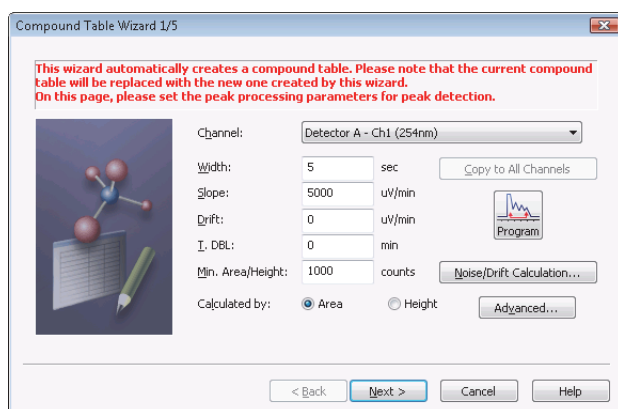
This section describes how to edit the data processing parameters of method files using standard samples data.

- 1 Click the  (Data Analysis) icon on the [Main] assistant bar in the [Postrun Analysis] program.



- 2 Drag-and-drop the data file of the standard sample from which data has already been acquired onto the [Data Analysis] window from the [Data Explorer] sub-window.
- 3 Click the  (Wizard) icon on the [Data Analysis] assistant bar.

4 Refer to "6.5.1 Compound Table Wizard" to set the data processing parameters using the Compound Table Wizard.



5 Click (View Mode) in [Method View].

The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the analysis results in [Chromatogram View] and [Results View].

6 Click the (Apply to Method) icon on the [Data Analysis] assistant bar.

The parameters are exported to the method file.

Reference

For details, see "6.7 Save (Export) to Method Files" P.171.

5.1.2 Edit Batch Tables

■ Create Batch Tables

This section describes how to create batch tables. There are two ways to create a Batch Table according to how data is acquired.


- New Batch Table
- Load the Batch Table used for data acquisition

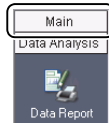
New Batch Table

1 Click the (Postrun Batch) icon on the [Main] assistant bar in the [Postrun Analysis] program.

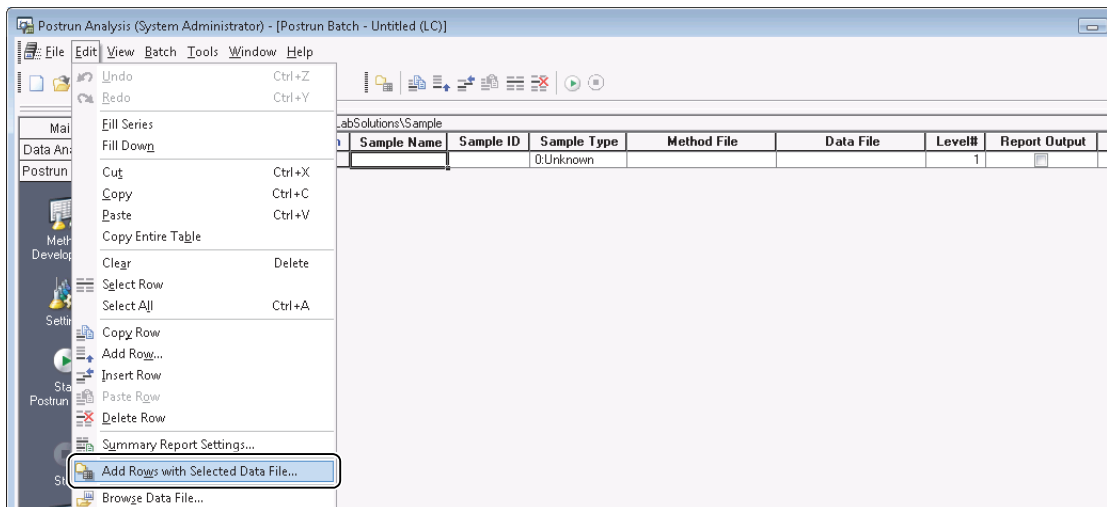


 **NOTE**

If the  (Postrun Batch) icon is not displayed on the assistant bar, click on the assistant bar title.



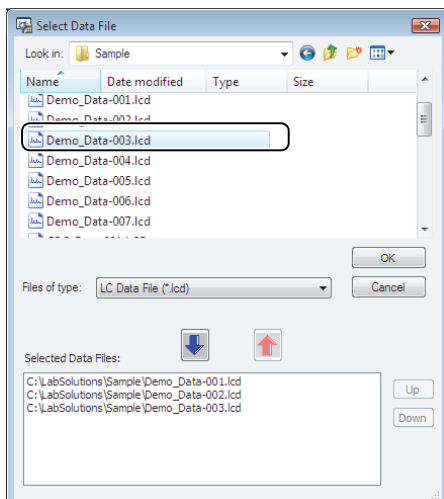
2 Click [Add Rows with Selected Data File] on the [Edit] menu.



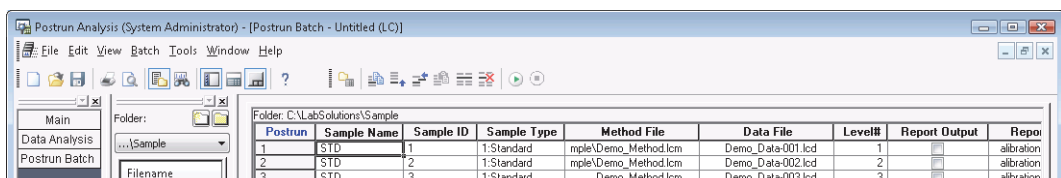
5

3 Select the data file name and then click .

The data file name is displayed in the [Selected Data Files] box. Repeat this procedure to select all of the files required for postrun batch.



The Batch Table is created from the information in the selected data file.




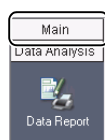
Load a Batch Table Used for Data Acquisition

- 1 Click the  (Postrun Batch) icon on the [Main] assistant bar in the [Postrun Analysis] program.

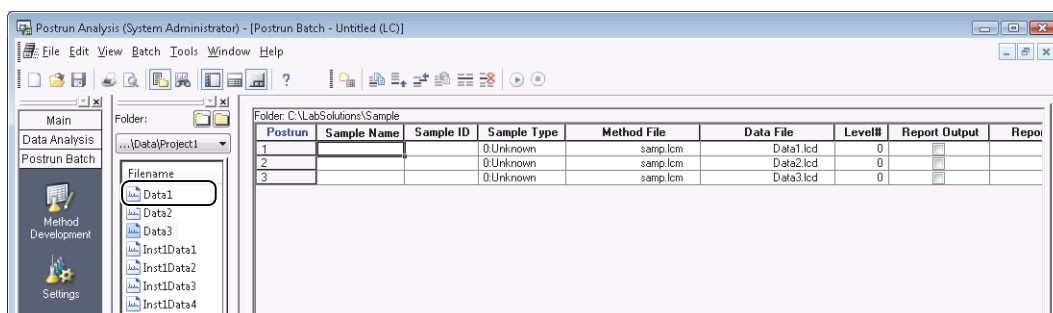


NOTE

If the  (Postrun Batch) icon is not displayed on the assistant bar, click on the assistant bar title.



- 2 Drag-and-drop the batch file used for data acquisition onto the [Postrun Batch] window from the [Data Explorer] sub-window.



■ Set the Sample Type

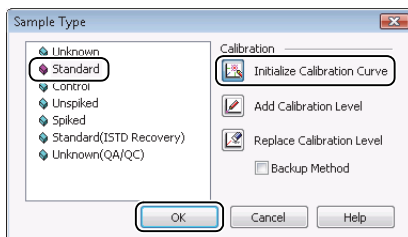
Set the type of sample to measure.

In the case of a standard sample, set the first standard sample to [Initialize Calibration Curve] and the next standard sample to [Add Calibration Level]. The default setting [0: Unknown] is used for unknown samples.

1 Click the [Sample Type] cell of the initial standard sample.

Postrun	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Report Output	Repor
1	STD1		0:Unknown (i)	samp.lcm	Data1.lcd	0	<input type="checkbox"/>	
2	STD2		0:Unknown	samp.lcm	Data2.lcd	0	<input type="checkbox"/>	
3	STD3		0:Unknown	samp.lcm	Data3.lcd	0	<input type="checkbox"/>	

2 Click [Standard], select [Initialize Calibration Curve] and click [OK].

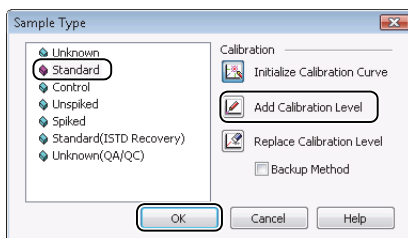


The initial cell for the sample type is displayed as [1: Standard (i)].

3 Click the [Sample Type] cell of the next standard sample.

Postrun	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Report Output	Repor
1	STD1		1:Standard(i)	samp.lcm	Data1.lcd	1	<input type="checkbox"/>	
2	STD2		0:Unknown (i)	samp.lcm	Data2.lcd	0	<input type="checkbox"/>	
3	STD3		0:Unknown	samp.lcm	Data3.lcd	0	<input type="checkbox"/>	

4 Click [Standard], select [Add Calibration Level] and click [OK].



The cell for the sample type is displayed as [1: Standard].

Repeat steps 3 and 4 for multiple standard samples.

Postrun	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Report Output	Repor
1	STD1		1:Standard(i)	samp.lcm	Data1.lcd	1	<input type="checkbox"/>	
2	STD2		1:Standard	samp.lcm	Data2.lcd	1	<input type="checkbox"/>	
3	STD3		0:Unknown	samp.lcm	Data3.lcd	0	<input type="checkbox"/>	

■ Set the Level#

Set the standard sample [Level#] according to the concentration value in the Compound Table of the method file. The calibration points are created from the level number of the Compound Table and the area and height values of the preset standard sample.



NOTE

[Level#] values are not used for unknown samples, even if they are set.

1

Click the [Level#] cell for the standard sample.

Postrun	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Report Output	Repor
1	STD1		1:Standard(I)	samp.lcm	Data1.lcd	1	<input type="checkbox"/>	
2	STD2		1:Standard	samp.lcm	Data2.lcd	1	<input type="checkbox"/>	
3	STD3		0:Unknown	samp.lcm	Data3.lcd	0	<input type="checkbox"/>	

2

Enter the level number.

Postrun	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Report Output	Repor
1	STD1		1:Standard(I)	samp.lcm	Data1.lcd	1	<input type="checkbox"/>	
2	STD2		1:Standard	samp.lcm	Data2.lcd	2	<input type="checkbox"/>	
3	STD3		0:Unknown	samp.lcm	Data3.lcd	0	<input type="checkbox"/>	

The level number is changed.

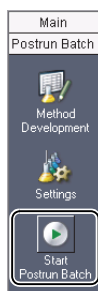
3

Set the [Level#] cell for other standard samples.

5.1.3 Postrun Analysis Using Batch Tables

1

Click the  (Start Postrun Batch) icon on the [Postrun Batch] assistant bar.




Postrun batch is started.

Postrun	Sample Name	Sample ID	Sample Type	Method File	Data File	Level#	Report Output	Repor
1	STD1		1:Standard(I)	samp.lcm	Data1.lcd	1	<input type="checkbox"/>	
2	STD2		1:Standard	samp.lcm	Data2.lcd	2	<input type="checkbox"/>	
3	STD3		0:Unknown	samp.lcm	Data3.lcd	0	<input type="checkbox"/>	

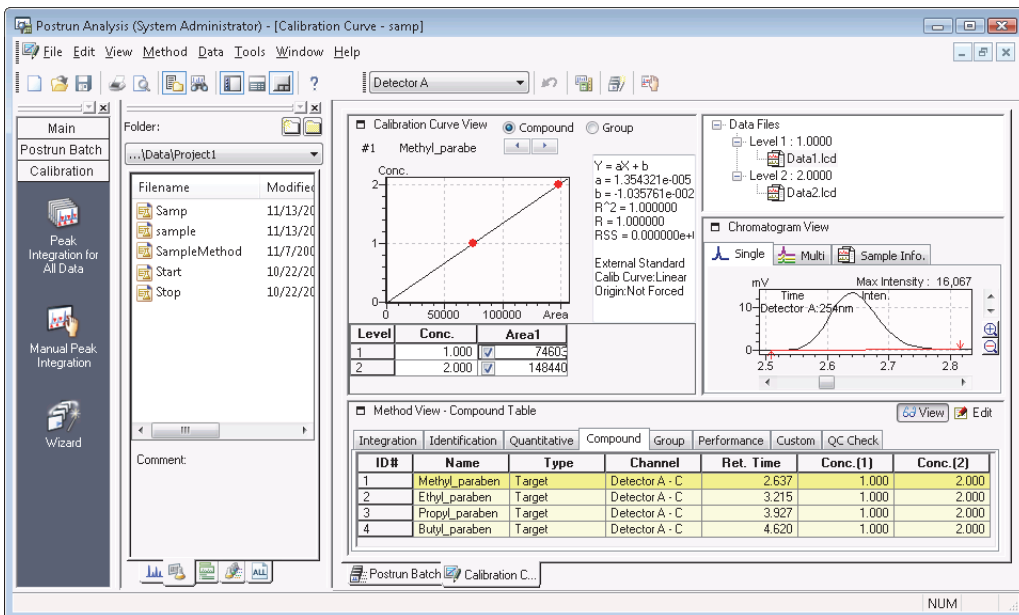
5.1.4 Check Calibration Curves

Check whether the calibration curve has been successfully drawn in the [Calibration Curve] window in "5.1.3 Postrun Analysis Using Batch Tables".

- 1 Select the [Method File] cell in the batch table, and click the  (Method Development) icon on the [Postrun Batch] assistant bar.

Postrun	Sample Type	Method File	Data File	Level#	Report Output	Report Forma
1	1:Standard(I)	samp.lcm	Data1.lcd	1	<input type="checkbox"/>	
2	1:Standard	samp.lcm	Data2.lcd	2	<input type="checkbox"/>	
3	0:Unknown	samp.lcm	Data3.lcd	0	<input type="checkbox"/>	

- 2 Check the calibration curve in the [Calibration Curve] window.



The screenshot shows the 'Calibration Curve - samp' window. The main graph plots Concentration (Conc.) on the y-axis (0 to 2) against Area on the x-axis (0 to 100,000). Two data points are shown: (74503, 1.000) and (149440, 2.000). The regression equation is $Y = aX + b$ with $a = 1.354321e-005$, $b = -1.035761e-002$, $R^2 = 1.000000$, $R = 1.000000$, and $RSS = 0.000000e+00$. The external standard is identified as Methylparaben with a linear calibration curve and no forced origin.

The 'Method View - Compound Table' at the bottom shows the following data:

ID#	Name	Type	Channel	Ret. Time	Conc.(1)	Conc.(2)
1	Methylparaben	Target	Detector A - C	2.637	1.000	2.000
2	Ethylparaben	Target	Detector A - C	3.215	1.000	2.000
3	Propylparaben	Target	Detector A - C	3.927	1.000	2.000
4	Butylparaben	Target	Detector A - C	4.620	1.000	2.000

The chromatogram view shows a single peak at 2.637 minutes with a maximum intensity of 16,067 mV. The x-axis is labeled 'Time' and 'Detector A: 254nm Inten.'.

5.2 [Calibration Curve] Window

Check calibration curves made in realtime or postrun batch in the [Calibration Curve View] window and make calibration curves by manually adding calibration points.

The [Calibration Curve] window has four views, [Calibration Curve View] displays calibration curves, [Method View] displays the data processing parameters, the [Data Files] tree view displays the data files used for calibration curves, and [Chromatogram View].

5.2.1 [Calibration Curve] window Description

This section describes how to view the [Calibration Curve] window.



NOTE

The layout of each view can be changed in the [Calibration Curve] window.

Two modes are provided for the display layout, [Normal Mode] and [Many Ingredients Mode], which is used when there are many identified peaks.

The screenshot shows the [Calibration Curve] window interface. Callout 1 points to the toolbar at the top. Callout 2 points to the Calibration Curve View, which includes a graph of Concentration vs. Area, a table of calibration points, and regression statistics. Callout 3 points to the Data Files tree view on the right. Callout 4 points to the Chromatogram View showing a peak at 2.54 minutes. Callout 5 points to the Method View - Compound Table at the bottom. Callout 6 points to the Method View - Compound Table.

Level	Conc.	Area
1	1.000	74600
2	2.000	148440


ID#	Name	Type	Channel	Ret. Time	Conc.[1]	Conc.[2]
1	Methyl_paraben	Target	Detector A - C	2.637	1.000	2.000
2	Ethyl_paraben	Target	Detector A - C	3.215	1.000	2.000
3	Propyl_paraben	Target	Detector A - C	3.927	1.000	2.000
4	Butyl_paraben	Target	Detector A - C	4.620	1.000	2.000

No.	Explanation
1	Displays the [Standard] and [Calibration Curve] toolbars.
2	Displays a calibration curve graph, calibration curve information and Calibration Table.
3	Displays the data files for the individual levels used to make the calibration curve. Calibration points for each level can be added or deleted. Add data files by dragging-and-dropping them from the [Data Explorer] sub-window.
4	Displays the chromatograms and sample information of the data files used to make the calibration curve.
5	Parameters are displayed in the [View] mode, and can be changed in the [Edit] mode.
6	Displays the data processing parameters in the method file.

5.2.2 Make Calibration Curves in the [Calibration Curve] Window

This section describes how to manually make calibration curves.

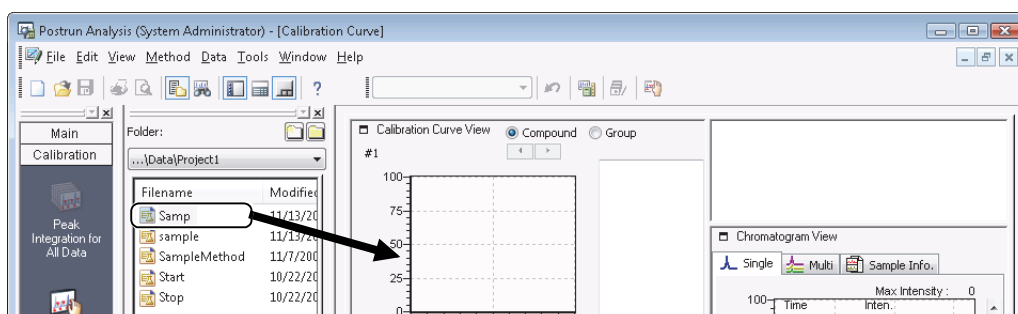
Data processing parameters must be set before calibration curves can be manually created in the [Calibration Curve] window.

1 Click the  (Calibration Curve) icon on the [Main] assistant bar in the [Postrun Analysis] program.


2 Select the method file.

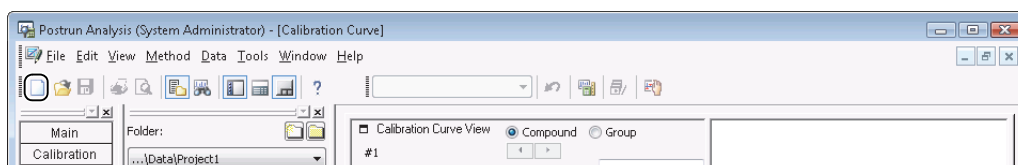
- Existing method file

1 Drag-and-drop the method file onto the [Calibration Curve] window from the [Data Explorer] sub-window.



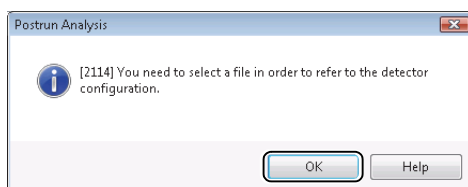
- New method file

1 Click the  (New) button on the toolbar.

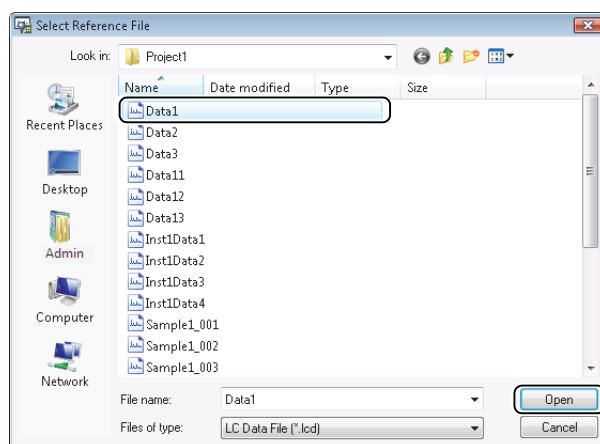


The following message is displayed.

2 Click [OK].



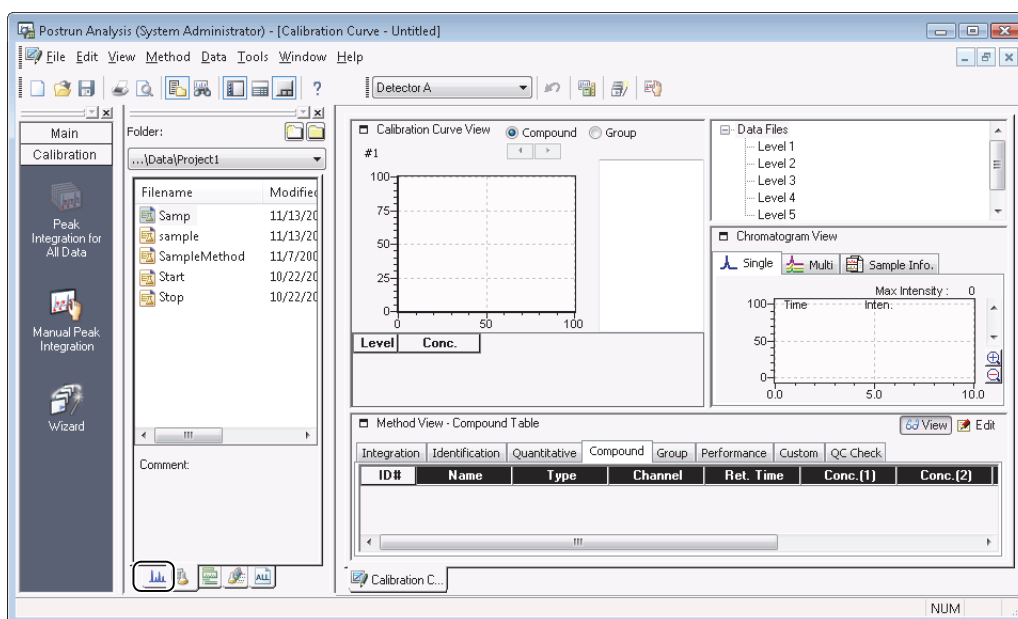
- 3 Select the method file used for data acquisition or a method file with the same system configuration, and click [Open].



The detector is set based on the system configuration information in this file.
The [Calibration Curve] window changes to [Untitled].



- 3 Click the [Data] tab at the bottom of the [Data Explorer] sub-window.

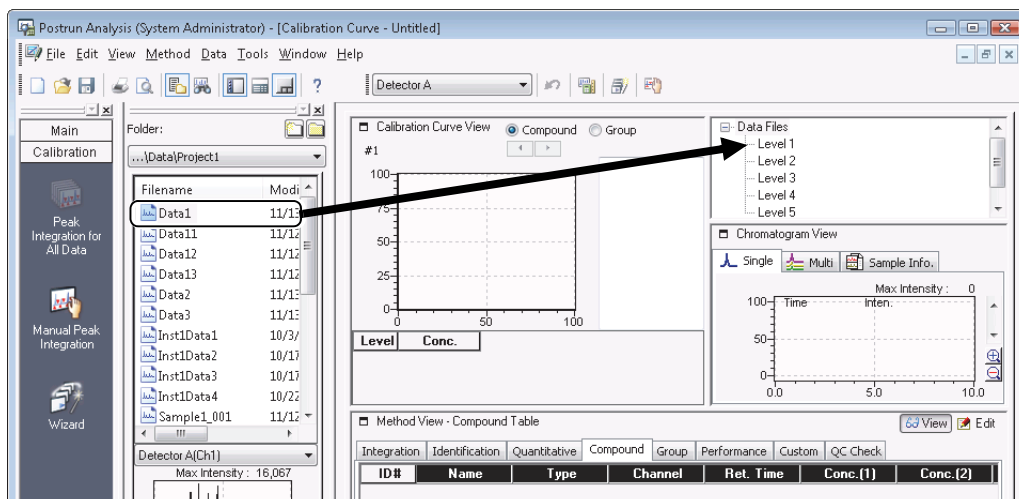


4 Drag-and-drop the data file of the standard sample onto the target level in the [Data Files] tree view from the [Data Explorer] sub-window.

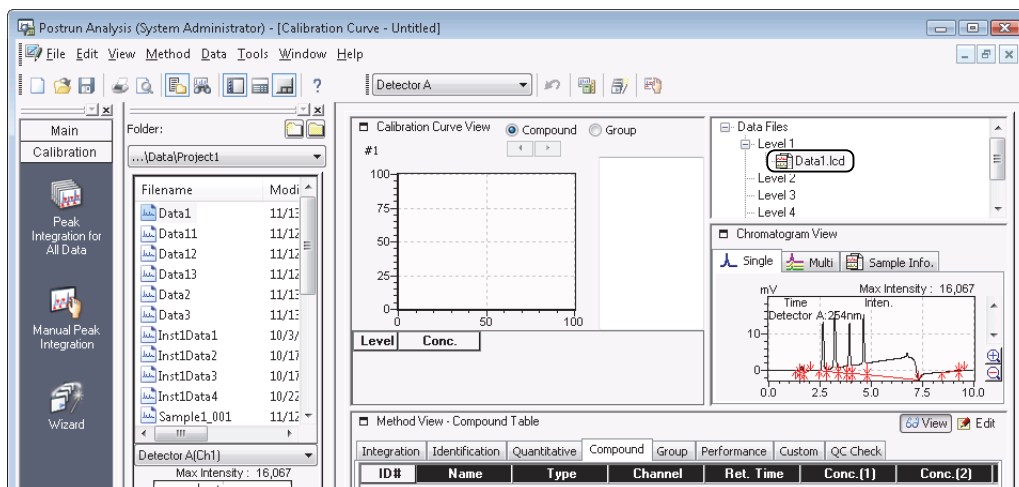


NOTE

Drag-and-drop the data file onto the same level position as the concentration set in the Compound Table of the method file.

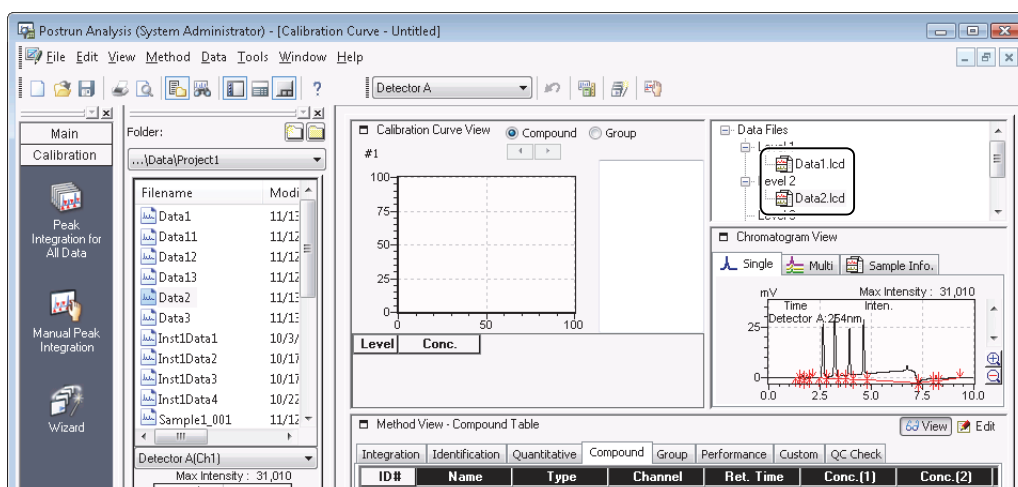


The data file is added to the level.

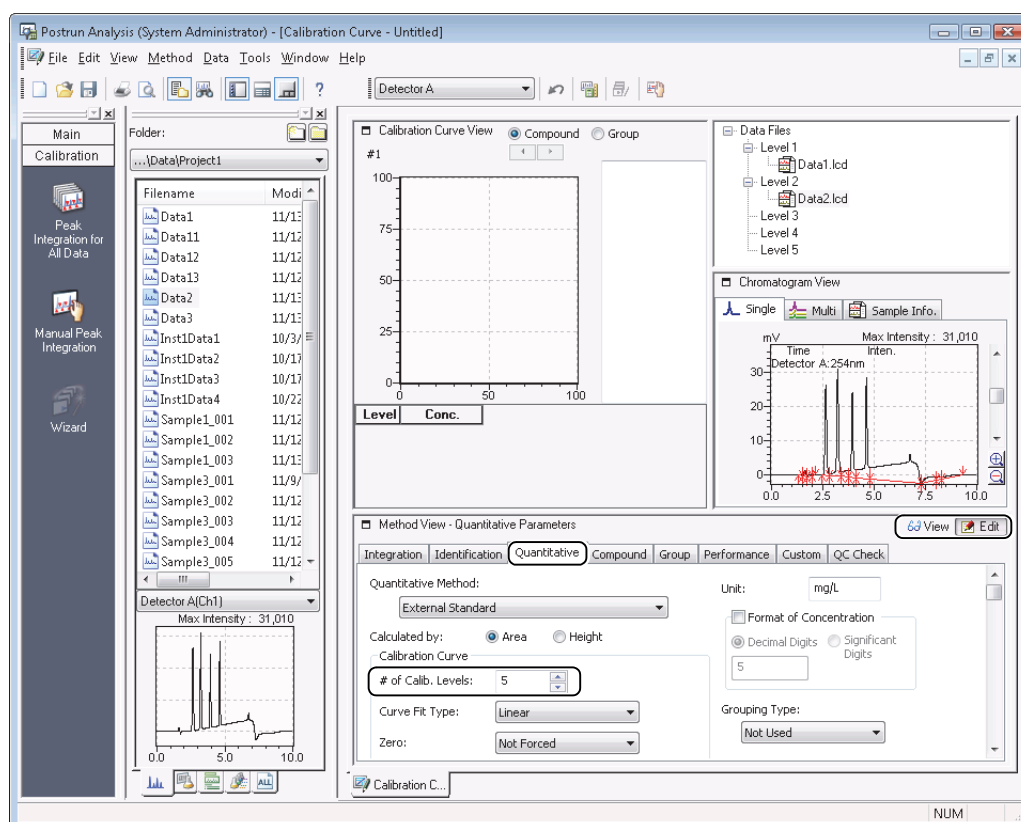


Repeat the above step and drag-and-drop the additional standard sample data file onto the target level when multiple standard samples are used.

5

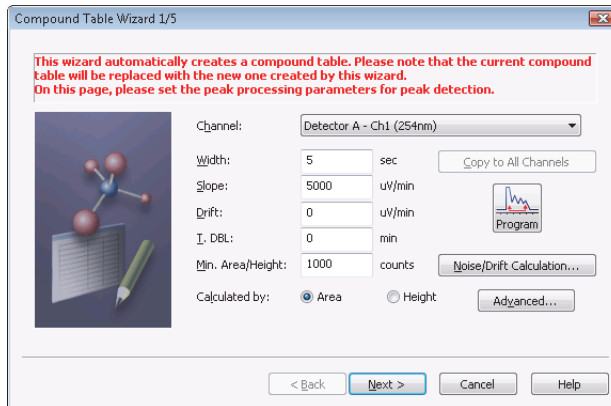
**NOTE**

Set the [# of Calib. Levels] on the [Quantitative] tab in the [Method View] to increase the number of levels in the calibration curve.

**5**

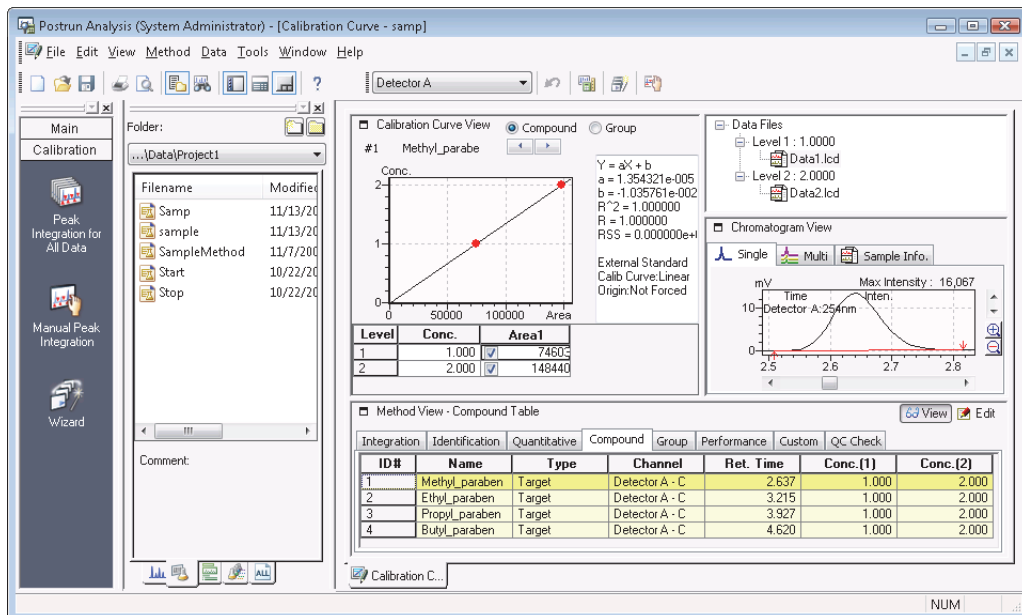
Click the  (Wizard) icon on the [Calibration] assistant bar.

6 Refer to "6.5.1 Compound Table Wizard" to set the data processing parameters using the Compound Table Wizard.



7 Click View (View Mode) in [Method View].

Data processing is performed on the data loaded in the [Data Files] tree view according to the parameters set in the Compound Table Wizard.

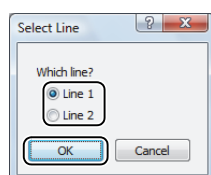


8 Click the (Save) button on the toolbar.

The method file and the data file(s) in the [Data Files] tree view are saved.

NOTE

In the case of a dual-line configuration GC, select the line to export the method from, and click [OK].



6

Data Analysis

This chapter describes how to display the results of acquired data and set data processing parameters during postrun analysis. The [Data Analysis] window displays the contents of a single data file.

Reference

- Use the [Quant Browser] window to display the contents of multiple data files, refer to "[9 Quant Browser](#)" P.259.
- Refer to "[5 Calibration Curves](#)" P.113 for details on creating calibration curves used for quantitative calculations.

6.1 [Data Analysis] Window

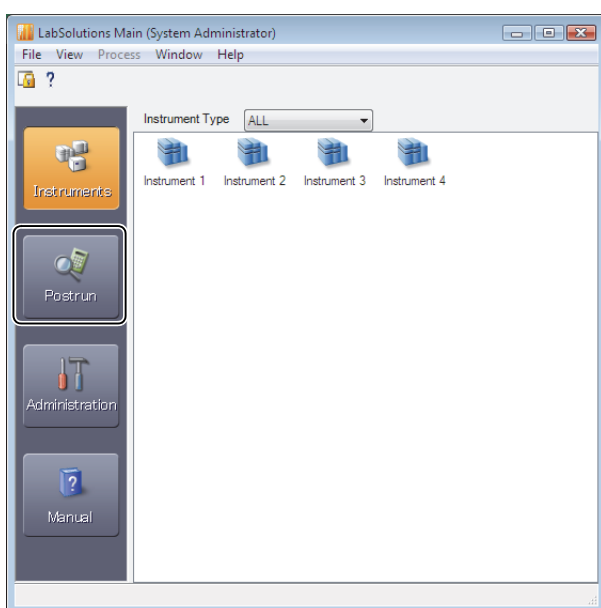
The [Data Analysis] window is comprised of the following views:

- [Chromatogram View] - displays chromatograms and instrument status
- [Results View] - displays Peak Tables and quantitative results
- [Method View] - displays the data processing parameters

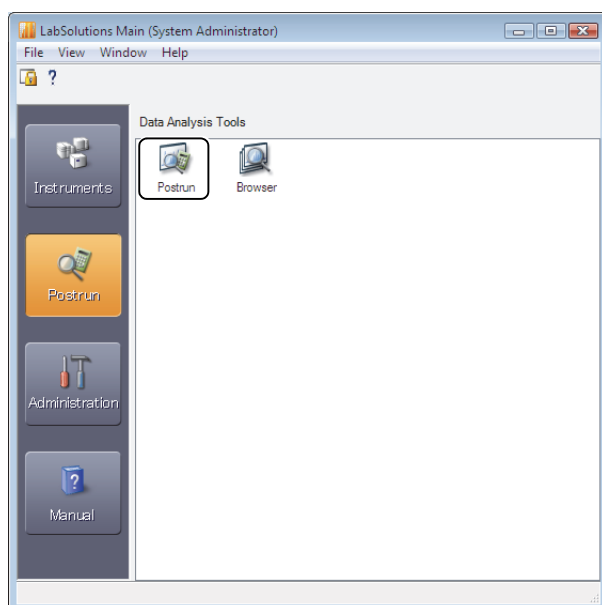
6

6.1.1 Open the [Data Analysis] Window


- 1 Click the  icon in the [LabSolutions Main] window.



2 Double-click [Postrun].



NOTE

The [Data Analysis] window can also be opened by clicking the  (Data Analysis) icon on the [Acquisition] assistant bar.

3 Drag-and-drop a data file onto the [Data Analysis] window from the [Data Explorer] sub-window.



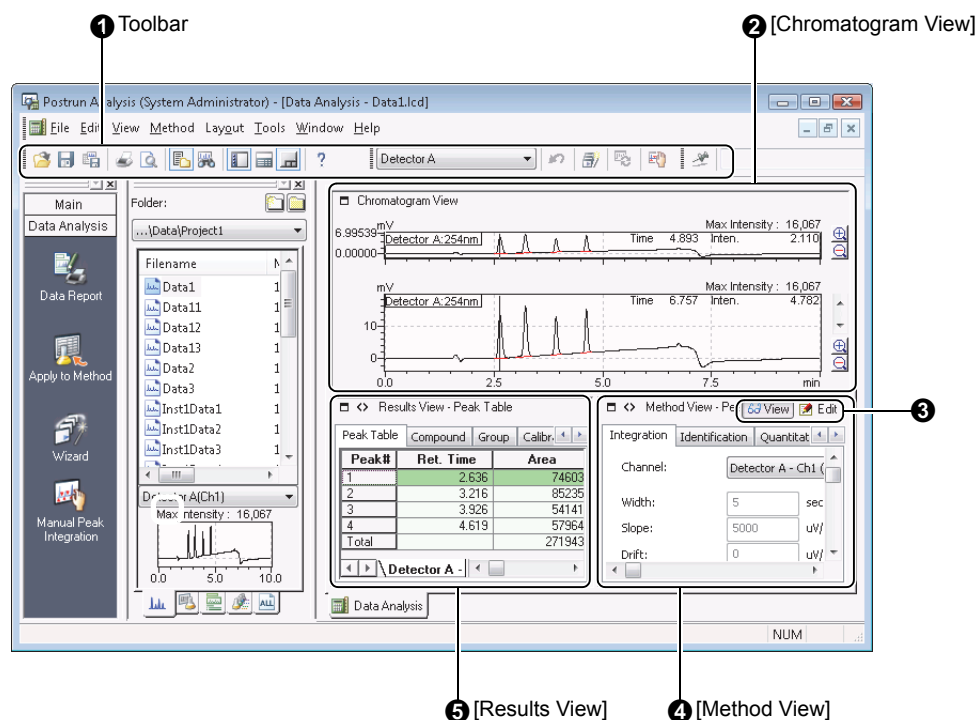
The content of the data file is displayed in the [Data Analysis] window.



6.1.2 [Data Analysis] Window Description

This section describes how to view and use the [Data Analysis] window.

NOTE

The size of each view can be changed. Click [Save Layout] on the [Layout] menu, and save the changed layout under a new name.

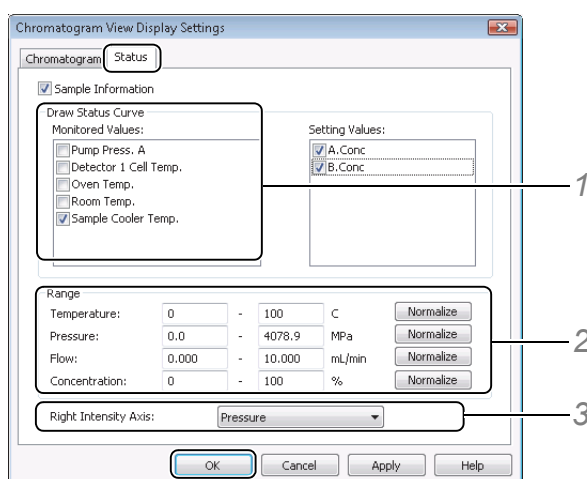


No.	Explanation
1	Displays the [Standard] toolbar, [Data Analysis] toolbar, and [Background Compensation Bar].
2	Displays the chromatogram for the currently open data file. [Chromatogram View] displays graphs with the [Full Chromatogram] on top and the [Zoomed Chromatogram] on the bottom. If the data has been acquired from multiple detectors, [Other Detector] graphs can also be displayed. [Pressure] and [Flow] can be set to overlaying [Chromatogram View] in the display settings.  Reference Refer to " Status Display in the [Chromatogram View] " P.130 for details.
3	Displays the parameters in the [View] mode. Switch to the [Edit] mode to change the parameters. Change back to the [View] mode to perform postrun analysis using edited parameters.
4	The data processing parameters are displayed on the [Integration], [Identification], [Quantitative], [Compound], [Group], [Performance], [Custom], and [QC Check] tabs.  Reference Refer to " 6.2 Peak Integration Parameters " P.132 for details.
5	The analysis results are displayed on the [Peak Table], [Compound], [Group], and [Calibration Curve] tabs.

■ Status Display in the [Chromatogram View]

The pressure, temperature and other conditions at the time of data acquisition are displayed and can be overlaid in the [Chromatogram View].

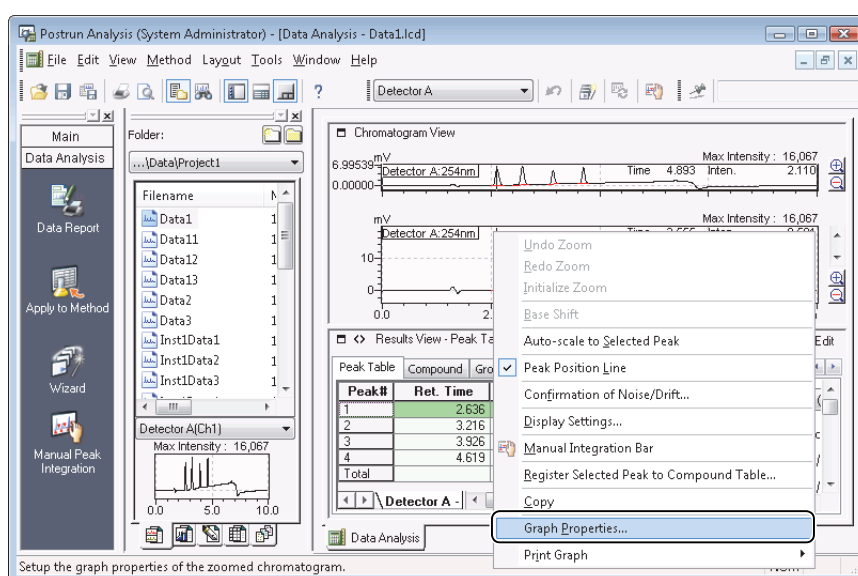
- 1 Right-click on the graph, and click [Display Settings].
- 2 Click the [Status] tab, make the necessary selections, and click [OK].



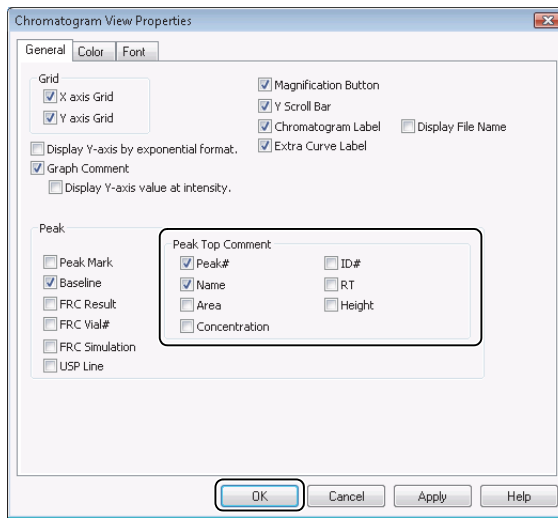
- 1 Select the status items to be overlaid on the chromatogram.
- 2 Set the display range of each status item or click [Normalize].
- 3 Select the parameter to display on the right axis of the graph (Intensity Axis).

■ Top of Peak Comment

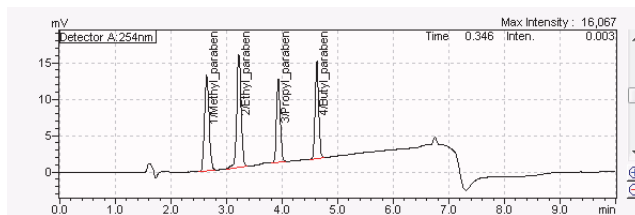
- 1 Right-click on the chromatogram, and click [Graph Properties].



2 Select the peak top comment that is displayed on zoomed chromatograms, and click [OK].



The selected comment is displayed at the top of the peak in the enlarged chromatogram.



6.2 Peak Integration Parameters

Change the peak integration parameters and repeat peak integration.



NOTE

While in the [Data Analysis] window, the changes to peak integration parameters are applied only to data processing parameters in the current data file.

The parameters must be exported to a method file before they can be applied to other data, then data processing using this newly saved method must be applied to all of the additional data. Refer to ["6.7 Save \(Export\) to Method Files" P.171](#).

6.2.1 Peak Integration of Detected Peaks

This section describes how to set peak integration parameters.

1

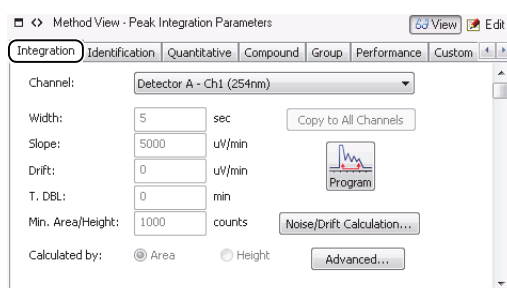
Click **Edit (Edit Mode) in [Method View]**.

Click the [Integration] tab, and change the parameters as required.

Click to change the integration time program and peak selection range.

If analysis was performed on multiple detectors, the parameter changes can be applied to the other channels by clicking [Copy to All Channels].

Click [Noise/Drift Calculation], and make changes to the [Noise/Drift Calculation Settings] in the sub-window that is displayed.



Reference

Refer to Help for details about each of the parameters.

2

Click **View (View Mode) in [Method View]**.


The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the processing results in the [Chromatogram View] and [Results View].

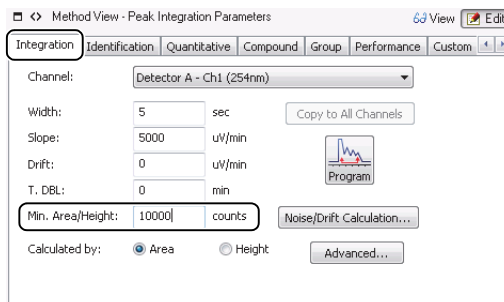
6.2.2 Remove Unwanted Peak Integration

■ Remove Integration of Unwanted Peaks with Minimum Area/Height

Use a larger [Min. Area/Height] value to exclude integration of small peaks.

The following example describes how to change the [Min. Area/Height] value from “1000” to “10000”.

- 1 Click  **Edit** (Edit Mode) in [Method View].
- 2 Click the [Integration] tab, and change the [Min. Area/Height] value to “10000”.



Method View - Peak Integration Parameters

Integration Identification Quantitative Compound Group Performance Custom

Channel: Detector A - Ch1 (254nm)

Width: 5 sec Copy to All Channels

Slope: 5000 uV/min

Drift: 0 uV/min

T. DBL: 0 min

Min. Area/Height: 10000 counts

Calculated by: Area Height

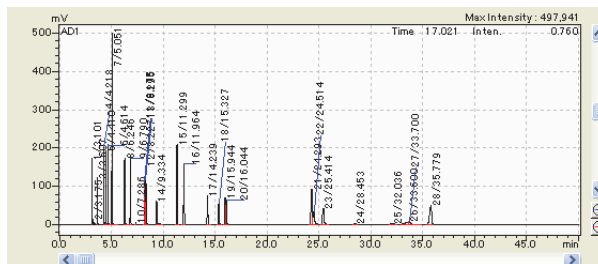
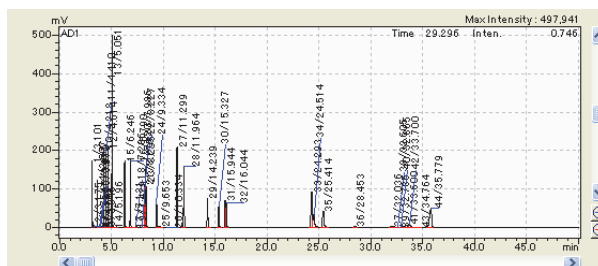


NOTE

Select [Height] at [Calculated by] to remove the integration of unwanted peaks based on peak height.

- 3 Click  **View** (View Mode) in [Method View].

The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the processing results in the [Chromatogram View] and [Results View].



Remove Integration of Unwanted Peaks with the Integration Time Program

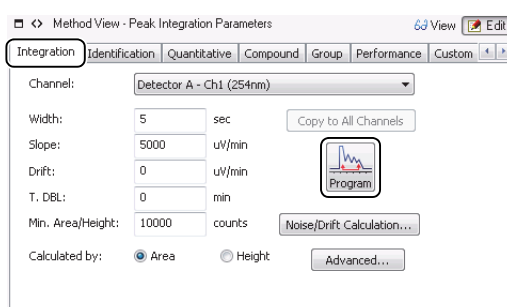
The integration time program allows for detailed peak integration, that is not normally possible with typical integration parameters.

The following example describes how to remove integration of unwanted peaks using the integration time program.

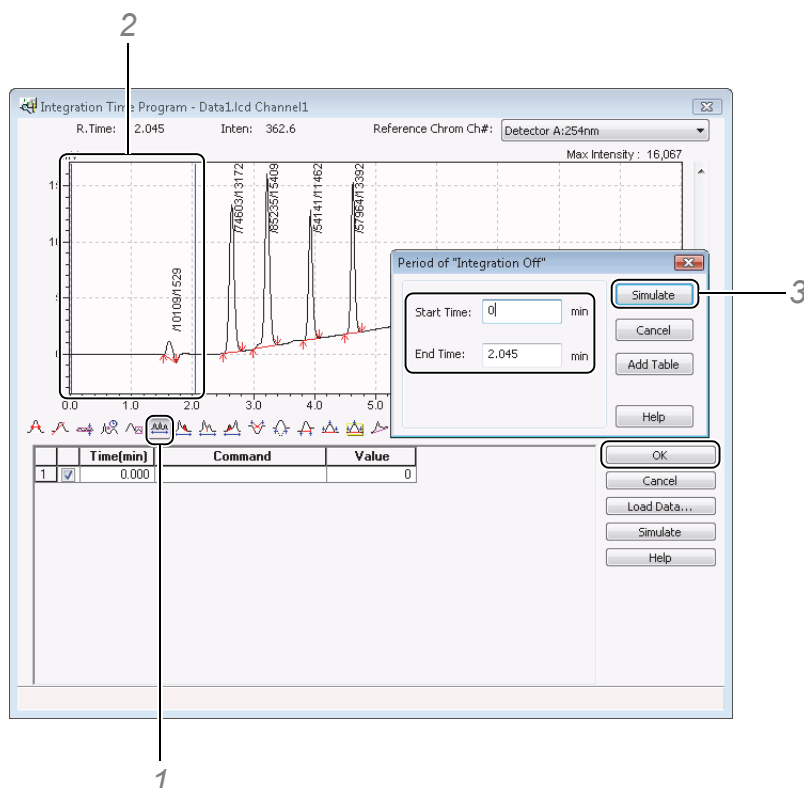
You can delete unwanted peaks by setting period in which peak detection is not performed in the Time Program Table in the [Integration Time Program] sub-window.


1 Click  (Edit Mode) in [Method View].

2 Click the [Integration] tab, and click .



3 Create an integration time program, and click [OK].

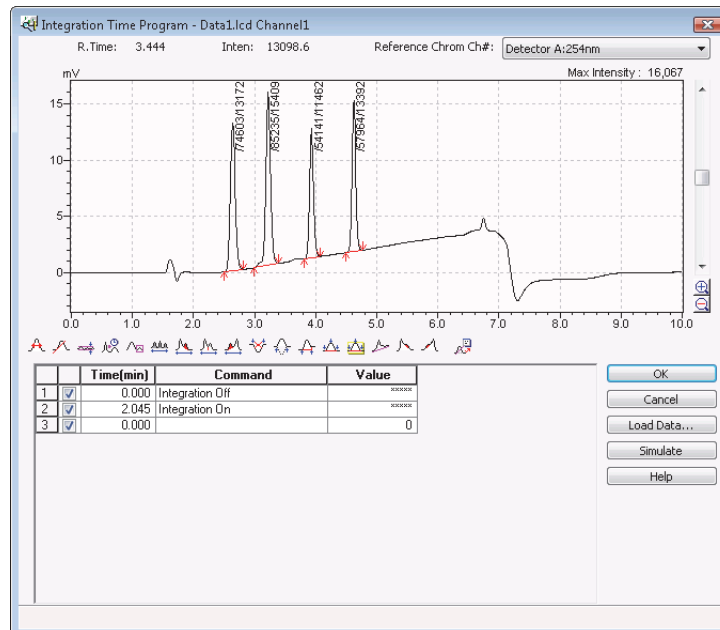


1 Click  (Period of "Integration Off").



2 Use the cursor to select the start and end positions of the range where integration is not performed.

3 Evaluate the [Start Time] and [End Time] in the [Period of "Integration Off"] sub-window, and click [Simulate].

The time and processing commands are added to the time program.
Examine the resulting integration.



NOTE

Use the mouse to click   to zoom in or out a chromatogram and change the display of the specified view area.

4 Click View (View Mode) in [Method View].

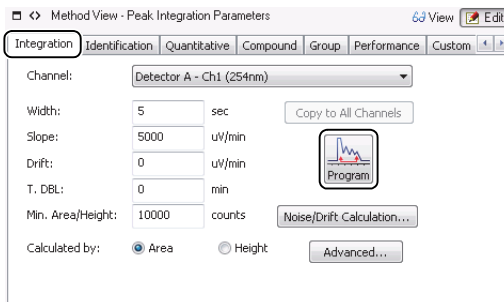
The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the processing results in the [Chromatogram View] and [Results View].

6.2.3 Analyze Tailing Peaks

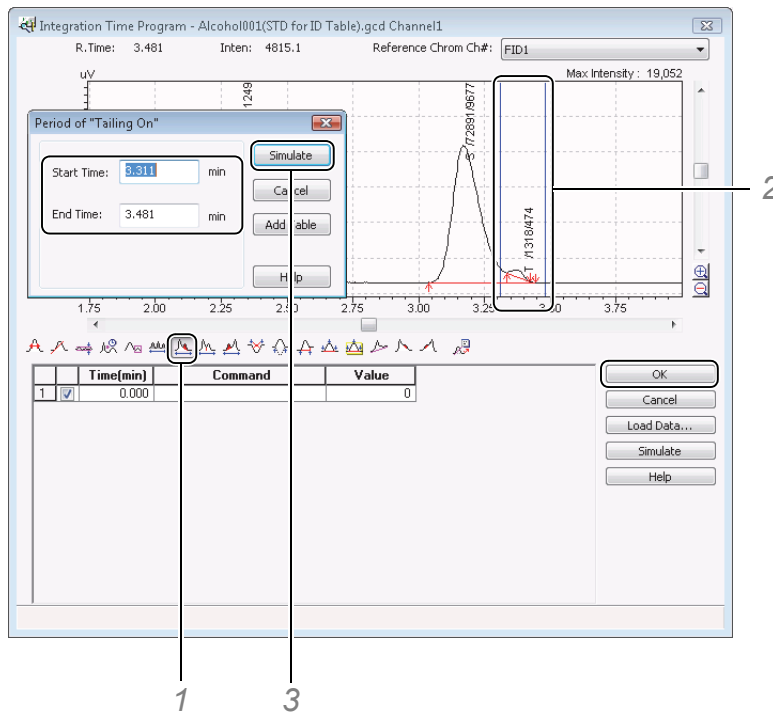
This section describes how to process a target peak that overlays the tail of the main peak.


1 Click  **Edit** (Edit Mode) in [Method View].

2 Click the [Integration] tab, and click .













3 Set the peak to perform tailing processing on, and click [OK].



- 1 Click  (Period of "Tailing On").
- 2 Use the cursor to select the start and end positions of the range where tailing processing is performed.
- 3 Evaluate the [Start Time] and [End Time] in the [Period of "Tailing On"] sub-window, and click [Simulate].

The time and processing commands are added to the time program.

Button	Name	Explanation
	Move BL	Moves the peak detection points (start or end) along the X-axis (time). Processing is executed on specified points.
	Move BL (Vertical)	Moves the peak detection points (start or end) along the Y-axis (intensity).
	Insert Peak	Inserts a peak by specifying the peak start and end times. Processing is executed on specified points.
	Insert Peak Start/End	Inserts a peak start and peak end point for a peak that was not previously integrated. Small peaks on the shoulders of larger peaks are easily integrated using this feature.
	Split Peak	Draws a vertical line to the split a peak at a specified point.
	Unify Peaks	Unifies all detected peak between 2 specified points into a single peak.
	Reject Peak	Select the top of a peak to remove the integration of that peak.
	Reject Peaks	Removes the integration of all of the detected peaks between 2 specified points.
	Force B/V	Selects between vertical division and baseline separation for the processing of two adjacent peaks.
	Force T/L/N/NB	Specifies the retention time (top of peak) of the target peak, and changes the peak integration method.

**NOTE**

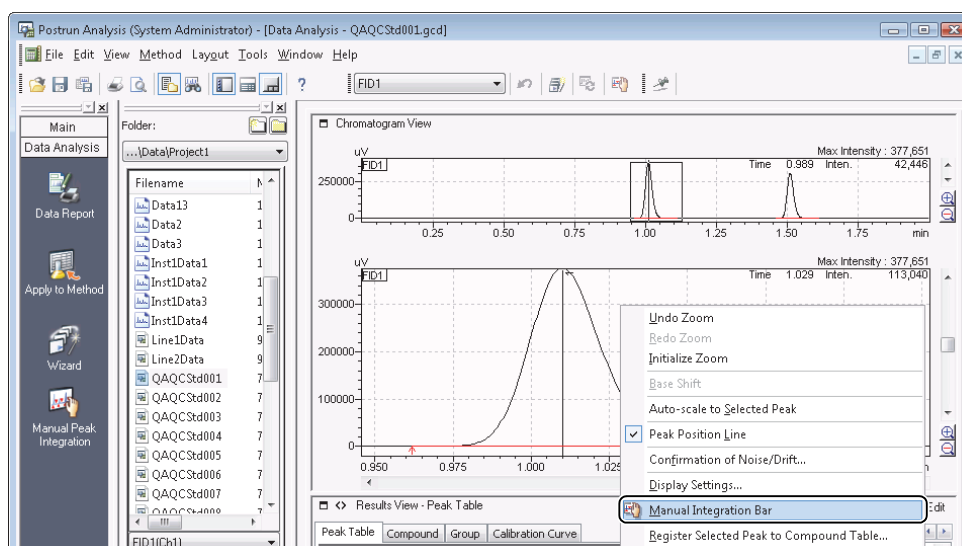
Right-click on the manual integration bar, and click [Advanced Toolbar] to switch the toolbar display to the Advanced toolbar.

Move Peak Detection Points

This section describes how to move peak detection points to change the baseline.

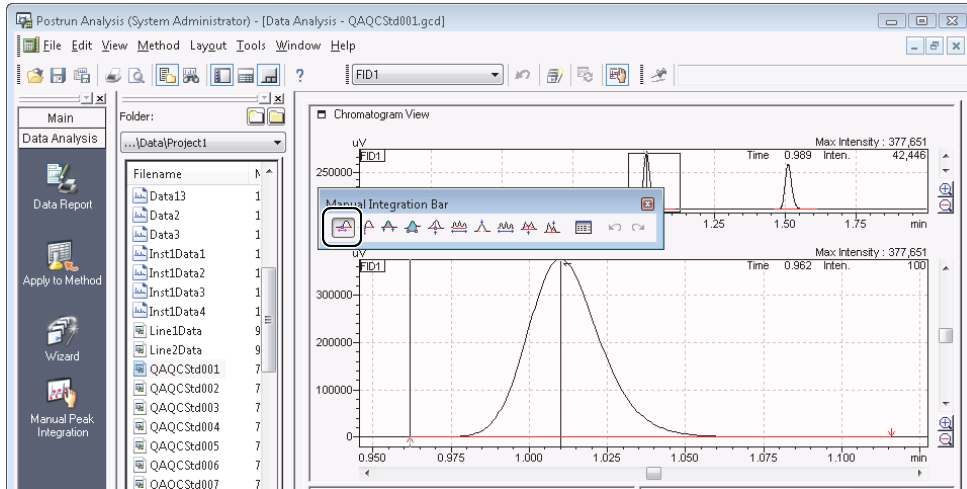
1

Right-click on a [Zoomed Chromatogram] in the [Data Analysis] window, and click [Manual Integration Bar].

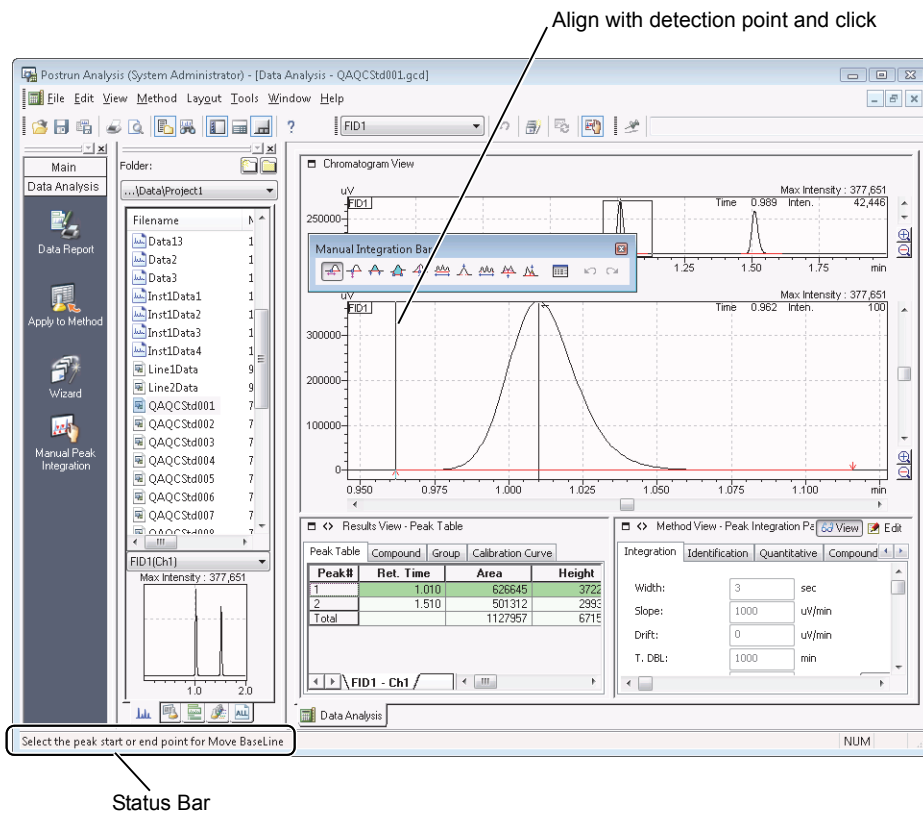


The screenshot displays the 'Data Analysis' window with a 'Chromatogram View' showing two peaks. The top peak is at 0.989 min with a maximum intensity of 377,651. The bottom peak is at 1.029 min with a maximum intensity of 113,040. A context menu is open over the bottom peak, listing options such as 'Undo Zoom', 'Redo Zoom', 'Initialize Zoom', 'Base Shift', 'Auto-scale to Selected Peak', 'Peak Position Line' (checked), 'Confirmation of Noise/Drift...', 'Display Settings...', and 'Manual Integration Bar'. The 'Manual Integration Bar' option is highlighted in blue.

2 Click (Move BL), and edit the processing of the chromatogram.



- Following the message displayed on the status bar, place the cursor displayed on the chromatogram at the peak detection point and click.



6

- 2 Following the message displayed on the status bar, place the cursor to the desired destination at the peak detection point and click.

Align with move destination and click

Select the point after moving BaseLine

Status Bar

Chromatogram View

Manual Integration Bar

Results View - Peak Table

Peak#	Ret. Time	Area	Height
1	1.010	626645	3722
2	1.510	501312	2993
Total		1127957	6715

Method View - Peak Integration Parameters

Integration Identification Quantitative Compound

Width: 3 sec

Slope: 1000 uV/min

Drift: 0 uV/min

T. DBL: 1000 min

The peak detection point is changed and the baseline is adjusted.

Chromatogram View

Manual Integration Bar

Results View - Peak Table

Peak#	Ret. Time	Area	Height
1	1.010	626645	3722
2	1.510	501312	2993
Total		1127957	6715

Method View - Peak Integration Parameters

Integration Identification Quantitative Compound

Width: 3 sec

Slope: 1000 uV/min

Drift: 0 uV/min

T. DBL: 1000 min

NOTE

- If a mistake is made when moving the peak detection point, click the (Undo) to undo the move.
- Click the (Toggle Manual Peak Integration Table) to display and edit the Integration Time Program Table.
- Manual peak integration parameters are only saved to the current data loaded in the [Data Analysis] window. Since the manual peak integration parameters cannot be saved to the method file, they cannot be applied to other data files.

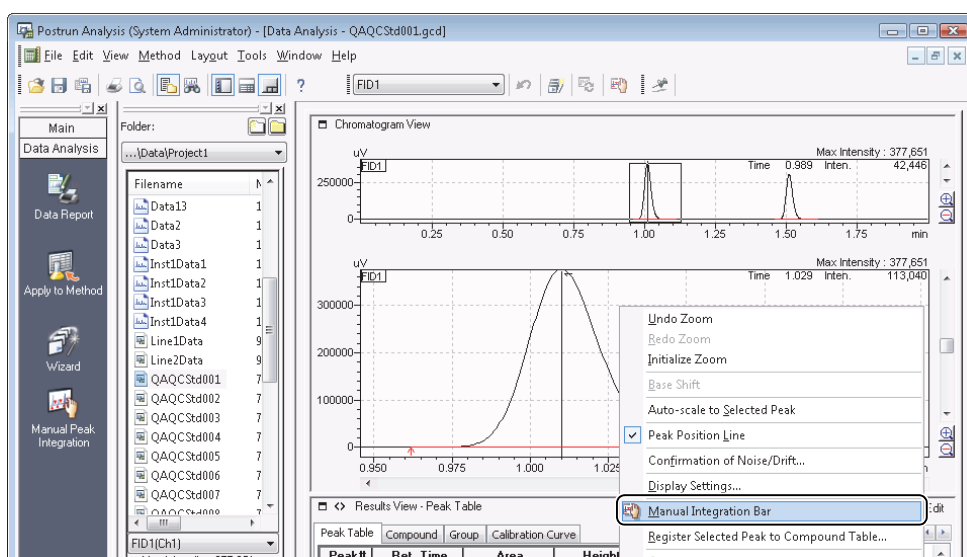
- The manual peak integration parameters are not overwritten, even if the data file is later reanalyzed with another method file.


■ Integrate Multiple Peaks as One

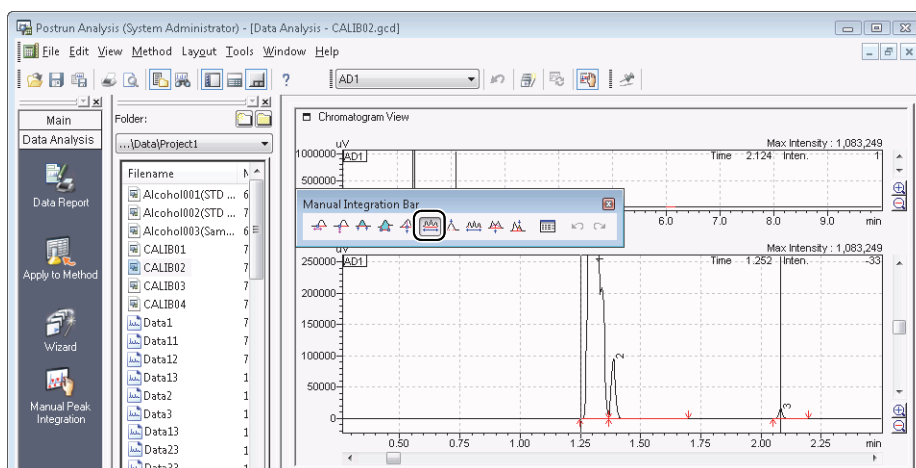
Multiple peaks can be integrated as a single peak.

This section describes how to integrate two separate peaks as a single peak.

- 1** Right-click on the [Zoomed Chromatogram] in the [Data Analysis] window, and click [Manual Integration Bar].



- 2** Click  (Unify Peaks), and select the beginning and end points for the area of the chromatogram where all of the peaks will be combined as one.



- Following the message displayed on the status bar, place the cursor displayed on the chromatogram at the peak unify start point and click.

Align with start point and click

Select the start point for Unify Peaks

Status Bar

The screenshot shows the 'Manual Peak Integration' dialog box with the following data:

Peak#	Ret. Time	Area	Heig
1	1.305	3042883	10
2	1.388	118011	
3	2.082	16710	
4	2.743	17056	
5	3.672	16989	
6	4.816	18222	

Integration parameters:

- Width: 2 sec
- Slope: 200 uW/min
- Drift: 0 uW/min
- T. DBL: 1000 min

- Following the message displayed on the status bar, place the cursor at the peak unify end point and click.

Align with end point and click

Select the end point for Unify Peaks

Status Bar

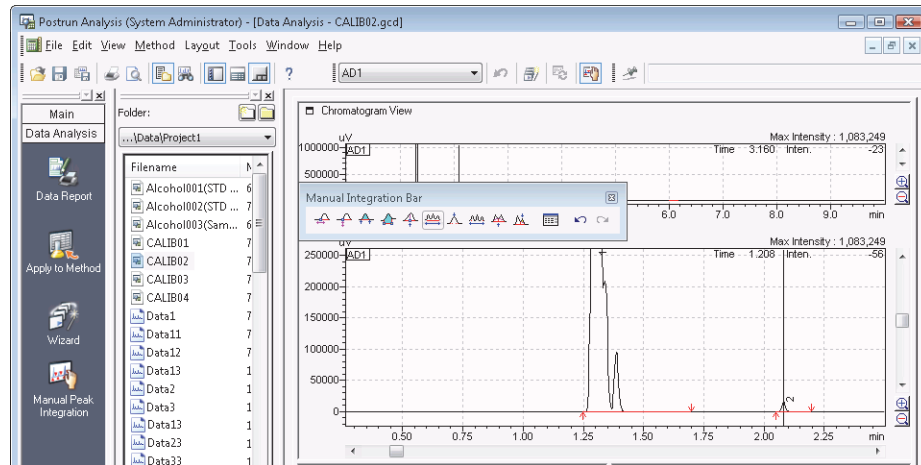
The screenshot shows the 'Manual Peak Integration' dialog box with the following data:

Peak#	Ret. Time	Area	Heig
1	1.305	3042883	10
2	1.388	118011	
3	2.082	16710	
4	2.743	17056	
5	3.672	16989	
6	4.816	18222	


Integration parameters:

- Width: 2 sec
- Slope: 200 uW/min
- Drift: 0 uW/min
- T. DBL: 1000 min

The peaks in the selected range are integrated and displayed as a single peak.



NOTE

- If a peak unification mistake is made, click the  (Undo) to undo the unification.
- Multiple peaks can also be integrated as a single peak by changing the [Width] value on the [Integration] tab.

Reference

Refer to Help for details on Width.

6

6.2.5 Remove Manual Peak Integration

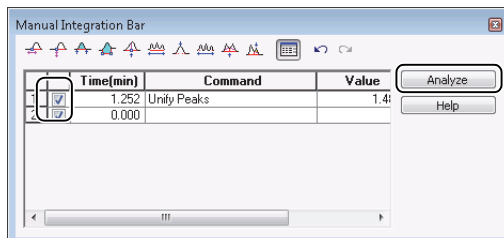
This section describes how to undo data that has undergone manual peak integration.

- 1 Click  (Toggle Manual Peak Integration Table) on [Manual Integration Bar].




The processing commands are displayed in the Time Program Table.

- 2 Deselect the manual integration commands, and click [Analyze].



The data returns to its previous state.

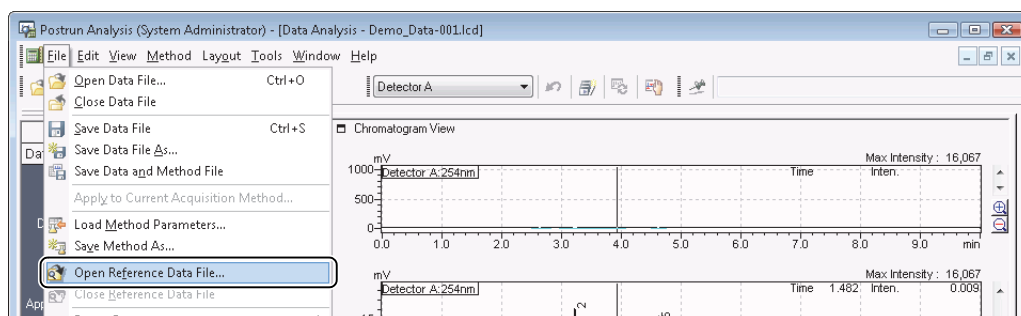
NOTE

- Data can also be returned to its previous state by clicking  (Toggle Manual Peak Integration Table).
- Selected Time Program Table rows can be deleted by pressing the keyboard [Delete] key.

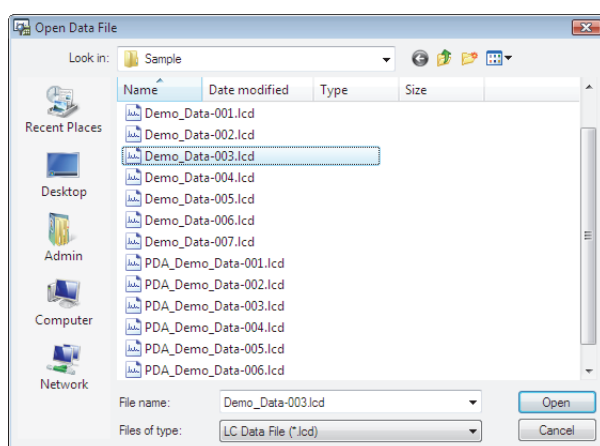
6.2.6 Overlay Data in the Analysis Sub-window

A reference data file can be opened on the current open data file and displayed as an overlay in the [Chromatogram View].

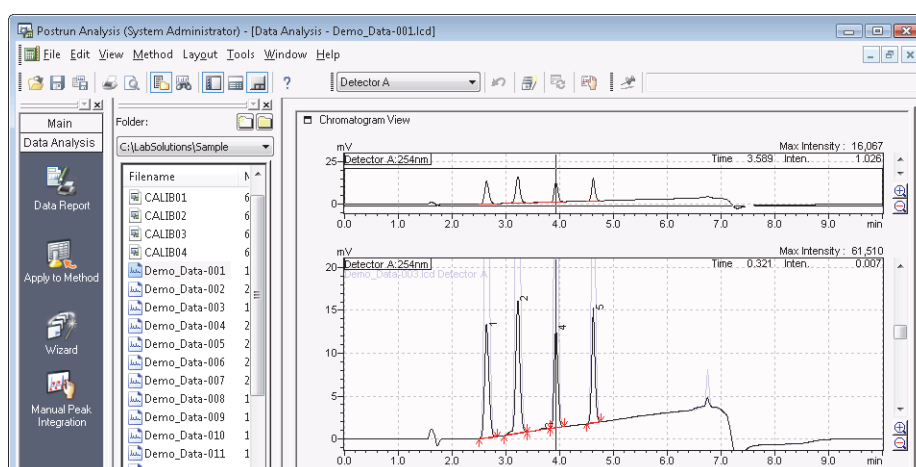
1 Select [Open Reference Data File] on the [File] menu.



2 Click the data file to display, and click [Open].



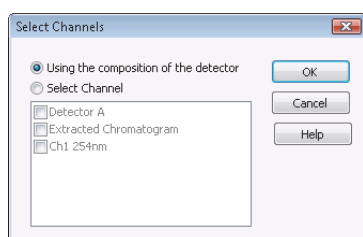
The chromatogram in the selected data file is displayed on the sub-window.



NOTE

- Up to 16 data files can be drawn overlaying each other as reference chromatograms.

- If the data file was obtained by data acquisition on multiple channels, the [Select Channels] sub-window opens to allow for proper chromatogram selection.



- To display the baseline of a reference chromatogram, right-click on the zoomed chromatogram, and select at [Graph Properties].

Reference


Refer to "6.1.2 [Data Analysis] Window Description" P.129 for details.

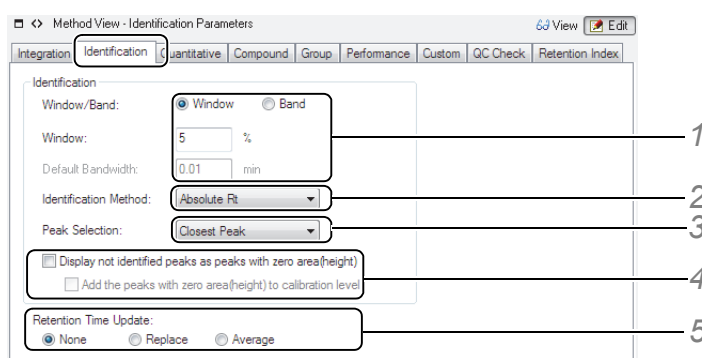
- The peak integration parameters for the reference chromatograms cannot be displayed or modified.

6.3 Peak Identification Parameters

6

This section describes how to set the allowable time width (window/band width) used for identifying peaks based on the Compound Table and which of the identification methods, absolute retention time method or relative retention time method is used.


- 1 Click  **Edit** (Edit Mode) in [Method View].
- 2 Click the [Identification] tab, and set each parameter.



- 1 Select either [Window] or [Band] at [Window/Band].
If [Window] is selected, enter [Window] in % units, and if [Band] is selected, enter [Default Band Time] in minutes.

Parameter	Contents
Window	The allowable time width for the peak top is set as a percentage (%) of the retention time. All peaks are calculated with the same window percentage. Allowable time width (min) = $\pm (\text{Compound Table retention time (min)} \times \text{window (\%)} + 0.02)$
Band	The allowable time width of the peak top is set as an absolute time. The allowable time width can be set to each peak in the Compound Table. Allowable time width (min) = $\pm \text{Default Band Time (min)}$

- 2 Select either [Absolute Rt] or [Relative Rt] as the peak identification method.

Parameter	Contents
Absolute Rt	Identifies target peaks from the retention time of each peak and their allowable times preset to the Compound Table.
Relative Rt	Compares the retention time of the sample peak to the retention time of the reference peak to compensate for retention time deviation caused by fluctuation of the data acquisition conditions. A reference peak must be set in the Compound Table.  Reference For details, see "6.5.4 Directly Edit the Compound Table" P.167.

- 3 Select the peak to identify from [All Peaks], [Closest Peak], and [Largest Peak].

Parameter	Contents
All Peaks	If multiple peaks fall within a single allowable time range, all peaks are identified as the target compound despite whether the Window method or Band method is set as the allowable time width setting method.
Closest Peak	If multiple peaks fall within a single allowable time range, only the peak closest to the retention time in the Compound Table is identified as the target compound, despite whether the Window method or Band method is set as the allowable time width setting method.
Largest Peak	If multiple peaks fall within a single allowable time range, only the peak with the largest peak area or height value is identified as the target compound, despite whether the Window method or Band method is set as the allowable time width setting method.
Similarity	[Similarity] can be selected when the photodiode array detector is used. The similarity between the spectrum at the retention time of the peaks in the allowable identification width and the standard spectrum registered in the Compound Table is calculated, and only the peak with the largest similarity value is identified as the target compound.

**NOTE**

If peak identification is based on internal standard substances or if peak identification is performed on reference substances, the peak having the maximum area or maximum height is automatically identified regardless of the [Peak Selection] setting.

- 4 Set [Display not identified peaks as peaks with zero area (height)].
If this checkbox is selected, the information of that compound is displayed at [Results View].
- 5 Set how the Compound Table retention time is automatically updated based on the retention time of an actually identified peak each time that data processing is performed on the standard sample.

Parameter	Contents
Replace	Replaces the retention time of each compound in the Compound Table with the retention time of the actually identified peak.
Average	Replaces the retention time with the value obtained by averaging the retention time of each compound in the Compound Table and the retention time of the actually identified peak.

3

- Click  (View Mode) in [Method View].

The data loaded in the [Data Analysis] window is reanalyzed according to the new parameter settings. Check the processing results in the [Chromatogram View] and [Results View].

6.4 Quantitative Parameters

This section describes how to set the quantitative parameters used to calculate the concentration values of the target peak.

Quantitative Processing	Reference
Quantitate by external standard method.	"6.4.1 External Standard Method" P.147
Quantitate by internal standard method.	"6.4.2 Internal Standard Method" P.149
Quantitate by standard addition method.	"6.4.3 Standard Addition Method" P.151
Calculate the percentage (%) of each component by corrected area normalization method.	"6.4.4 Corrected Area Normalization Method" P.153
Quantitate multiple compound peaks as a group	"6.4.5 Grouping" P.155
Make the calibration curve of the natural logarithmic axis	"6.4.6 Calibration Curve for Exponential Calculation" P.156
Correct the concentration value of a standard sample using the standard concentration factor.	"6.4.7 Standard Concentration Factor" P.157
Quantitate using the calibration curve of other components.	"6.4.8 Reference Standard ID and Correction Factor" P.158

6

6.4.1 External Standard Method

This method involves calculating concentrations from the peak area or height of unknown samples using a calibration curve based on a standard sample. This is the most frequently used quantitative calculation method.

Data acquisition is performed on a fixed volume of multiple concentrations of a standard solution that were prepared to bracket the anticipated concentration of the substance in the unknown sample.

A calibration curve is made using the absolute concentration of the standard solution (absolute amount) as the vertical axis and the respective peak area or height as the horizontal axis.

(The X- and Y-axes display can be changed using [X Axis Calib. Curve].)

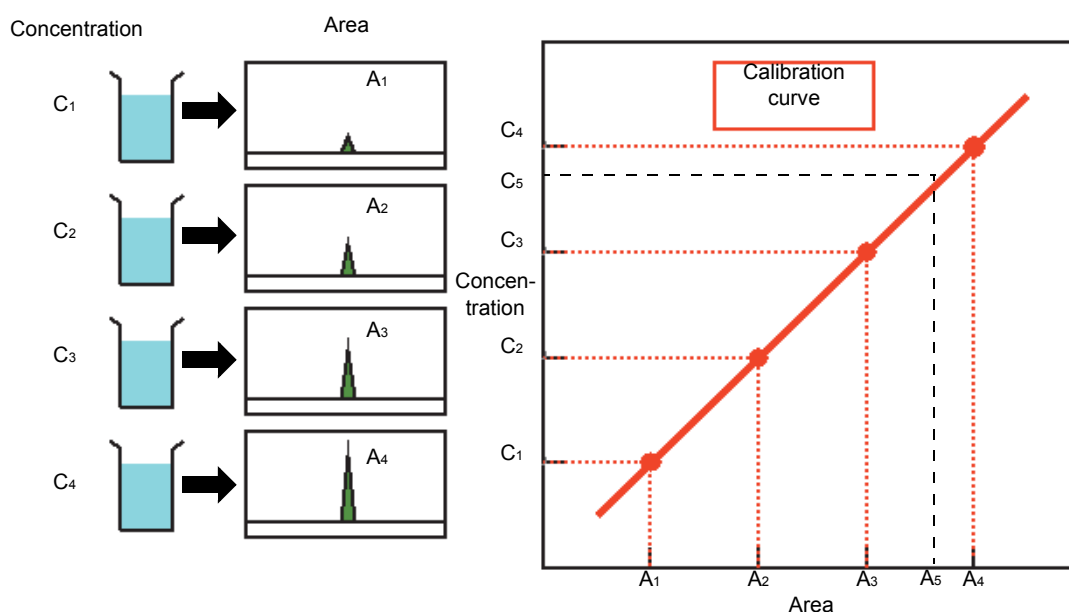



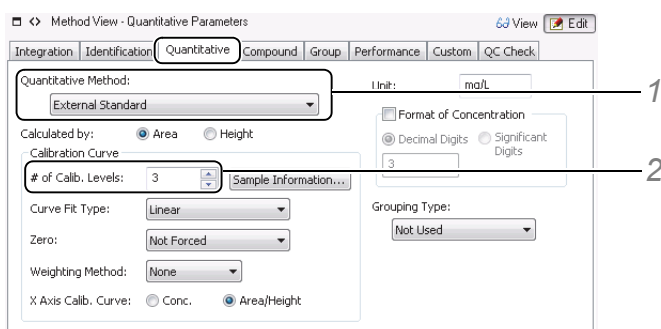
Fig.6-1 External Standard Method (Absolute Calibration Curve Method)

After the calibration curve is created, the same volume of the unknown sample solution is analyzed under the same conditions used to analyze the standard solutions.

The peak area or height (A5) of the unknown sample is determined and the concentration (C5) of the substance in the unknown sample can be calculated from the calibration curve.

This section describes how to quantitate using the “external standard method”.

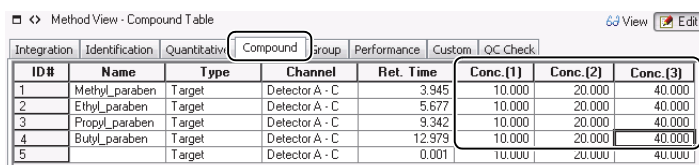
- 1 Click  **Edit (Edit Mode)** in **[Method View]**.
- 2 Click the **[Quantitative]** tab, and set each parameter.



- 1 Select **[External Standard]** for the **[Quantitative Method]**.
- 2 Enter the number of concentration levels (calibration points) at **[# of Calib. Levels]**.

- 3 Click the **[Compound]** tab, and enter the concentration for each of the standard samples in the **[Conc. (1)]**, **[Conc. (2)]** and **[Conc. (3)]** columns.

This example uses a 3-point calibration curve.




ID#	Name	Type	Channel	Ret. Time	Conc.(1)	Conc.(2)	Conc.(3)
1	Methyl_paraben	Target	Detector A - C	3.945	10.000	20.000	40.000
2	Ethyl_paraben	Target	Detector A - C	5.677	10.000	20.000	40.000
3	Propyl_paraben	Target	Detector A - C	9.342	10.000	20.000	40.000
4	Butyl_paraben	Target	Detector A - C	12.979	10.000	20.000	40.000
5		Target	Detector A - C	0.001	10.000	20.000	40.000



NOTE

[Not Used] is displayed if the concentration cell is selected and the keyboard [Delete] key is pressed or if “-1” is entered in the cell.

Use this method when separate standard samples are prepared for individual target components.

- 4 Click  **(View Mode)** in **[Method View]**.
- 5 Save the method file before creating the calibration curve.

Reference

For details on how to make calibration curves, refer to *"4 Realtime Batch" P.63* or *"5 Calibration Curves" P.113*.

6.4.2 Internal Standard Method

This highly precise method involves performing quantitative calculation with an area ratio or height ratio to correct for injection volume errors.

The internal standard (ISTD) substance should be a stable compound that separates completely from other peaks in the sample, has a similar chemical nature and elutes near the substance to be quantitated.

The standard solutions are prepared with 1 or more known concentrations of the target substance (“X” from here on) and a specified concentration of the internal standard substance (“ISTD” from here on). Then data acquisition is performed on fixed amounts of these standard solutions.

A calibration curve is created using the ratio of “X concentration/ISTD concentration” in the standard solution as the vertical axis and the ratio of “peak area of X/peak area of ISTD” as the horizontal axis. (The X- and Y-axes display can be changed using [X Axis Calib. Curve].)

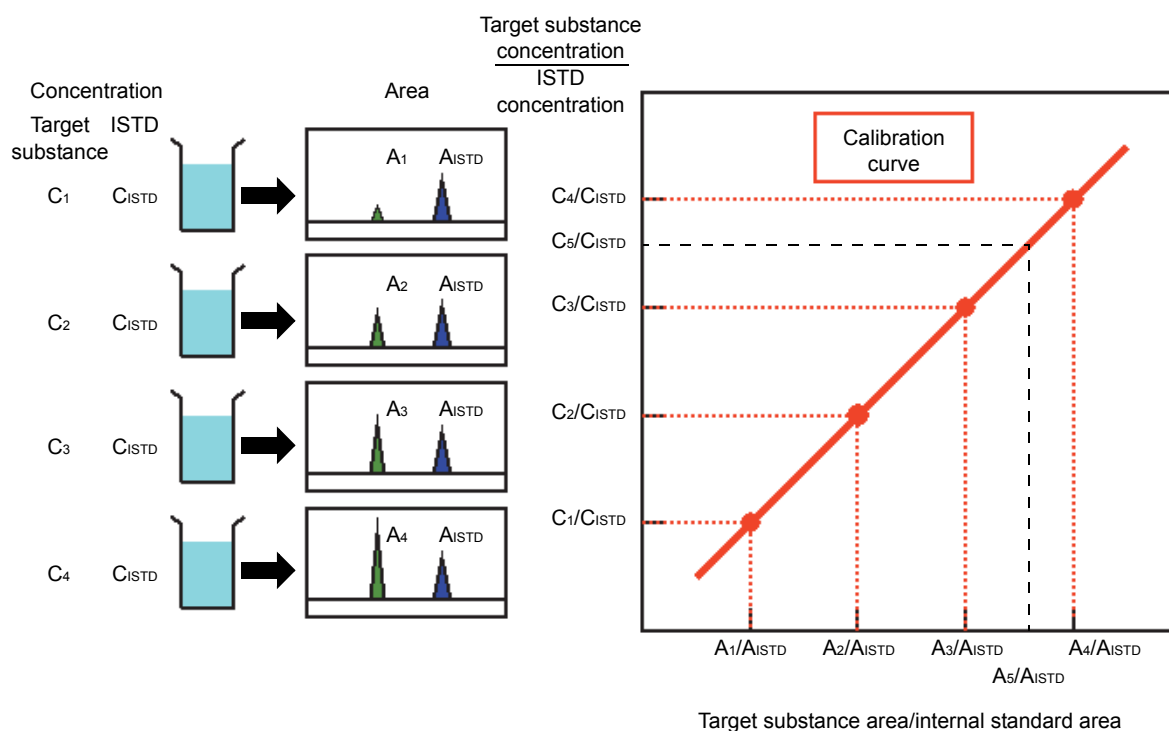


Fig.6-2 Internal Standard Method

A sample solution is prepared by spiking the unknown sample with the same concentration of ISTD as was used in the standard solution preparation. Data acquisition is performed on the same volume of unknown sample solution under the same conditions used to analyze the standard solutions.

The peak area ratio between X and ISTD (A₅/A_{1STD}) for the unknown sample is calculated and the concentration ratio (C₅/C_{ISTD}) is calculated from the calibration curve.

This section describes how to quantitate using the “internal standard method”.

1

Click  Edit (Edit Mode) in [Method View].

6

2 Click the [Quantitative] tab, and set each parameter.

- 1 Select [Internal Standard] for the [Quantitative Method].
- 2 Enter the number of concentration levels (calibration points) at [# of Calib. Levels].

3 Click the [Compound] tab, and set the [Type], [Conc.], and [ISTD Group] for each compound.

This example uses the following calibration curve parameters.

ID#	Name	Type	Channel	Ret. Time	Conc.[1]	Conc.[2]	Conc.[3]	ISTD Group
1	PeakA	ISTD	Detector A - C	3.945	1.000	1.000	1.000	1
2	PeakB	Target	Detector A - C	5.677	1.000	2.000	4.000	1
3	PeakC	ISTD	Detector A - C	9.342	1.000	1.000	1.000	2
4	PeakD	Target	Detector A - C	12.979	1.000	2.000	4.000	2

Make a calibration curve using 3 concentrations of standard solution:

- Peak A: ISTD
- Peak B: Target substance. Quantitated using Peak A.
- Peak C: ISTD
- Peak D: Target substance. Quantitated using Peak C.

NOTE

- The ISTD concentration values are used to calculate the calibration curve as the ISTD amount.
- If multiple ISTDs are used, number the substances in the [ISTD Group] column so that the ISTDs corresponding to the target substance are in the same ISTD group.

4 Click (View Mode) in [Method View].

NOTE

- The amount of ISTD in the standard sample is entered in the Compound Table. The amount of ISTD in unknown samples is entered in the Batch Table and in single run. Refer to "[4.6.2 Edit Batch Tables](#)" P.101 for details on entering the ISTD amount.
- To make a calibration curve with multiple calibration points (levels) add equivalent amounts of ISTD to standard solutions of different concentrations. If the standard solution is spiked with the ISTD before it is diluted, only a 1-point calibration curve is created.
- Prepare standard sample solutions by diluting a stock solution in stages to achieve multiple concentrations of the target substance. Prepare the unknown sample solution at the appropriate concentration. Spike all of the diluted standard samples and the unknown sample with equal amounts of the ISTD.

When the unknown sample is spiked with the same amount of ISTD as the standard solution, quantitative calculation can be performed by comparing the sample amount and ISTD amount with all levels of the ISTD concentration fields set to "1".

5 Save the method file before creating the calibration curve.

Reference

For details on how to make calibration curves, see ["4 Realtime Batch" P.63](#) or ["5 Calibration Curves" P.113](#).

6.4.3 Standard Addition Method

This method involves analyzing an unknown sample that has been spiked with a known amount of the target substance and an unspiked unknown sample. Quantitation is performed using the difference between the measured peak areas or heights.

Equivalent aliquots of the same unknown sample solution are prepared. One aliquot remains unspiked and the other aliquots are spiked with differing known concentrations of the target substance. All of the unknown sample solutions are analyzed and the results are used to quantitatively calculate the amount of target substance in the unspiked unknown sample. The calibration curve created with the spiked amount of substance (concentration) as the horizontal axis and peak area or height as the vertical axis.

This method is often used in situations where the components of unknown sample matrix compromise the sensitivity of the target substance.

The sample solution (source solution) is divided into several equal parts, and each part is spiked with standard solution and used for data acquisition.

(Example C1: unspiked, C2: 1.0 mg/L, C3: 2.0 mg/L)

The calibration points of the peak area (A1, A2, A3) and spiked amount (0, 1.0 mg/L, 2.0 mg/L) from the data acquisition results, are used to make a 3-point calibration curve (linear).

The absolute value where the calibration curve intersects the X-axis (point of intersection - C4) indicates the concentration (X) of the target component.

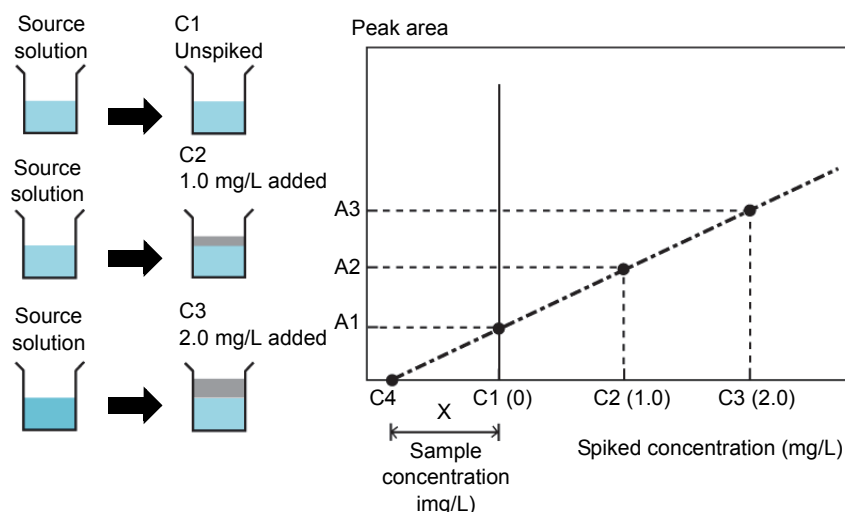
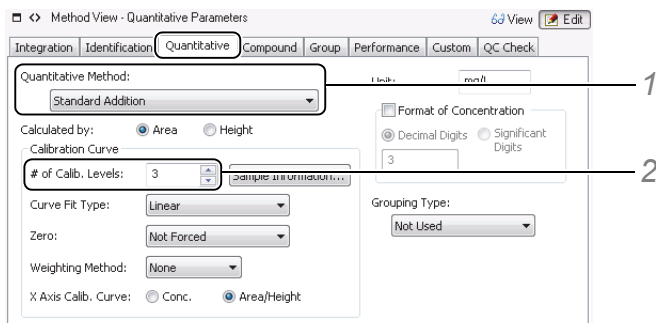


Fig.6-3 Standard Addition Method

This section describes how to quantitate using “standard addition method”.

1 Click  **Edit** (**Edit Mode**) in **[Method View]**.

2 Click the **[Quantitative]** tab, and set each parameter.



1 Select **[Standard Addition]** for the **[Quantitative Method]**.

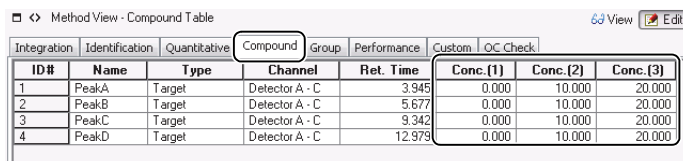
2 Enter the number of concentration levels (calibration points) at **[# of Calib. Levels]**.

 **NOTE**

The unspiked sample is one calibration point and 2 spiked samples are used, making the number of calibration points, 3. (1 unspiked sample + 2 spiked samples = 3). Therefore, set the number of levels to “3”.

3 Click the **[Compound]** tab, and enter the **[Conc.]** of the standard sample.

This example uses the following calibration curve parameters.



ID#	Name	Type	Channel	Ret. Time	Conc.[1]	Conc.[2]	Conc.[3]
1	PeakA	Target	Detector A - C	3.945	0.000	10.000	20.000
2	PeakB	Target	Detector A - C	5.677	0.000	10.000	20.000
3	PeakC	Target	Detector A - C	9.342	0.000	10.000	20.000
4	PeakD	Target	Detector A - C	12.978	0.000	10.000	20.000

- Level 1: Unspiked sample “concentration = 0”
- Level 2: 10 mg/L spiked sample
- Level 3: 20 mg/L spiked sample

 **NOTE**

- Enter “0” for **[Conc. (1)]** since it is used for the unspiked sample calibration point.
- Set **[Type]** to standard for the unspiked and all of the spiked samples, and perform data acquisition using the method file saved above. (Perform post-run batch analysis if the data has already been acquired.)
Then, change **[Type]** to **[Unknown]** for only the unspiked sample, and reprocess the data using the using the method file that contains this calibration curve to obtain the quantitative results.

4 Click  **View** (**View Mode**) in **[Method View]**.

6.4.4 Corrected Area Normalization Method

This method involves, first, correcting the peak area or height of each component peak in an unknown sample and totaling these values. The percentage of the corrected area or height for each component with is calculated with respect to that total value is assumed to be the quantitative value.

This section describes how to obtain the sensitivity correction factor using a standard sample of known concentration and how to perform quantitation by the “corrected area normalization” method by manually entering that sensitivity correction factor.




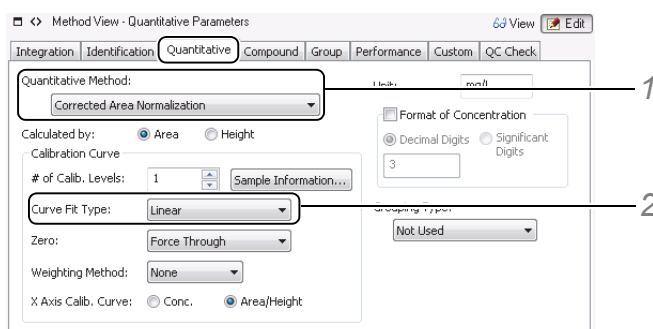
NOTE

With corrected area normalization, the percentage of the area or height value of all detected peaks is assumed to be the quantitative value.

■ Sensitivity Correction Factor Using a Standard Sample

This section describes use of a mixed sample as the standard sample.

- 1 Click  **Edit** (Edit Mode) in [Method View].
- 2 Click the [Quantitative] tab, and set each parameter.



- 1 Select [Corrected Area Normalization] for the [Quantitative Method].
- 2 Select [Linear] for the [Curve Fit Type].

- 3 Enter the concentration in the [Conc.(1)] cell for each compound in the [Compound] tab.

ID#	Name	Type	Channel	Ret. Time	Conc.(1)
1	PeakA	Target	Detector A - C	3.945	20.000
2	PeakB	Target	Detector A - C	5.677	20.000
3	PeakC	Target	Detector A - C	9.342	20.000
4	PeakD	Target	Detector A - C	12.979	20.000

- 4 Click  **View** (View Mode) in [Method View].




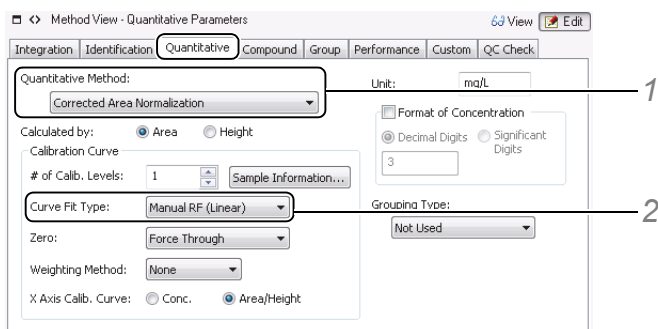
NOTE

Refer to *"5.1 Calibration Curves by Postrun Batch"* and use the standard sample data to make a calibration curve. The 1st coefficient obtained is the sensitivity correction factor.

■ Enter the Sensitivity Correction Factor

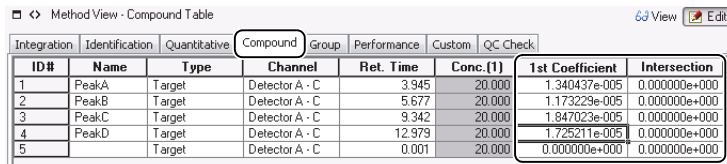
This section describes how to manually enter the sensitivity correction factor if it is known.

- 1 Click  **Edit (Edit Mode)** in [Method View].
- 2 Click the [Quantitative] tab, and set each parameter.



- 1 Select [Corrected Area Normalization] for the [Quantitative Method].
- 2 Select [Manual RF (Linear)] for the [Curve Fit Type].

- 3 Enter the sensitivity correction factor in the [1st Coefficient] cell for each compound in the [Compound] tab.



ID#	Name	Type	Channel	Ret. Time	Conc.(1)	1st Coefficient	Intersection
1	PeakA	Target	Detector A - C	3.945	20.000	1.340437e-005	0.000000e+000
2	PeakB	Target	Detector A - C	5.677	20.000	1.173229e-005	0.000000e+000
3	PeakC	Target	Detector A - C	9.342	20.000	1.847023e-005	0.000000e+000
4	PeakD	Target	Detector A - C	12.979	20.000	1.725211e-005	0.000000e+000
5		Target	Detector A - C	0.001	20.000	0.000000e+000	0.000000e+000


- 4 Click  **View (View Mode)** in [Method View].

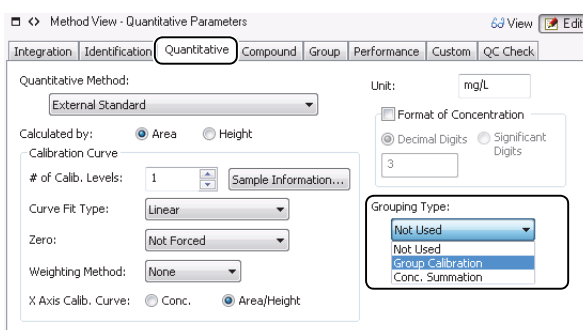
6.4.5 Grouping

Bundling homologs or isomers when there are multiple compounds is called “grouping”.

Grouping is effective in dividing the peaks into groups to perform quantitative analysis only on individual groups or when measuring the amount of impurities in a certain main component as a single group.

This section describes how to perform grouping quantitation.

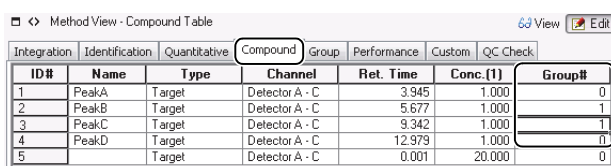
- 1 Click  **Edit** (**Edit Mode**) in **[Method View]**.
- 2 Click the **[Quantitative]** tab, and select **[Group Calibration]** or **[Conc. Summation]** for the **[Grouping Type]**.



NOTE

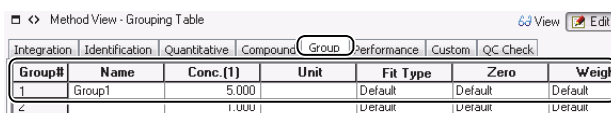
- The sum of the peak areas or heights of the grouped compounds is used with [Group Calibration], a calibration curve is created for each group, and quantitation is performed for each group.
- A calibration curve is created for each compound and quantitation is performed for each compound, with [Conc. Summation]. Then the sum of the concentrations of the grouped compounds is used as the concentration of the group.

- 3 Click the **[Compound]** tab, and enter the same group number in the **[Group#]** column of all of the compounds in a group.



ID#	Name	Type	Channel	Ret. Time	Conc.(1)	Group#
1	PeakA	Target	Detector A - C	3.945	1.000	1
2	PeakB	Target	Detector A - C	5.677	1.000	1
3	PeakC	Target	Detector A - C	9.342	1.000	1
4	PeakD	Target	Detector A - C	12.979	1.000	1
5		Target	Detector A - C	0.001	20.000	1

- 4 Click the **[Group]** tab, and enter **[Name]**, **[Conc.]**, and **[Unit]**.




Group#	Name	Conc.(1)	Unit	Fit Type	Zero	Weight
1	Group1	5.000	mg/L	Default	Default	Default
2		1.000		Default	Default	Default

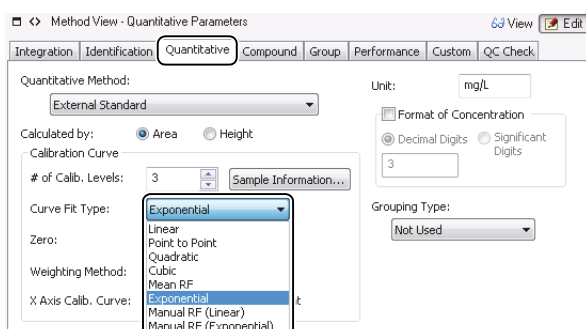
- 5 Click  **View** (**View Mode**) in **[Method View]**.

6.4.6 Calibration Curve for Exponential Calculation

Since the sample concentration and sensitivity are not directly proportional when using an LC-ELSD detector or the GC-FPD detector S mode, make a calibration curve using the exponential function.

This section describes how to perform quantitative calculation using a calibration curve calculated from the exponential function.

- 1 Click  **Edit** (**Edit Mode**) in **[Method View]**.
- 2 Click the **[Quantitative]** tab, and select **[Exponential]** for the **[Curve Fit Type]**.



NOTE

- At least 2 standard samples (i.e. 2 calibration points) are required to create a calibration curve with the exponential calculation. Select 2 or higher at **[# of Calb. Levels]**.
- **[Zero]** cannot be set for the exponential calibration curve since the curve does not pass through the origin.
- Both of the axes of the graph for the exponential calibration curve are logarithmic.

- 3 Click the **[Compound]** tab, and enter the **[Conc.](s)**.


ID#	Name	Type	Channel	Ret. Time	Conc.[1]	Conc.[2]	Conc.[3]
1	PeakA	Target	Detector A - C	3.945	1.000	10.000	1000.000
2	PeakB	Target	Detector A - C	5.677	1.000	10.000	1000.000
3	PeakC	Target	Detector A - C	9.342	1.000	10.000	1000.000
4	PeakD	Target	Detector A - C	12.978	1.000	10.000	1000.000

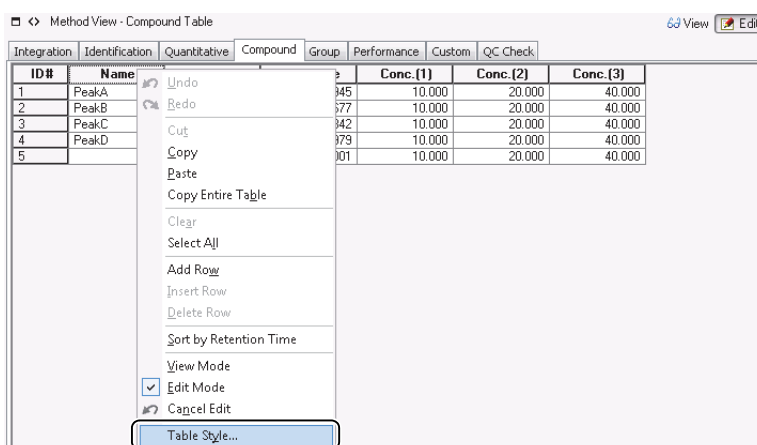
- 4 Click  **View** (**View Mode**) in **[Method View]**.

6.4.7 Standard Concentration Factor

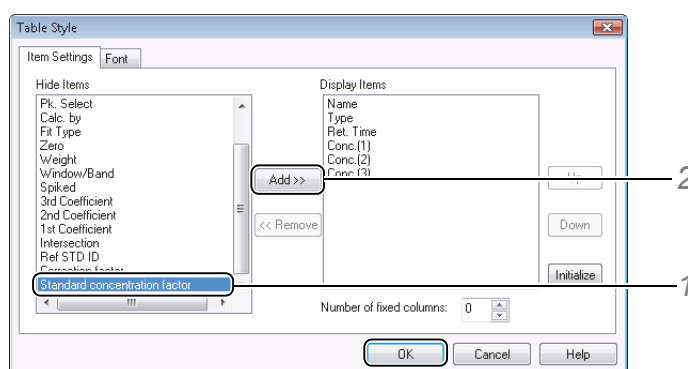
Make a calibration curve using values obtained by multiplying concentration values of each level with compensation factors.

This section describes how to set the standard concentration factor.

- 1 Click  **Edit** (**Edit Mode**) in **[Method View]**.
- 2 Click the **[Compound]** tab.
- 3 Right-click on the **Compound Table**, and click **[Table Style]**.



- 4 Add the **[Standard concentration factor]** column to the **Compound Table** in the **[Table Style]** sub-window, and click **[OK]**.

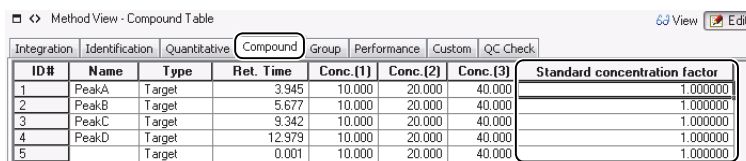


- 1 Select **[Standard concentration factor]** in the **[Hide Items]** list.
- 2 Click **[Add]**.
The **[Standard concentration factor]** item is added to **[Display Items]** list.

NOTE

Change the display order of items in the **Compound Table**, by selecting the item in the **[Display Items]** list and then clicking **[Up]** or **[Down]**.

5 Enter the [Standard concentration factor] column.



ID#	Name	Type	Ret. Time	Conc. (1)	Conc. (2)	Conc. (3)	Standard concentration factor
1	PeakA	Target	3.945	10.000	20.000	40.000	1.000000
2	PeakB	Target	5.677	10.000	20.000	40.000	1.000000
3	PeakC	Target	9.342	10.000	20.000	40.000	1.000000
4	PeakD	Target	12.979	10.000	20.000	40.000	1.000000
5		Target	0.001	10.000	20.000	40.000	1.000000

6 Click (View Mode) in [Method View].

6.4.8 Reference Standard ID and Correction Factor

If standards cannot be prepared for impurities or related substances, create a calibration curve using a standard substance with the same (or proportional) response factor, and quantitate the concentration of the impurities or related substances using that calibration curve.



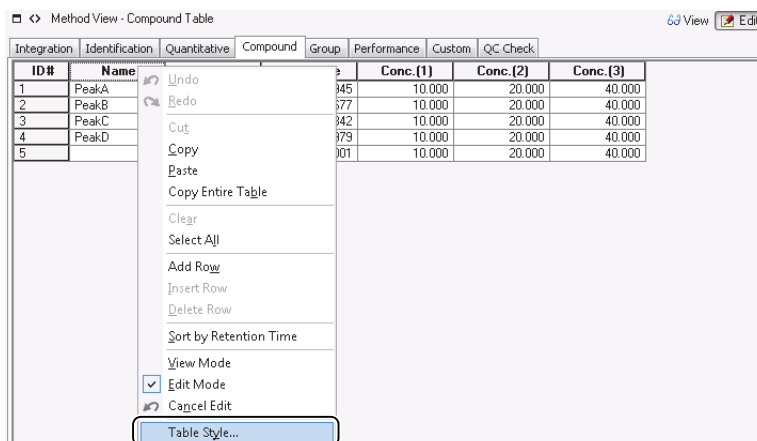
NOTE

Use the value obtained by multiplying the peak area or height or the peak area or height ratio of the internal standard by the correction factor, to create the reference standard calibration curve specified by ID.

1 Click (Edit Mode) in [Method View].

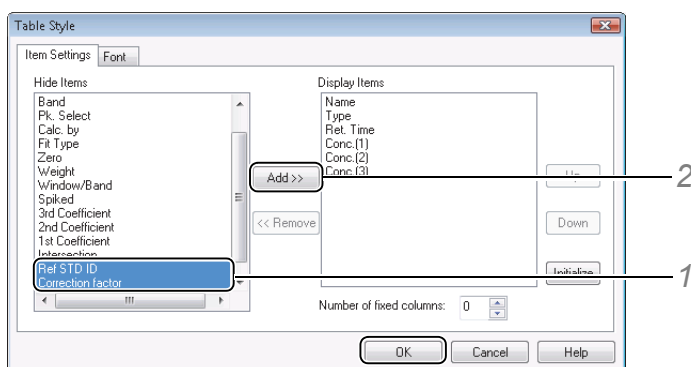
2 Click the [Compound] tab.

3 Right-click on the Compound Table, and click [Table Style].



ID#	Name	Conc. (1)	Conc. (2)	Conc. (3)
1	PeakA	345	10.000	20.000
2	PeakB	377	10.000	20.000
3	PeakC	342	10.000	20.000
4	PeakD	379	10.000	20.000
5		301	10.000	20.000

4 Add the [Ref STD ID] and the [Correction factor] column to the Compound Table in the [Table Style] sub-window, and click [OK].



- 1 Select [Ref STD ID] and [Correction factor] in the [Hide Items] list.
- 2 Click [Add].
The [Ref STD ID] and [Correction factor] item are added to the [Display Items] list.



NOTE

Change the display order of items in the Compound Table, by selecting the item in the [Display Items] list and then clicking [Up] or [Down].

5 Enter the [Ref STD ID] and [Correction factor] column.

Method View - Compound Table

ID#	Name	Type	Ret. Time	Conc.(1)	Conc.(2)	Conc.(3)	Ref STD ID	Correction factor
1	PeakA	Target	3.945	10.000	20.000	40.000	2	0.9538600
2	PeakB	Target	5.677	10.000	20.000	40.000		1.0000000
3	PeakC	Target	9.342	10.000	20.000	40.000	2	0.8648200
4	PeakD	Target	12.979	10.000	20.000	40.000		1.0000000
5		Target	0.001	10.000	20.000	40.000		1.0000000

6 Click (View Mode) in [Method View].

6.5 Compound Table

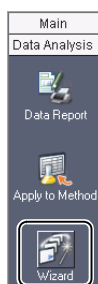
The Compound Table must be completed to identify detected peaks or to perform quantitative calculation on the detected peaks. There are various ways of entering data into the Compound Table. Use the method that is the most convenient.

- ["Compound Table Wizard"](#)
- ["Compound Table from the Peak Table"](#)
- ["Compound Table Retention Times Using the Mouse"](#)
- ["Directly Edit the Compound Table"](#)

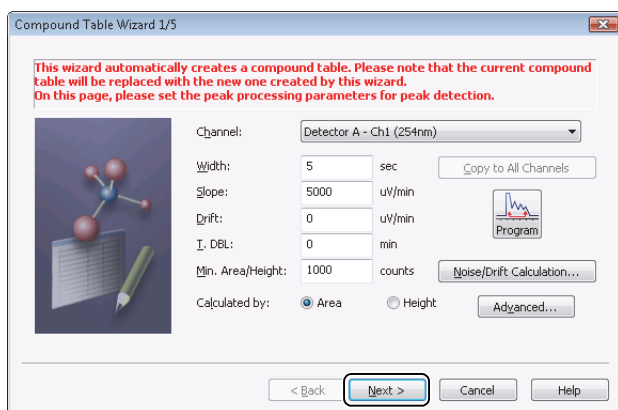
6.5.1 Compound Table Wizard

This section describes how to complete a Compound Table using the wizard. Using the wizard also allows the peak integration, peak identification, and quantitative parameters to be entered in the consecutive sub-windows.

- 1 Click the  (Wizard) icon on the [Data Analysis] assistant bar.



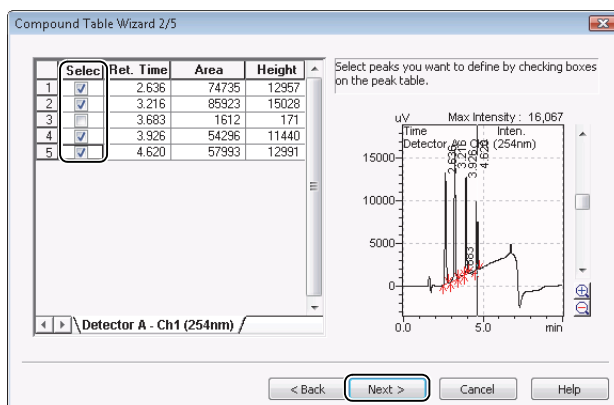
- 2 Enter the peak integration parameters, and click [Next].



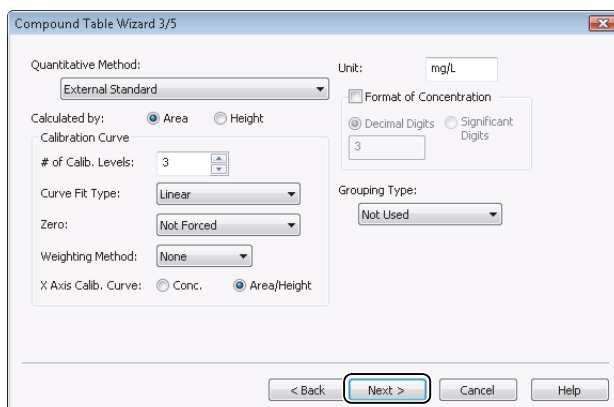
Reference

Refer to ["6.2 Peak Integration Parameters" P.132](#) for details on setting the peak integration parameters.

3 Select the [Select] column to register a peak in the Compound Table, and click [Next].



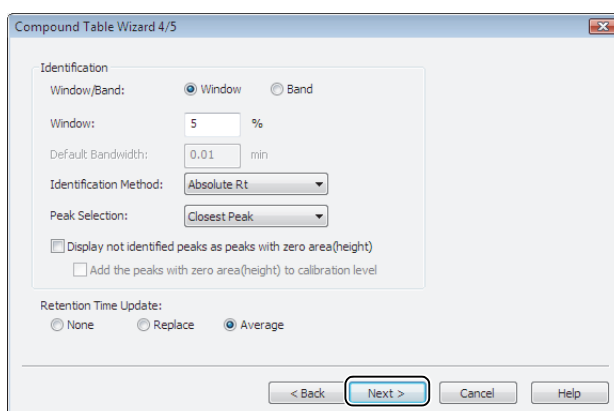
4 Enter the quantitative parameters, and click [Next].



Reference

Refer to ["6.4 Quantitative Parameters" P.147](#) for details on setting the quantitative parameters.

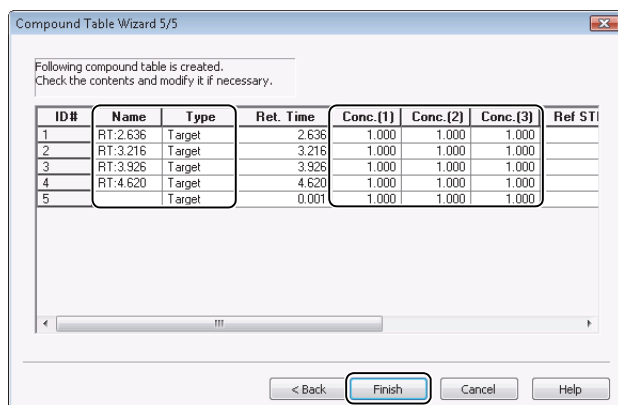
5 Enter the peak identification parameters, and click [Next].



Reference

Refer to ["6.3 Peak Identification Parameters" P.145](#) for details on setting the peak identification parameters.

6 Enter the [Name], [Type] and [Conc.] column in the Compound Table, and click [Finish].



NOTE

- The default [Name] is "RT (Retention Time) + peak retention time".
- Edit the Compound Table to match the parameters set in quantitative processing.

The settings made in the wizard are saved to the data processing parameters in the open data file.

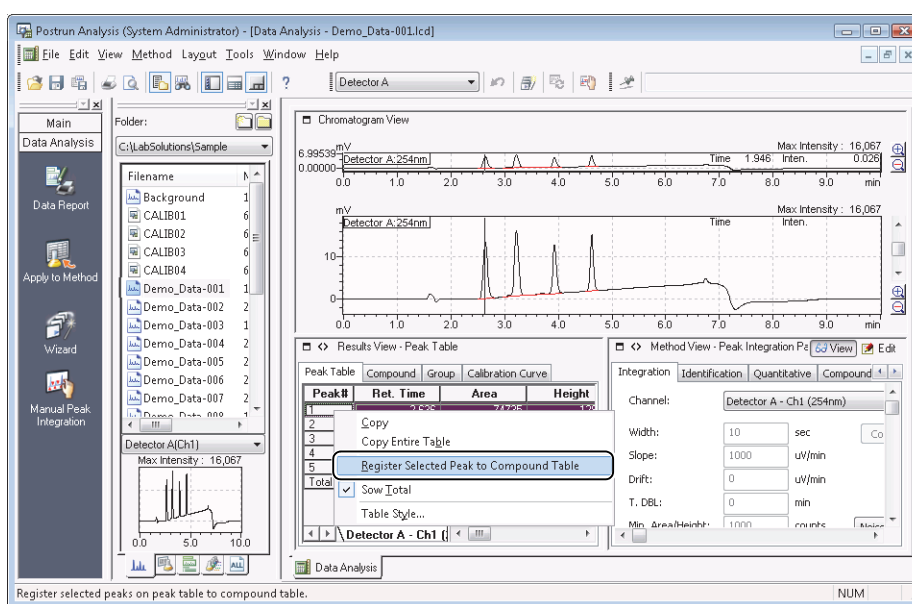
Reference

- Refer to ["6.7 Save \(Export\) to Method Files" P.171](#) to save settings made in the wizard to method file.
- Refer to ["5 Calibration Curves" P.113](#) for details on creating calibration curves.

6.5.2 Compound Table from the Peak Table

Peaks displayed in [Chromatogram View] can be registered to the [Compound] tab in [Method View]. This section describes how to register peaks in [Chromatogram View] to the Compound Table.

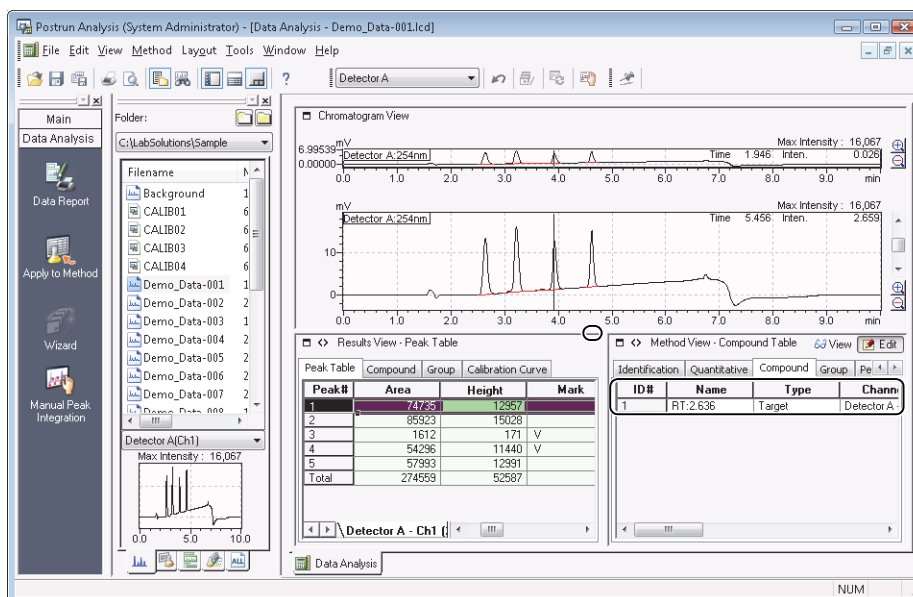
- 1 Click the [Peak Table] tab in [Results View].
- 2 Right-click [Peak#] for the desired peak, and click [Register Selected Peak to Compound Table].



The selected peaks in the Peak Table are registered to the Compound Table.

- 3 Click the [Compound] tab in [Method View].

4 Enter [Name] and [Conc.] of the registered peak in the Compound Table.



Click the (Wide Size) button to maximize the view width. Click the (Normal Size) button to restore the view size.

The close-up shows the "Method View - Compound Table" with the following data:

ID#	Name	Type	Channel	Ret. Time	Conc. [1]	Conc. [2]
1	RT:2.636	Target	Detector A - C	2.636	10.000	20.000


5 Click (View Mode) in [Method View].

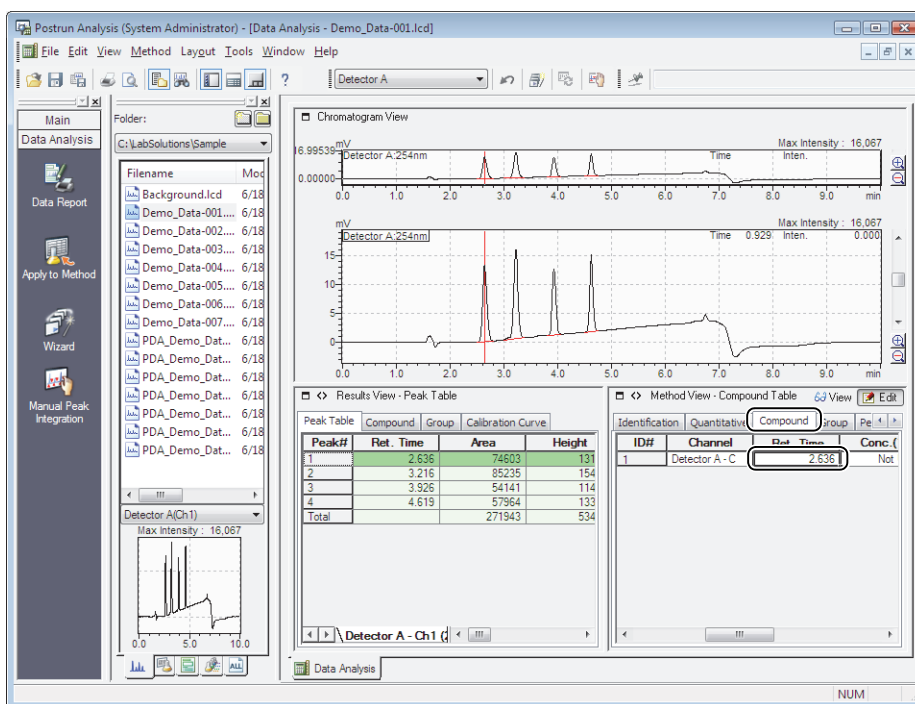
Reference

- Refer to "6.7 Save (Export) to Method Files" P.171 for details on saving to the method file.
- Refer to "5 Calibration Curves" P.113 For details on creating calibration curves.

6.5.3 Compound Table Retention Times Using the Mouse

Retention times in the Compound Table can be easily set with the mouse in [Chromatogram View].

- 1 Click  **Edit** (Edit Mode) in [Method View].
- 2 Click the [Compound] tab, and select the desired [Ret. Time] cell.

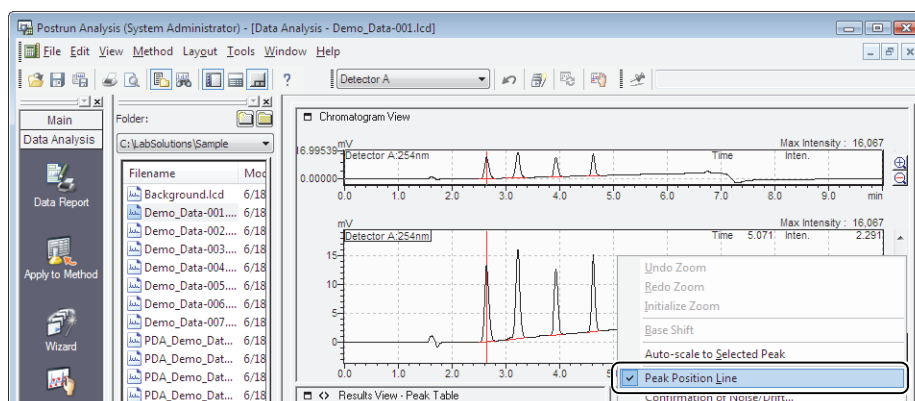


The peak position lines are displayed in red in the [Chromatogram View].



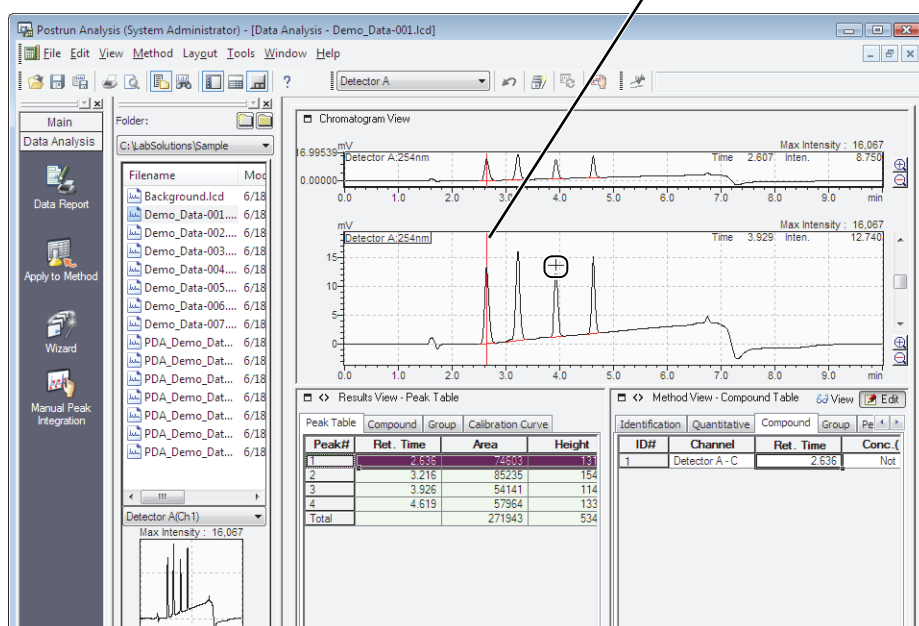
NOTE

Right-click on the chromatogram, and if [Peak Position Line] on the displayed menu is not selected, select [Peak Position Line] to display the peak position line.

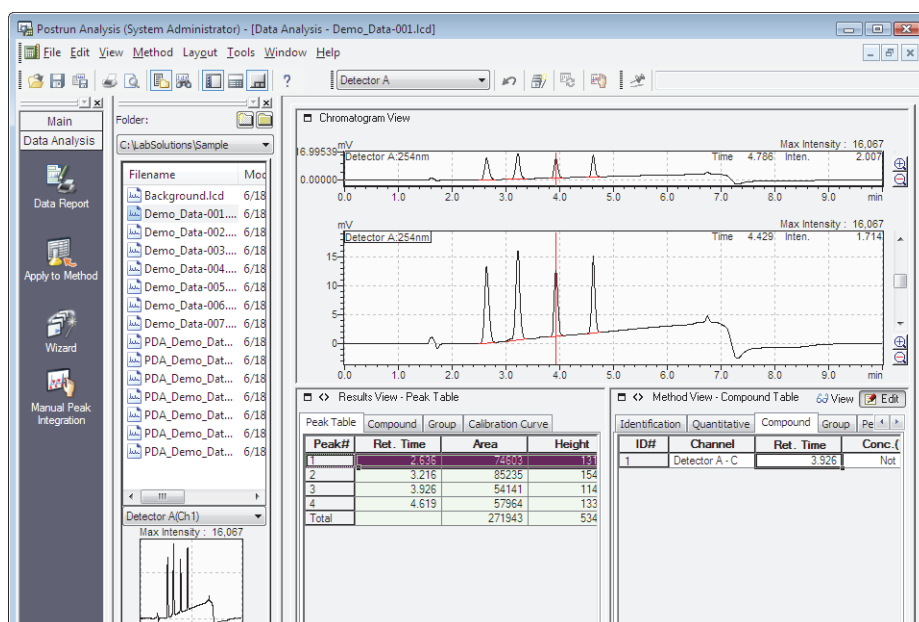


3 Select the peak whose retention time is to be changed.

Display position check line



The retention time change is automatically registered to the Compound Table.



NOTE

Fine-adjust the peak position line by dragging the line with the [Shift] key held down.

4 Click (View Mode) in [Method View].

Reference

- Refer to "6.7 Save (Export) to Method Files" P.171 for details on saving to the method file.
- Refer to "5 Calibration Curves" P.113 for details on creating calibration curves.


6.5.4 Directly Edit the Compound Table

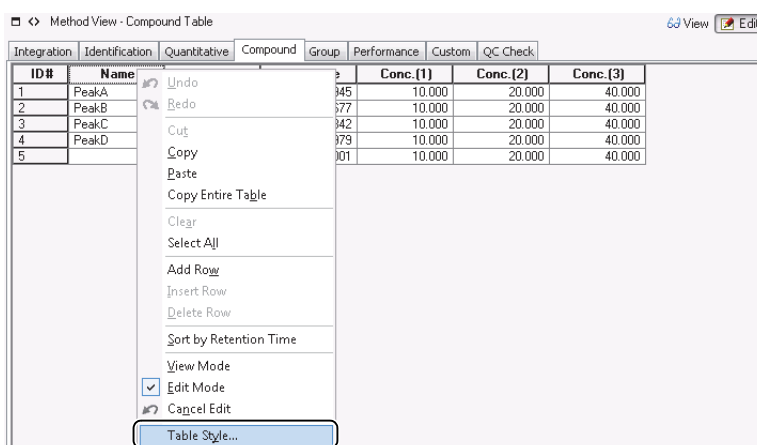
Click the target compound cell to edit a cell in the Compound Table.

This section describes how to select the Window/Band method and compound type.

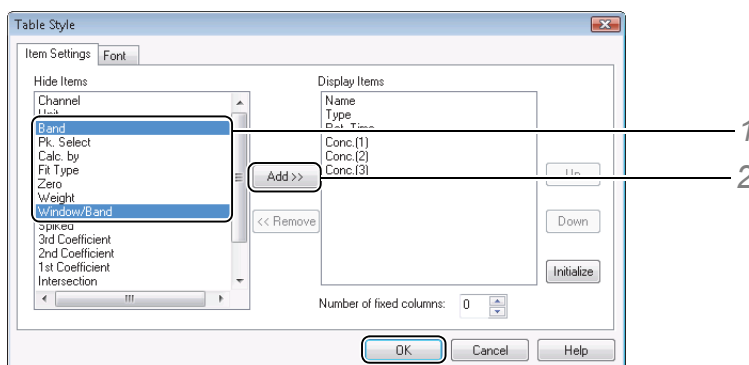
■ Select the Window/Band Method for Each Compound

The identification method set on the [Identification] tab in [Method View] is used for all of the compounds. It can also be set to each compound in the Compound Table.

- 1 Click  **Edit** (Edit Mode) in [Method View].
- 2 Click the [Compound] tab.
- 3 Right-click on the Compound Table, and click [Table Style].



- 4 Add the [Window/Band] and the [Band] column to the Compound Table in the [Table Style] sub-window, and click [OK].



- 1 Select [Window/Band] and [Band] in the [Hide Items] list.
- 2 Click [Add].
The [Window/Band] and the [Band] item are added to the [Display Items] list.

NOTE

Change the display order of items in the Compound Table, by selecting the item in the [Display Items] list and then clicking [Up] or [Down].

5 Set [Window/Band] and [Band] parameters.

ID#	Ret. Time	Conc.(1)	Conc.(2)	Conc.(3)	Window/Band	Band
1	2.636	10.000	20.000	40.000	Band	2.000
2	3.216	10.000	20.000	40.000	Default	Default
3	3.926	10.000	20.000	40.000	Default	Default
4	4.620	10.000	20.000	40.000	Window	Default
5	0.001	10.000	20.000	40.000	Band	Default

- 1 Click the [Window/Band] cell for the desired compound, and select [Default], [Window] or [Band].
- 2 Enter the allowable time width in the [Band] cell, if [Band] is selected.

NOTE

If [Window/Band] is set to [Default], the value set on the [Identification] tab is used.

6 Click View (View Mode) in [Method View].

Reference

- Refer to "6.7 Save (Export) to Method Files" P.171 for details on saving to the method file.
- Refer to "5 Calibration Curves" P.113 for details on creating calibration curves.

■ Compound Type

This section describes how to set the reference compound for peak identification using the relative retention time method.

1 Click Edit (Edit Mode) in [Method View].

2 Click the [Compound] tab, and select the [Type].

Click the [Type] cell of the desired compound, and select [Reference].

NOTE

Use this method to set the ISTD as the reference for the internal standard method. Click the [Type] cell of the ISTD, and select [ISTD & Ref.].

ID#	Name	Type	Ret. Time	Conc.(1)	Conc.(2)	Conc.(3)	Wi
1	PeakA	Label	2.636	10.000	20.000	40.000	Bar
2	PeakB	Label	3.216	10.000	20.000	40.000	Def
3	PeakC	ISTD	3.926	10.000	20.000	40.000	Def
4	PeakD	Reference	4.620	10.000	20.000	40.000	Def
5		ISTD&Ref.	0.001	10.000	20.000	40.000	Def

3 Click View (View Mode) in [Method View].

NOTE

If changes are made to the parameters such as [Type] on the [Compound] tab, the calibration curve will change. In this case, the current calibration curve information saved in the data file is automatically deleted.

Reference

- Refer to "6.7 Save (Export) to Method Files" P.171 for details on saving to the method file.
- Refer to "6.7 Save (Export) to Method Files" P.171 for details on creating calibration curves.

6.6 Column Performance Parameters

This section describes how to set the various calculation methods for supporting the system suitability test and how to check calculation results.

- USP
- USP2
- JP
- JP2
- EP
- BP
- DAB
- EMG
- EMG (50%)
- area/height
- user-defined

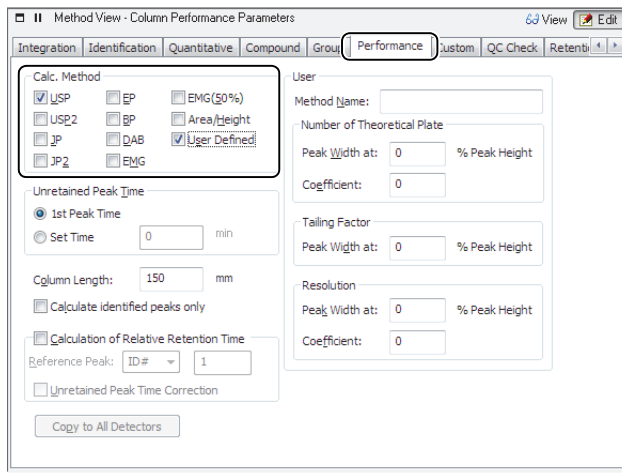
Reference

For details about the column performance equations, refer to Help or the Data Acquisition & Processing Theory Guide.

6

1 Click  **Edit** (**Edit Mode**) in **[Method View]**.

2 Click the **[Performance]** tab, and select the appropriate checkbox(es) at **[Calc. Method]**.



NOTE

- Select **[User Defined]** to display the **[User]** parameters box.
- Either select **[1st Peak Time]** or enter a **[Set Time]** at **[Unretained Peak Time]**.
- Select **[Column Length]** to calculate the number of theoretical plates.

3 Click  **View** (**View Mode**) in **[Method View]**.

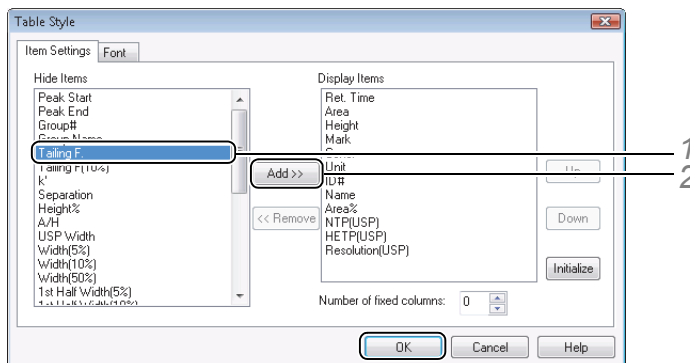
- 4** Click the [Peak Table] tab in [Results View], and check the number of theoretical plates and resolution.

Peak#	ID#	Name	Area%	NTP(USP)	HETP(USP)	Resolution(USP)
1	1	PeakA	27.220	4159	36.068	--
2	2	PeakB	31.295	6706	22.366	3.619
3			0.587	4211	35.618	2.431
4	3	PeakC	19.776	12715	11.797	1.325
5	4	PeakD	21.122	21054	7.125	5.203
Total			100.000			

- 5** To check the tailing factor, right-click on the Peak Table, and click [Table Style].

Peak#	ID#	Name	Area%	NTP(USP)	HETP(USP)	Resolution(USP)
1	1	PeakA	27.220	4159	36.068	--
2		Copy		706	22.366	3.619
3		Copy Entire Table		211	35.618	2.431
4		Register Selected Peak to Compound Table		715	11.797	1.325
5				054	7.125	5.203
Total						

- 6** Add the [Tailing F.] in the [Hide Items] column to the Compound Table in the [Table Style] sub-window, and click [OK].



- 1 Select [Tailing F.] in the [Hide Items] list.
 - 2 Click [Add].
- The [Tailing F.] item is added to the [Display Items] list.



NOTE

Change the display order of items in the Compound Table, by selecting the item in the [Display Items] list and then clicking [Up] or [Down].

[Tailing F.] is displayed in the Peak Table.

Peak#	Name	Area%	NTP(USP)	HETP(USP)	Resolution(USP)	Tailing F.
1	PeakA	27.220	4159	36.068	--	1.206
2	PeakB	31.295	6706	22.366	3.619	1.134
3		0.587	4211	35.618	2.431	--
4	PeakC	19.776	12715	11.797	1.325	1.175
5	PeakD	21.122	21054	7.125	5.203	1.182
Total		100.000				



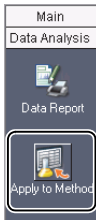
NOTE

Add [Tailing Factor] or [Resolution] display settings to the [Quantitative Results] report items to print the results in the output report.

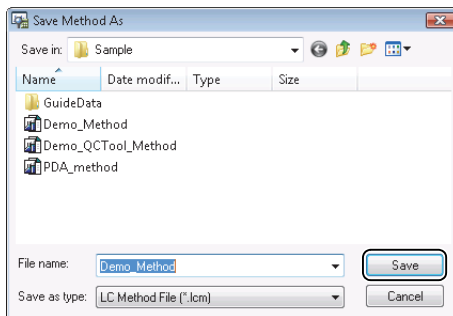
6.7 Save (Export) to Method Files

After setting the quantitative parameters and the Compound Table, save (export) the new settings to the method file.

- 1 Click the  (Apply to Method) icon on the [Data Analysis] assistant bar.



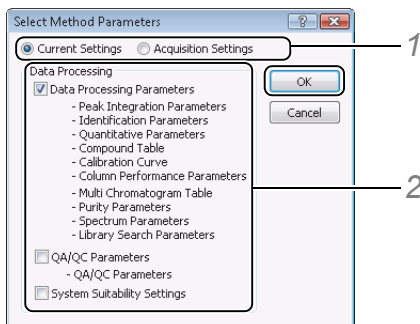
- 2 The name of the method file used for data acquisition is displayed. Click [Save].



NOTE

Enter a new name at [File name] to create a new method file.

- 3 Select the method items to save, and click [OK].

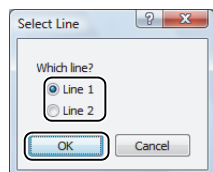


- 1 Select [Current Settings].
[Current Settings] saves the latest currently displayed method parameters.
[Acquisition Settings] saves the method parameters used for data acquisition.
- 2 Select the method items to save.

The selected method items are saved to the method file.

 **NOTE**

In the case of a dual-line configuration GC, select the line to export the method from, and click [OK].



7

PDA Data Analysis


This chapter describes how to analyze chromatograms or spectra obtained by data acquisition with the PDA (photodiode array) detector, execute purity calculations on detected peaks, and perform library searches.

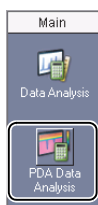
7.1 [PDA Data Analysis] Window

The [PDA Data Analysis] window is comprised of the following views:

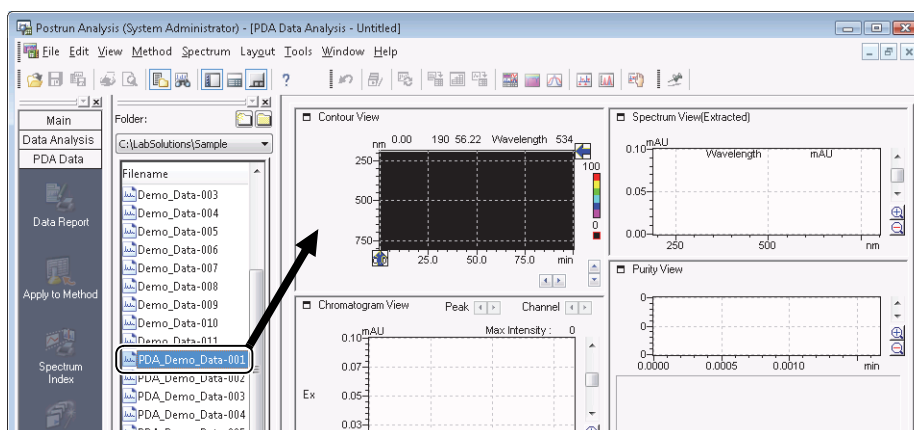
- [Contour View] - displays a contour view with absorbance color-coded
- [Chromatogram View] - displays chromatograms and status curves
- [Spectrum View] - displays the UV spectra
- [Purity View] - displays the purity calculation results of detected peaks
- [Results View] - displays quantitative calculation results
- [Method View] - displays and editing data processing parameters

7.1.1 Open the [PDA Data Analysis] Window

- 1 Click the  (PDA Data Analysis) icon on the [Main] assistant bar in the [Postrun Analysis] program.



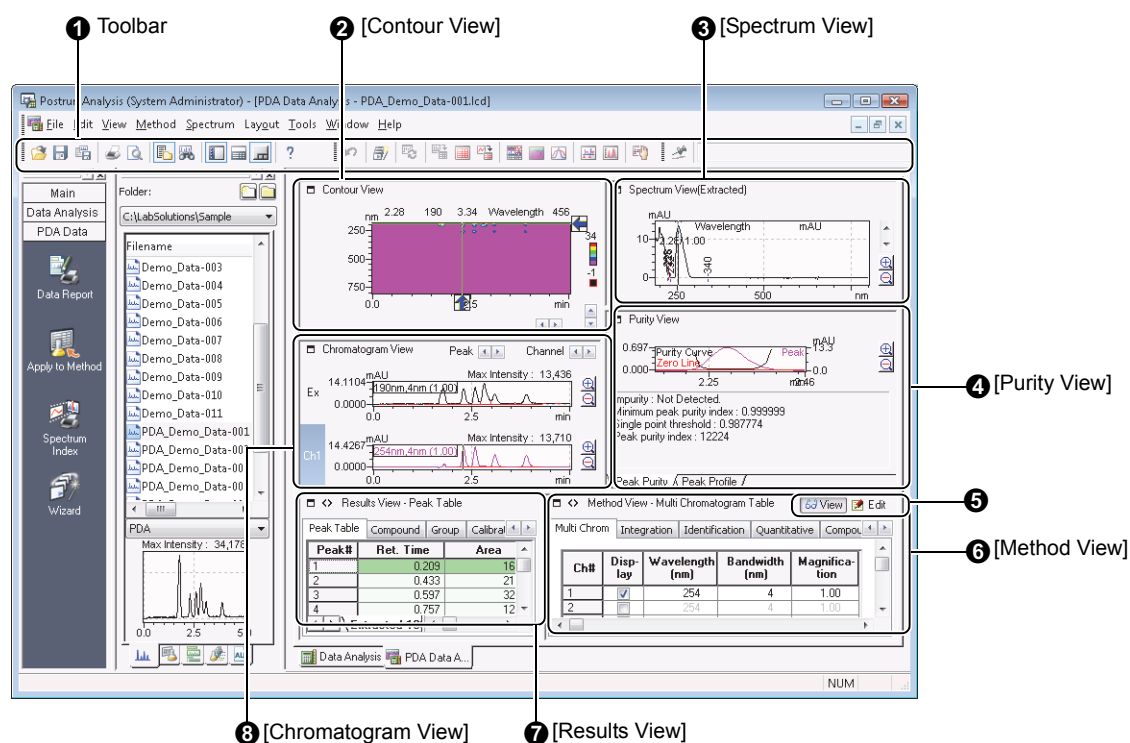
- 2 Drag-and-drop the data file onto the [PDA Data Analysis] window from the [Data Explorer] sub-window.



The contents of the data file is displayed in the [PDA Data Analysis] window.

7.1.2 [PDA Data Analysis] Window Description

This section describes how to view and use the [PDA Data Analysis] window.



No.	Explanation
1	Displays the [Standard] and [PDA Data Analysis] toolbars.
2	Displays the contour graph with PDA data color-coded into absorbance ranges. Drag the and to display the chromatograms and spectra extracted at that position in [Chromatogram View] and [Spectrum View].
3	Displays the UV spectrum at selected retention time or a selected peak. Right-click the [Spectrum View] to select operations such as switching of the view mode (Extracted or Registered) and UV library search for selected spectra.
4	The [Peak Purity] tab displays the purity result for the selected peak. The [Peak Profile] tab displays the overlaid chromatogram for the selected peak at multiple wavelengths.
5	Select the [Edit] mode to change various parameters in [Method View].
6	Displays the data processing parameters of the currently open data file. The [Multi Chrom], [UV Spectrum], [Library Search], and [Purity] tabs are displayed in addition to the tabs displayed in the [Data Analysis] window.
7	Displays the peak integration and quantitative results. The display content is the same as [Results View] in the [Data Analysis] window.
8	Displays the chromatogram at the wavelength on the [Multi Chrom] tab in the data processing parameters and the chromatogram extracted from the contour. Right-click on the graph in [Chromatogram View] to select operations such as switching the view mode (Overlay Chromatograms, Stack Chromatograms and Single Chromatogram), registration of multi chromatograms, and manual peak integration. Use to change the channel and peak position.

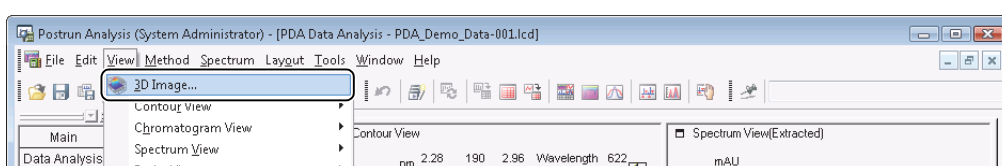
 **NOTE**

- Only data file can be displayed in the [PDA Data Analysis] window. Drag-and-drop the other data files onto the [PDA Data Analysis] window to change to the content of their data files.
- If the data file was acquired by simultaneous use of another detector, the chromatogram acquired by that detector is also displayed in the [Data Analysis] window.

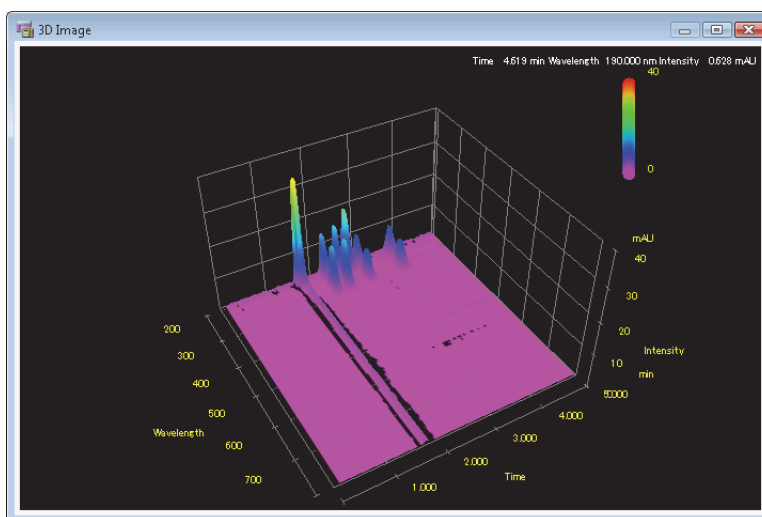
■ View the Data in Its Entirety (3D Image)

PDA data can be shown in its entirety as a 3D image.


1 Click [3D Image] on the [View] menu.



The [3D Image] sub-window opens.



 **NOTE**



- Click  in the top right corner of the sub-window to close the [3D Image] sub-window.
- The [3D Image] sub-window can be enlarged by dragging on the sub-window, and the display angle can be changed by dragging on the periphery of the 3D display area.
- The [3D Image] sub-window does not support the [256 Colors] Windows graphic mode. Use it in environments with the [High Color] setting or above. Do not change the number of colors for graphics while the [3D Image] sub-window is displayed.

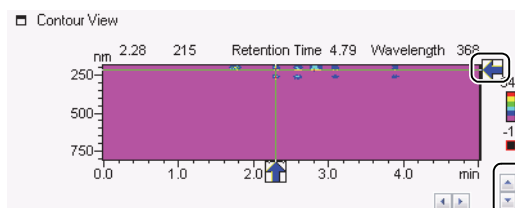
7.1.3 Display Chromatograms Extracted from [Contour View]

In [Contour View], the chromatograms or spectra can be extracted from [Contour View] by using the extraction lines.

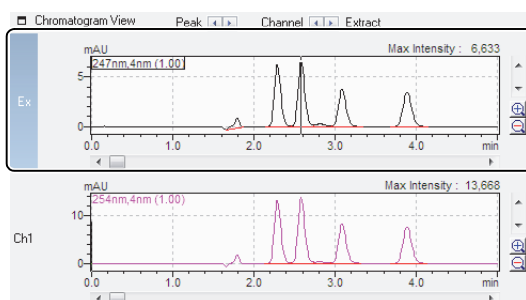
This section describes how to change the extraction position of the wavelength (Y-axis) and display the chromatogram at that position in the [Chromatogram View].

1


- Drag  to move to the target position.
 (Click  to fine-adjust the wavelength extraction position.)



The extracted chromatogram is displayed in the [Ex] (extracted chromatogram) region in the [Chromatogram View].



NOTE

- The wavelength extraction position can be checked by the wavelength displayed by  on [Contour View] or by the wavelength displayed in the [Ex] region in [Chromatogram View].
- Right-click on [Contour View] and select [Graph Properties] to adjust the Contour Properties. Select [Display Settings] to adjust the Contour View Display Settings.
- The extracted chromatogram is only displayed if [Display Extracted chromatogram] is selected on the [Multi Chrom] tab in [Method View].

Ch#	Display	Type	Wavelength (nm)	Bandwidth +/- (nm)	Magnification
1	<input checked="" type="checkbox"/>	Absorbance	254	4	1.00
2	<input type="checkbox"/>	Absorbance	254	4	1.00
3	<input type="checkbox"/>	Absorbance	254	4	1.00
4	<input type="checkbox"/>	Absorbance	254	4	1.00
5	<input type="checkbox"/>	Absorbance	254	4	1.00
6	<input type="checkbox"/>	Absorbance	254	4	1.00
7	<input type="checkbox"/>	Absorbance	254	4	1.00
8	<input type="checkbox"/>	Absorbance	254	4	1.00
9	<input type="checkbox"/>	Absorbance	254	4	1.00
10	<input type="checkbox"/>	Absorbance	254	4	1.00
11	<input type="checkbox"/>	Absorbance	254	4	1.00
12	<input type="checkbox"/>	Absorbance	254	4	1.00
13	<input type="checkbox"/>	Absorbance	254	4	1.00
14	<input type="checkbox"/>	Absorbance	254	4	1.00
15	<input type="checkbox"/>	Absorbance	254	4	1.00
16	<input type="checkbox"/>	Absorbance	254	4	1.00

Reference Correction

Ref. Wavelength: nm

Ref. Bandwidth: nm

Display Extracted Chromatogram

Extraction Settings

Absorbance Derivative




Bandwidth: nm

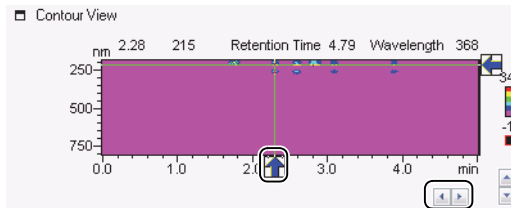
Magnification:

7.1.4 Display Spectra Extracted from [Contour View]

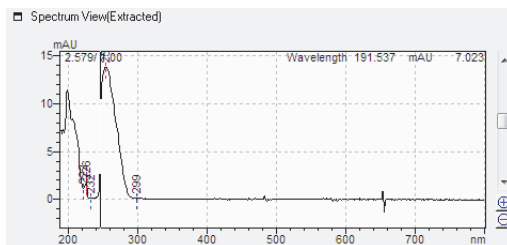
The chromatograms or spectra can be extracted from [Contour View] by using the extraction line.

This section describes how to change the extraction position of the time (X-axis) and display the spectrum at that position in the [Spectrum View].


- 1 Drag  to move to the target position.
(Click   to fine-adjust the time extraction position.)

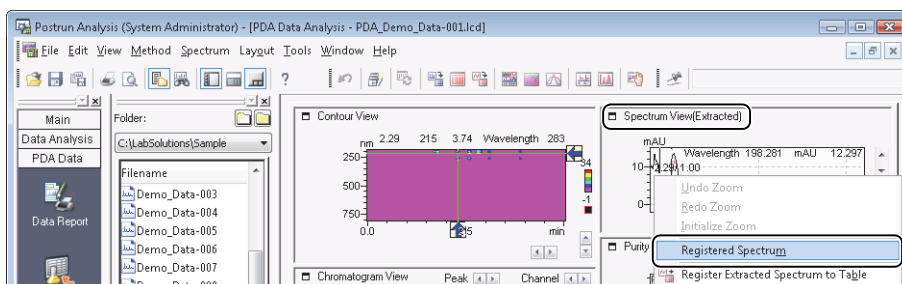


The extracted spectrum is displayed in [Spectrum View].



NOTE

- The wavelength extraction position can be checked by the wavelength displayed by  on [Contour View] or by the retention time displayed in [Spectrum View].
- Right-click on [Contour View] and select [Graph Properties] to adjust the Contour Properties. Select [Display Settings] to adjust the Contour View Display Settings.
- Right-click on the spectrum and select or deselect [Registered Spectrum] and switch between [Spectrum View (Registered)] and [Spectrum View (Extracted)].

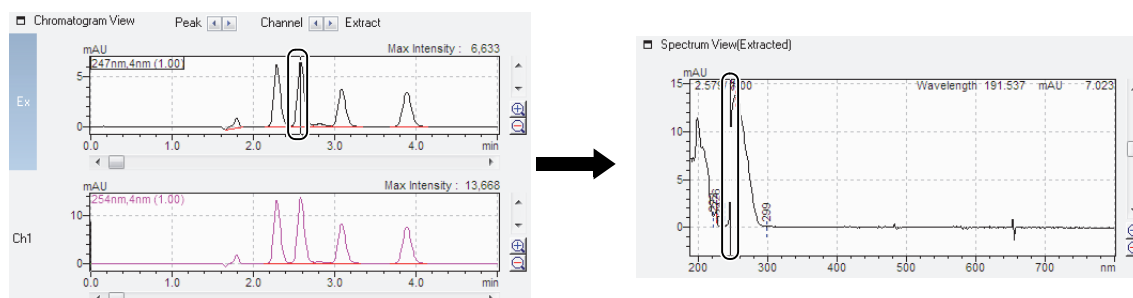


7.1.5 Manipulate Extracted Chromatograms and Spectra

Double-click anywhere on a chromatogram (or spectrum) display to check the chromatogram waveform or spectrum shape.

■ Display the Spectrum of a Desired Retention Time Extracted from the Chromatogram

Double-click a selected chromatogram at a desired retention time to display the spectrum of that retention time in [Spectrum View].

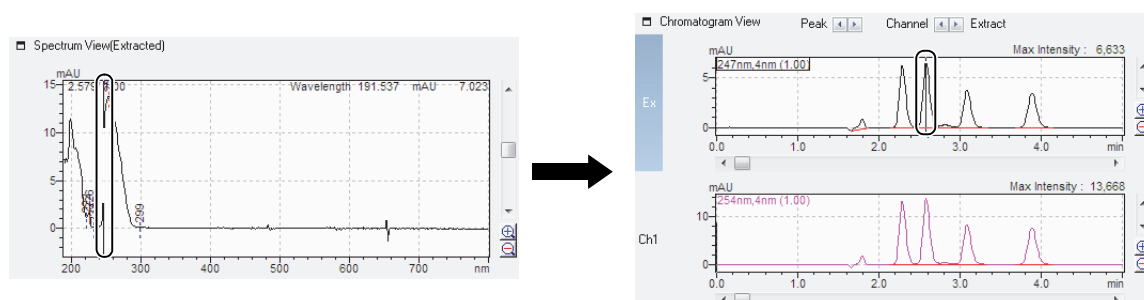


NOTE

To check the spectrum of a time at the top of a detected peak, click [Peak]. The spectrum moves to the top of the detected peak.

■ Display the Chromatogram of a Desired Wavelength Extracted from the Spectrum

Double-click a desired wavelength of a spectrum to display the chromatogram at that wavelength in the [Ex] (extracted chromatogram) section of the [Chromatogram View].



NOTE

- Chromatograms extracted from [Spectrum View] cannot be displayed if a channel other than [Ex] (extracted chromatogram) is selected in [Chromatogram View].
- The extracted chromatogram cannot be displayed if [Display Extracted chromatogram] is deselected on the [Multi Chrom] tab in [Method View].

7.2 Register Chromatograms

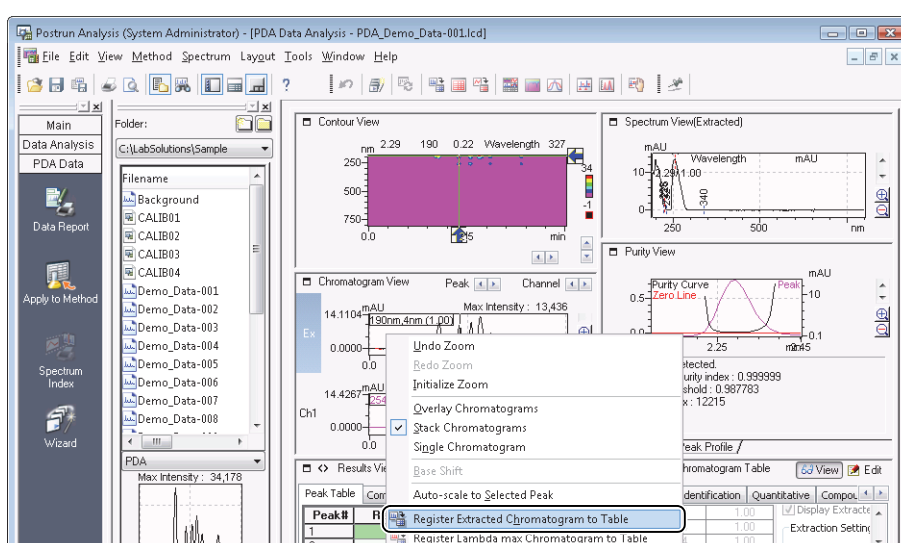
Chromatograms extracted from 3D data can be registered in the Multi-Chromatogram Table.

7.2.1 Register Chromatograms to the Multi-Chromatogram Table

Register a chromatogram to the Multi-Chromatogram Table to perform operations such as comparison of multiple chromatograms, output of reports and peak integration.

This section describes how to register chromatograms to the Multi-Chromatogram Table.


- 1 Right-click on the chromatogram in [Ex] (extracted chromatogram), and select [Register Extracted Chromatogram to Table].

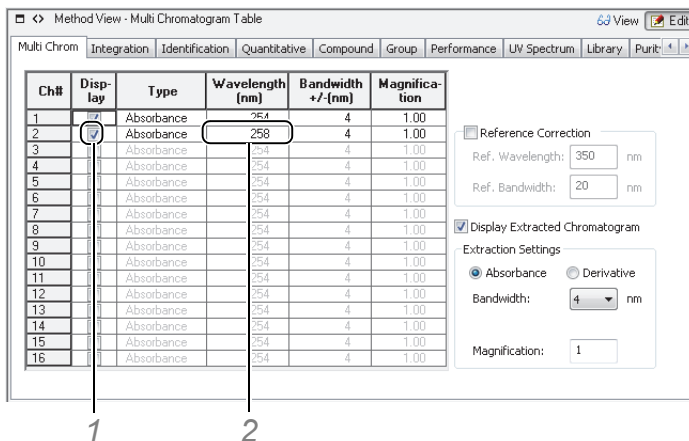


The extracted chromatogram is registered to a channel in the Multi Chromatogram Table.

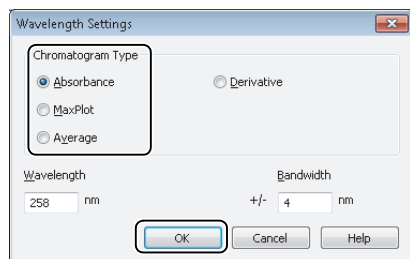
NOTE

- The extracted chromatogram cannot be displayed if [Display Extracted chromatogram] is deselected on the [Multi Chrom] tab in [Method View].
- Right-click on the chromatogram, and select [Register Lambda max Chromatogram to Table] to register the lambda max chromatogram for the target peak to the Multi Chromatogram Table. Then, double-click near the peak top of the target peak in [Chromatogram View]. The chromatogram is registered to the Multi Chromatogram Table.
- If the chromatogram display mode is [Overlay Chromatograms] or [Stack Chromatograms], new chromatograms are displayed in [Chromatogram View] as they are registered to a channel in the Multi Chromatogram Table.

- 2 Click  **Edit** (**Edit Mode**) in **[Method View]**.
- 3 Click the **[Multi Chrom]** tab in **[Method View]**, and select the registered chromatograms.



- 1 Select **[Display Extracted chromatogram]** to display the chromatogram in **[Chromatogram View]**.
- 2 Click the **[Wavelength]** cell.
Select **[Max Plot]** from the **[Types of Chromatograms]** and enter a **[Start Wavelength]** and an **[End Wavelength]** to display that chromatogram as a Max Plot.

**NOTE**


Max Plot refers to the chromatogram obtained by plotting the intensity of the maximum absorbance in the specified wavelength range.

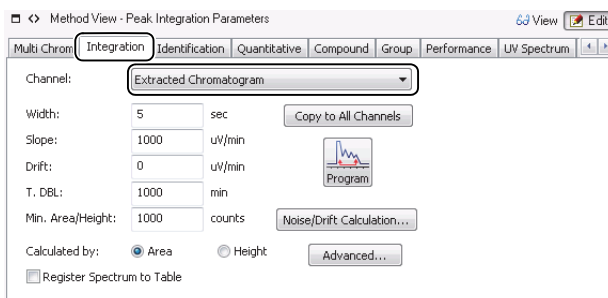
- 4 Click  **View** (**View Mode**) in **[Method View]**.
The chromatogram is displayed in **[Chromatogram View]**.

7.2.2 Peak Integration Parameters

The peak integration parameters for PDA data can be individually edited for each channel in the Multi Chromatogram Table.

This section describes how to select a channel and perform data processing on that channel.

- 1 Click  **Edit** (**Edit Mode**) in **[Method View]**.
- 2 Click the **[Integration]** tab, and select the target channel from the **[Channel]** list.



- 3 **Edit the peak integration parameters.**

Reference

Refer to ["6.2 Peak Integration Parameters" P.132](#) for details on peak integration operations.

- 4 Click  **View** (**View Mode**) in **[Method View]**.

The chromatogram in the selected channel is reintegrated with the new peak integration parameters.

NOTE

Right-click on the chromatogram in **[Chromatogram View]**, and select **[Manual Integration Bar]** to manually integrate the chromatograms for each channel. Refer to ["6.2.4 Manual Peak Integration" P.137](#) for details on manual peak integration.

7.3 Register Spectra

Register spectra extracted from 3D data to the Spectrum Table to perform a library search and calculate the similarity between each spectrum and the reference spectrum.

7.3.1 Register Spectra to the Spectrum Table

If the displayed spectra are registered to the Spectrum Table, they can be compared with other spectra and their similarity can be calculated.

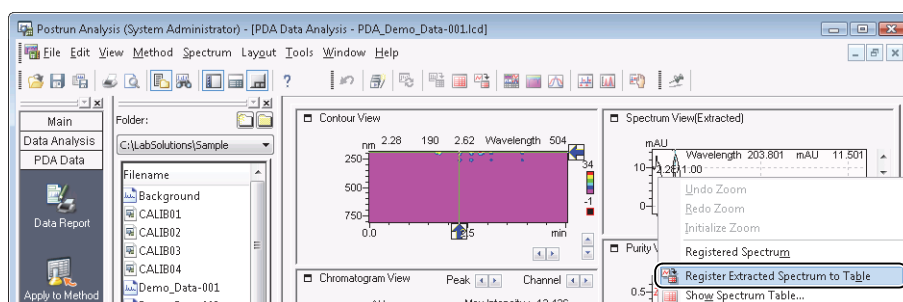
This section describes how to register extracted spectrum to the Spectrum Table.



NOTE

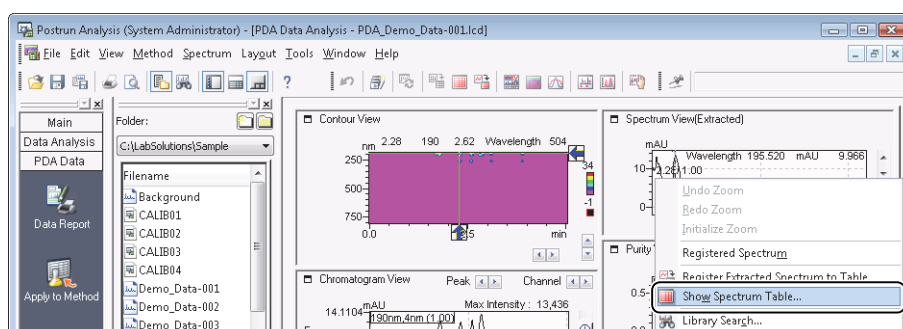
Right-click on the spectrum and select or deselect [Registered Spectrum] and switch between [Spectrum View (Registered)] and [Spectrum View (Extracted)].

1 Right-click on [Spectrum View], and click [Register Extracted Spectrum to Table].



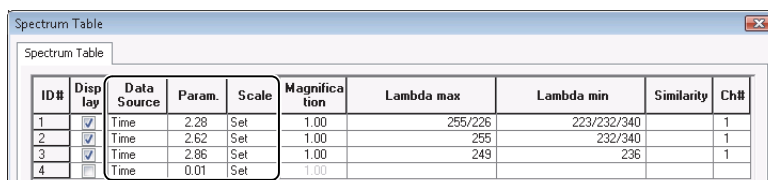
The extracted spectrum is registered to the Spectrum Table.

2 Right-click on [Spectrum View], and click [Show Spectrum Table].



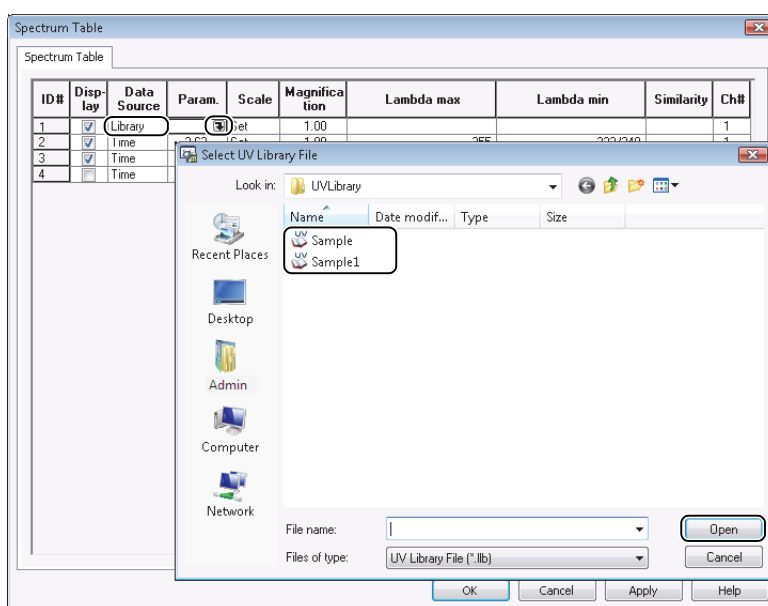
3 Edit the Spectrum Table.

- 1 Check the content of the [Data Source], [Param.], and [Scale] cells of the registered spectrum.
If an extracted spectrum has been registered, [Time] is displayed at [Data Source], and the retention time when it was extracted from the chromatogram is displayed at [Param.].

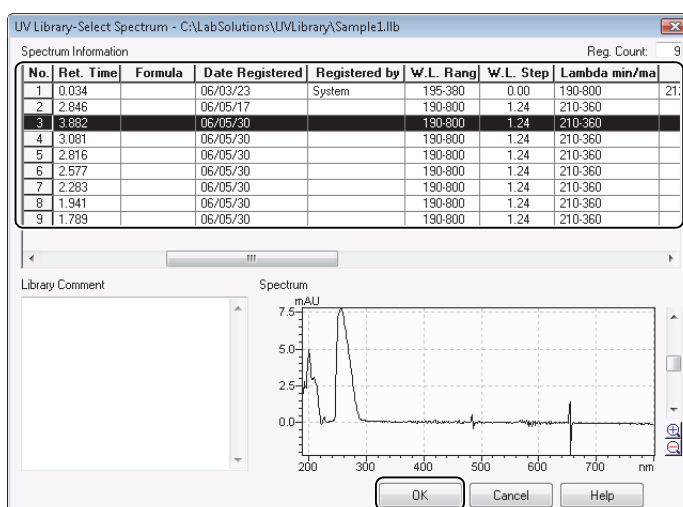


ID#	Display	Data Source	Param.	Scale	Magnification	Lambda max	Lambda min	Similarity	Ch#
1	<input checked="" type="checkbox"/>	Time	2.28	Set	1.00	255/226	223/232/340		1
2	<input checked="" type="checkbox"/>	Time	2.62	Set	1.00	255	232/340		1
3	<input checked="" type="checkbox"/>	Time	2.86	Set	1.00	249	236		1
4	<input type="checkbox"/>	Time	0.01	Set	1.00				

- 2 Click the [Data Source] cell and select [Library] and select the UV library file to register a spectrum in a library file to the Spectrum Table.



- 3 Select the spectrum in the library file from the [UV Library-Select Spectrum] sub-window, and click [OK].



4 Click [Apply], check the display in [Spectrum View], and then click [OK].

ID#	Display	Data Source	Param.	Scale	Magnification	Lambda max	Lambda min	Similarity	Ch#
1	<input checked="" type="checkbox"/>	Library	le1.lib	Set	1.00	234/278	251/331		1
2	<input checked="" type="checkbox"/>	Time	2.62	Set	1.00	255	232/340		1
3	<input checked="" type="checkbox"/>	Time	2.86	Set	1.00	249	236		1
4	<input checked="" type="checkbox"/>	Time	2.86	Set	1.00	249	236		1
5	<input type="checkbox"/>	Time	0.01	Set	1.00				



NOTE

- If [Spectrum View (Registered)] is displayed, double-click anywhere in [Chromatogram View] to register the extracted spectrum to the Spectrum Table.
- Select [Register Spectrum to Table] on the [Integration] tab in [Method View] to automatically register the spectrum at all peak top times to the Spectrum Table.

7.3.2 Calculate Spectrum Similarity

The similarity between the reference spectrum and another spectrum in the Spectrum Table can be calculated if a reference spectrum ([Ref]) is registered to the Spectrum Table.

This section describes how to register a reference spectrum to calculate similarity.

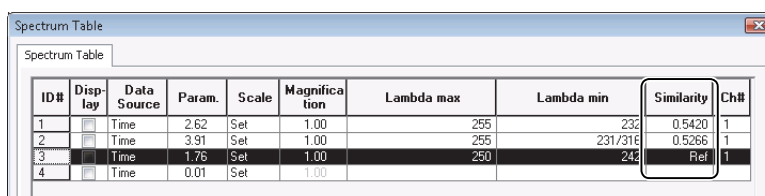
1

Right-click the ID No. to be used as the reference spectrum, and click [Set to Reference Spectrum for Similarity].

[Ref] is displayed in the [Similarity] for the selected ID#.

ID#	Display	Data Source	Param.	Scale	Magnification	Lambda max	Lambda min	Similarity	Ch#
1	<input type="checkbox"/>	Time	2.62	Set	1.00	255	232		1
2	<input type="checkbox"/>	Time	3.91	Set	1.00	255	231/316		1
3	<input type="checkbox"/>	Time	1.75	Set	1.00	250	242		1
4	<input type="checkbox"/>								

- 2** Click [Apply], and check [Similarity] of the spectrum currently registered to the Spectrum Table.

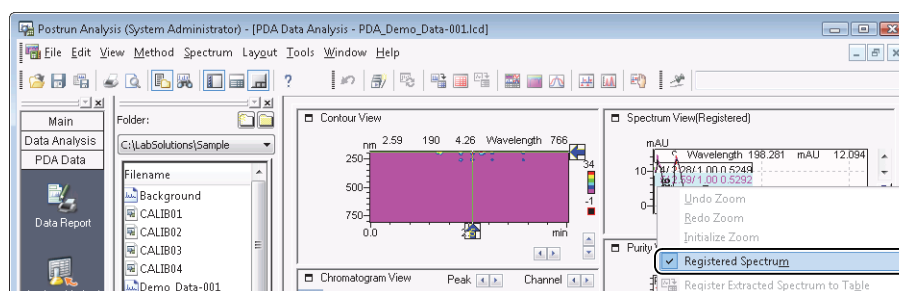


ID#	Display	Data Source	Param.	Scale	Magnification	Lambda max	Lambda min	Similarity	Ch#
1		Time	2.62	Set	1.00	255	232	0.5420	1
2		Time	3.91	Set	1.00	255	231/318	0.5266	1
3		Time	1.76	Set	1.00	250	243	Ref	1
4		Time	0.01	Set	1.00				

NOTE
[Similarity] is displayed as a value with respect to [Ref] = 1.

- 3** Click [OK].

NOTE
Right-click on the [Spectrum View] and select [Registered Spectrum] to display the spectrum currently registered in the Spectrum Table.



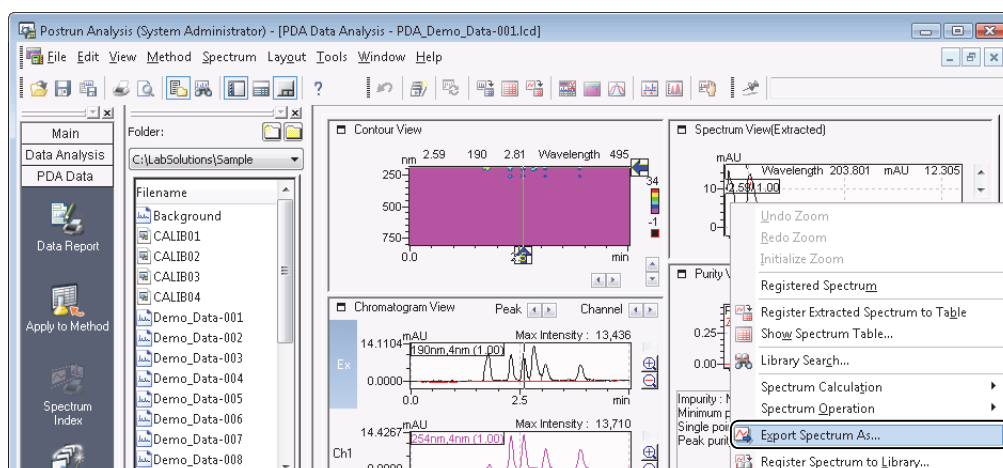
7.3.3 Create a Spectrum File

Spectra can be exported to common format (.jcm) files. Exported files are used to register to library files and to perform peak identification based on similarity.

This section describes how to export a spectrum in [Spectrum View] to a file, and how to export spectra registered to the Spectrum Table to files.

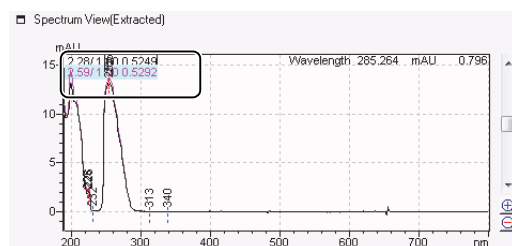
■ Export a Spectrum in [Spectrum View]

1 Right-click on [Spectrum View], and click [Export Spectrum As].

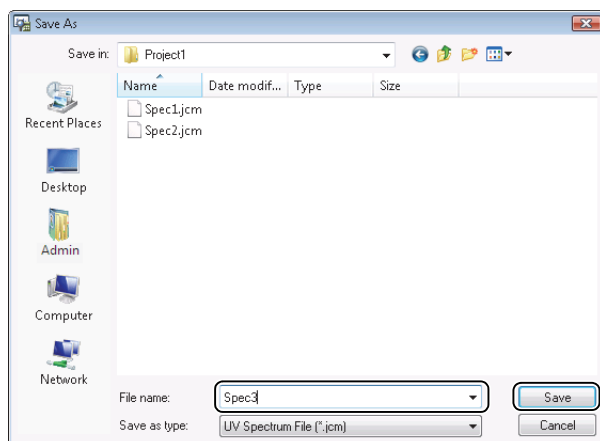


NOTE

If the view mode is [Spectrum View (Registered)], select the spectrum label before right-clicking on [Spectrum View].



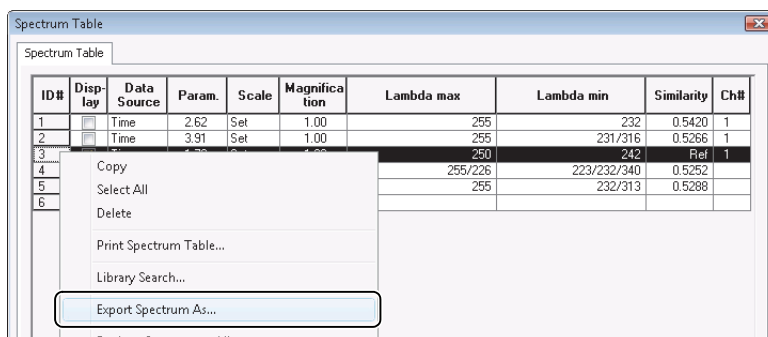
2 Enter the file name, and click [Save].



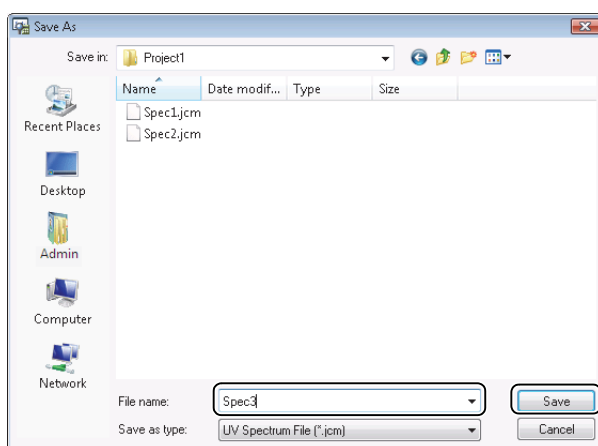
The spectrum file is created.

■ Export Spectra Registered to the Spectrum Table

- 1 Right-click on the ID No. of the spectrum to export, and click [Export Spectrum As].



- 2 Enter the file name, and click [Save].



The spectrum file is created.

7.4 UV Spectrum Library

A file that contains multiple UV spectra is called a library file. Library file allow for the comparison of unknown spectra to a library of known spectra to identify the unknown compound.

This section describes how to make a library file according to the following procedures.


1. "Create a Library File"
2. "Register a UV Spectrum to the Library File"
3. "Edit a Library File"

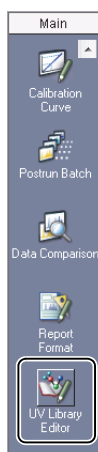
Reference

Refer to "7.5.1 Identify Peaks by Spectrum Similarity" P.194 or "7.5.2 Use [Library Search] to Search for Spectra" P.197 for more details.

7.4.1 Create a Library File

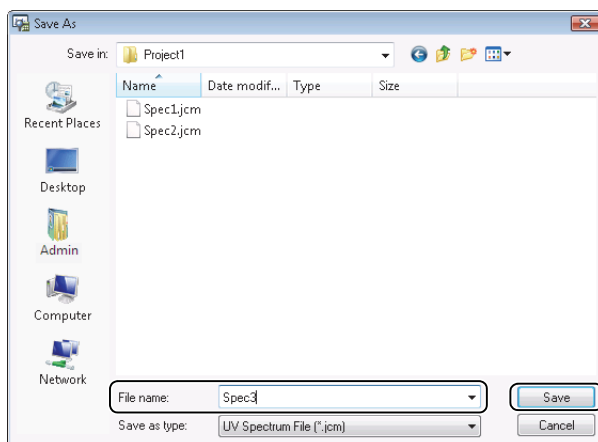
A UV spectra library file must be created before extracted spectra can be added to it.

- 1 Click the  (UV Library Editor) icon on the [Main] assistant bar in the [Postrun Analysis] program.



- 2 Click  (New) on the toolbar.

3 Enter a [File name], and click [Save].



The UV library file is created.

7.4.2 Register a UV Spectrum to the Library File

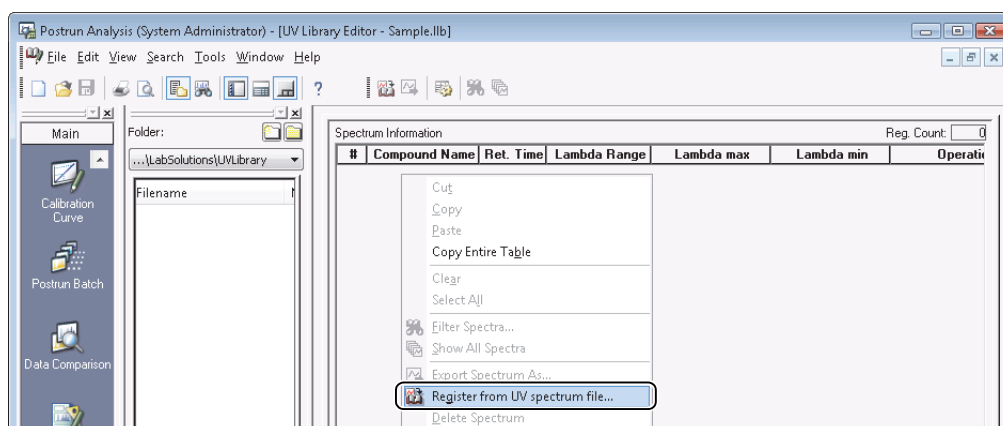
This section describes how to register the UV spectra displayed in the [Spectrum View] and spectra files to the library file made in "7.4.1 Create a Library File".

Register a UV Spectrum File

Reference

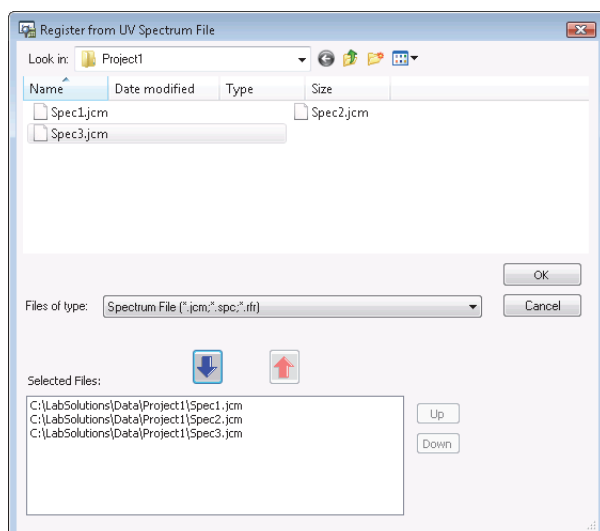
Refer to "7.3.3 Create a Spectrum File" P.186 for details.

- 1 Right-click on [Spectrum Information] in the [UV Library Editor] window, and click [Register from UV spectrum file].



- 2 Select the desired UV spectrum file and then click .

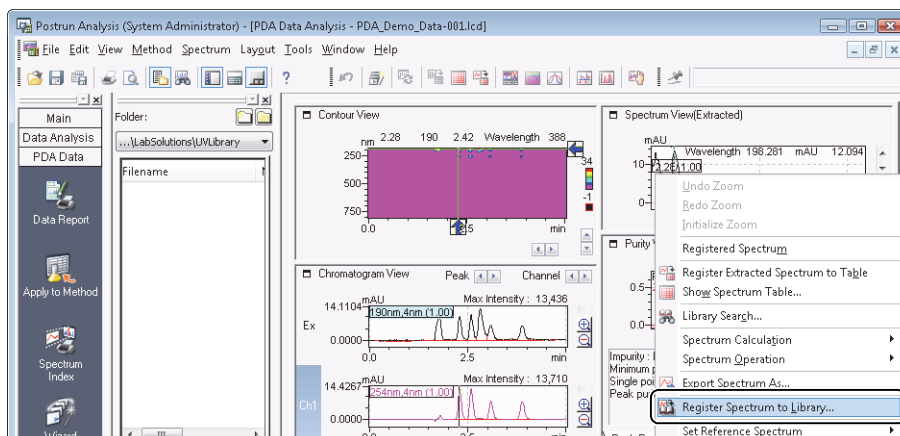
The UV spectrum file name is displayed in the [Selected Files] box. Repeat this procedure to select all files required for the UV library.



The selected UV spectra files are registered to the UV library file.

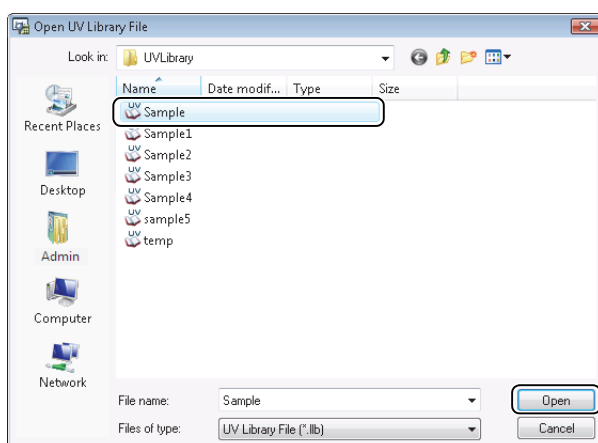
■ Register a UV Spectrum

- 1 Right-click on [Spectrum View] in the [PDA Data Analysis] window, and click [Register Spectrum to Library].



The spectrum is added to the UV library file.

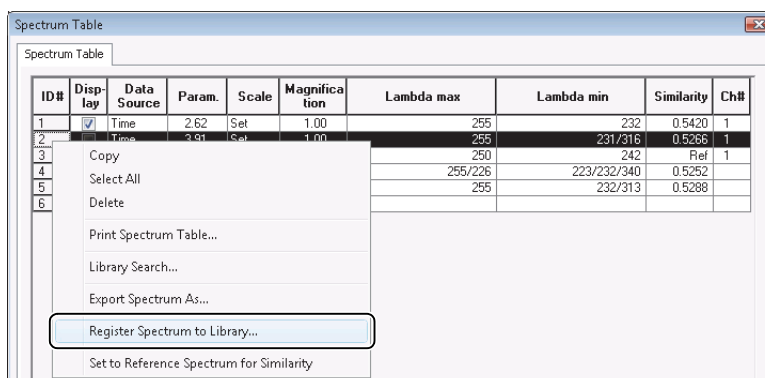
- 2 Select the desired UV library file, and click [Open].



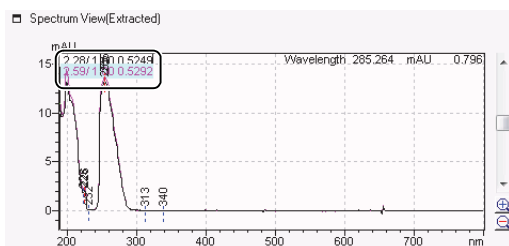
The spectrum is added to the UV library file.

NOTE

- Right-click on the ID No. of the desired spectra, and select [Register Spectrum to Library] to add spectra in the Spectrum Table to the library file.




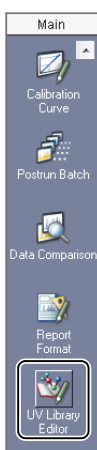
- If the view mode is [Spectrum View (Registered)], select the spectrum label before right-clicking on [Spectrum View], and then select [Register Spectrum to Library].



7.4.3 Edit a Library File

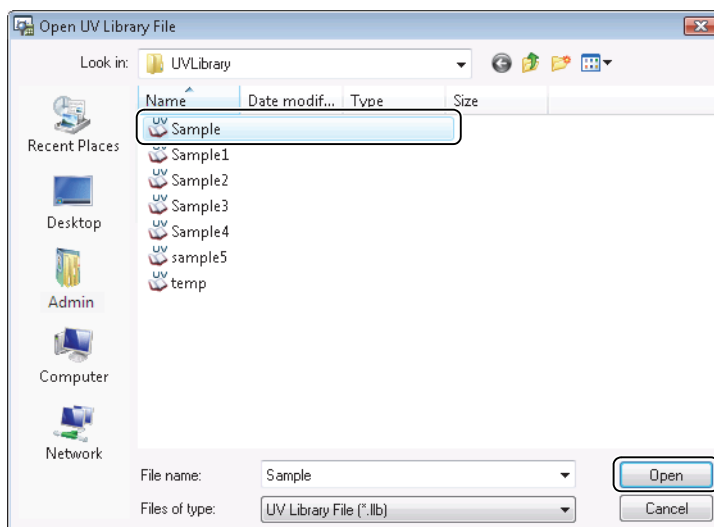
This section describes how to edit the spectrum files registered at ["7.4.2 Register a UV Spectrum to the Library File"](#).

- 1 Click the  (UV Library Editor) icon on the [Main] assistant bar in the [Postrun Analysis] program.

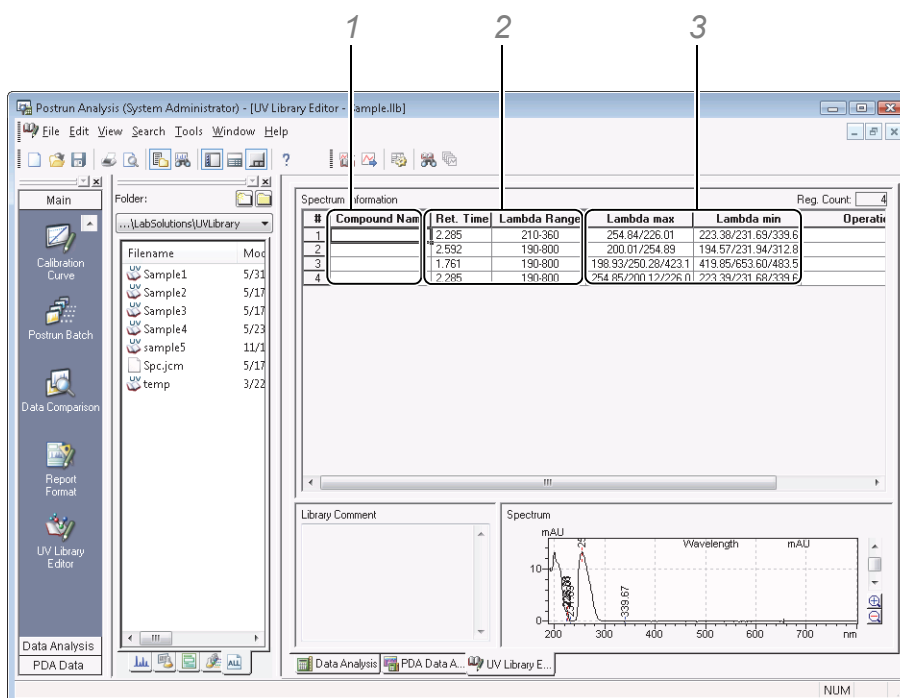


- 2 Click the  (Open) button on the toolbar.

3 Select the desired UV library file, and click [Open].



4 Edit the [Spectrum Information] in the UV library file.



- 1 Enter the [Compound Name] if one was not already entered.
- 2 Enter the wavelength range in the [Lambda Range] column for use the library search.
- 3 Check the [Lambda max] and [Lambda min] values.



NOTE

The items displayed at [Spectrum Information] can be edited with [Table Style]. Right-click on [Spectrum Information], and select [Table Style].

5 Click the (Save) button on the toolbar.

The UV library file is saved.

7.5 Specify a Compound From a Spectrum


Compare the spectra of known compounds with the spectrum of an unknown compound to identify and specify the compounds from a spectrum.

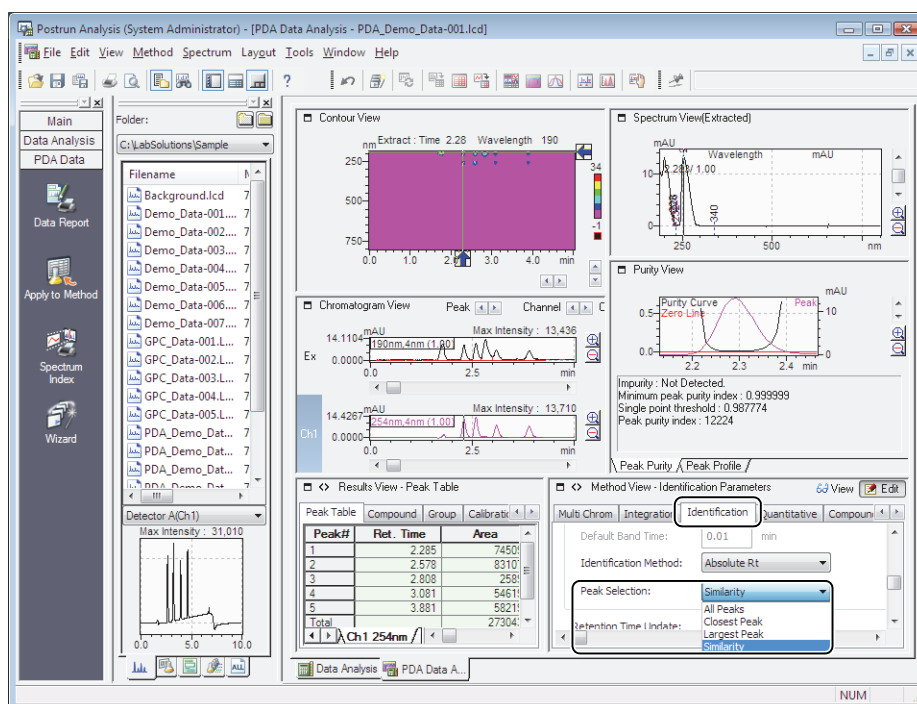
This section describes the following operations.

- *"Identify Peaks by Spectrum Similarity"*
- *"Use [Library Search] to Search for Spectra"*
- *"Spectrum Conditions of the Search Target"*

Set the spectrum conditions of the search target to perform higher precision similarity and library searches.

7.5.1 Identify Peaks by Spectrum Similarity

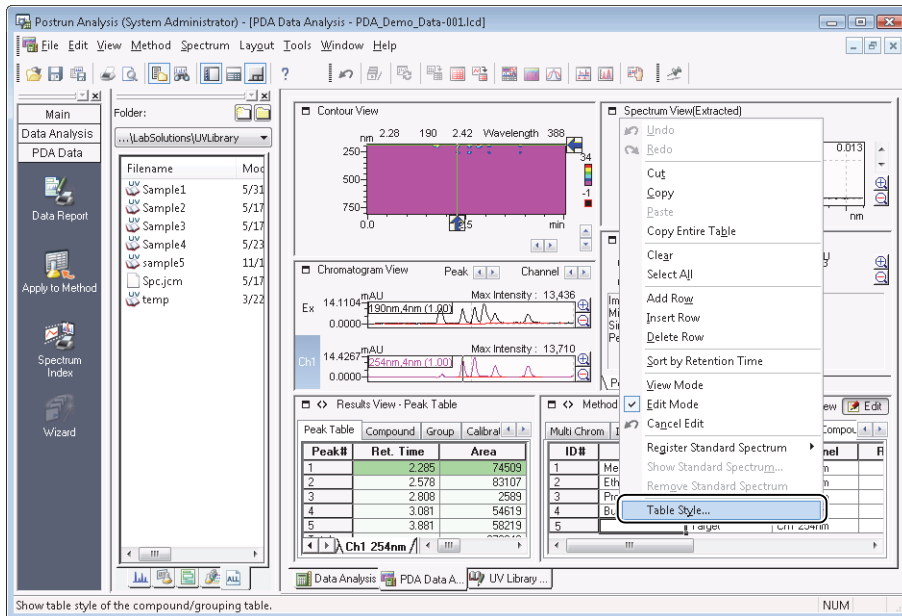
- 1 Click  **Edit** (Edit Mode) in [Method View].
- 2 Click the [Identification] tab, and select [Similarity] in the [Peak Selection] list.



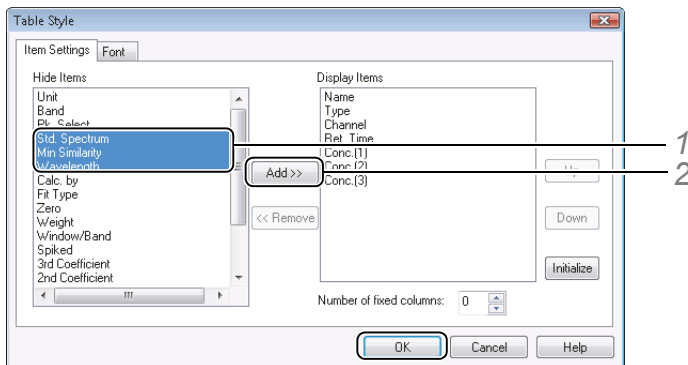
The screenshot displays the Postrun Analysis software interface. The main window shows a chromatogram with a peak at 2.28 minutes. The 'Identification Parameters' dialog box is open, showing the 'Identification' tab. The 'Peak Selection' list is set to 'Similarity'. The 'Method View - Identification Parameters' section shows the 'Identification Method' set to 'Absolute Rt' and the 'Peak Selection' dropdown menu open, with 'Similarity' selected. The 'Retention Time Tolerance' is set to 'Largest Peak'.

Peak#	Ret. Time	Area
1	2.285	74501
2	2.578	83101
3	2.808	2581
4	3.081	54811
5	3.881	58211
Total		273041

3 Click the [Compound] tab, right-click on the Compound Table, and click [Table Style].



4 Make the settings in the [Table Style] sub-window, and click [OK].



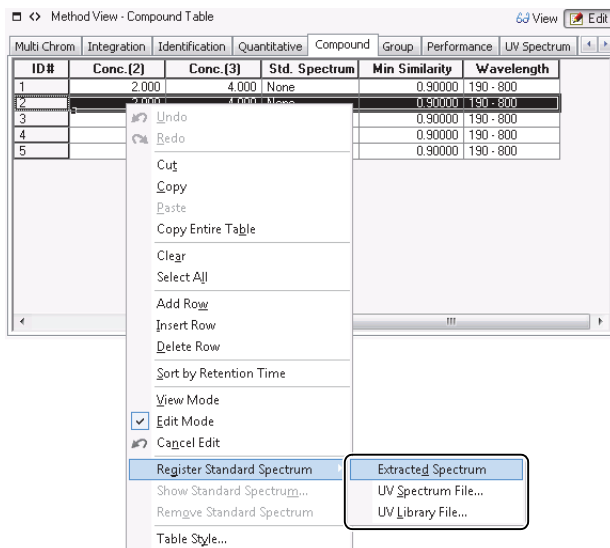
- 1 Select [Std. Spectrum], [Min Similarity], and [Wavelength] in the [Hide Items] box.
- 2 Click [Add].
[Std. Spectrum], [Min Similarity], and [Wavelength] are added to the [Display Items] box.



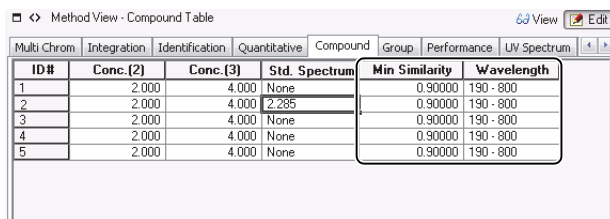
NOTE

Change the display order of items in the Compound Table, by selecting the item in the [Display Items] box and then clicking [Up] or [Down].

- 5** Right-click the [ID#] of the compound whose similarity is to be identified, click [Extracted Spectrum], [UV Spectrum File] or [UV Library File] at [Register Standard Spectrum], and register the standard spectrum for the compound.



- 6** Enter the [Min Similarity] and [Wavelength] that is associated with the [Std. Spectrum].



- 7** Click  (View Mode) in [Method View].



NOTE

- Right-click and select [Show Standard Spectrum] to check a registered spectrum.
- The peak is not identified if the similarity between the standard spectrum and the spectrum of the time at the top of the detected peak falls below the threshold.


7.5.2 Use [Library Search] to Search for Spectra

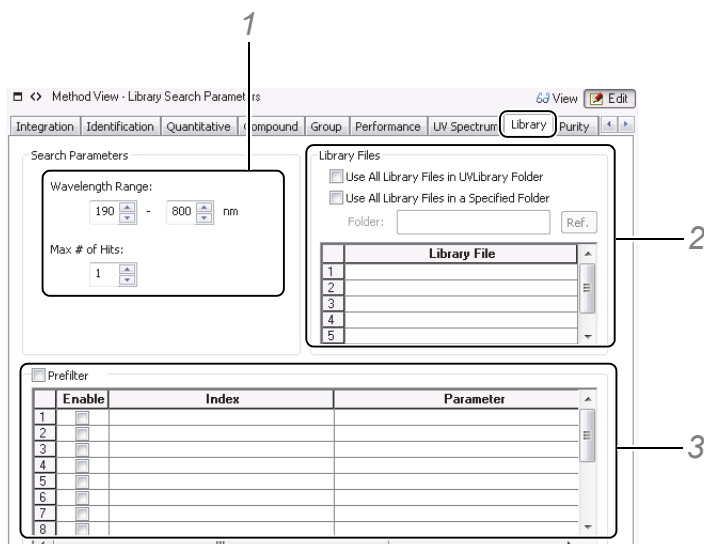
This section describes how to perform a library search.

1. Set library search criteria
2. Execute the library search

Library Search Criteria

The following example describes how to set the criteria to search the similarity between an unknown spectrum and the spectra registered to the library file.

- 1 Click  **Edit** (**Edit Mode**) in **[Method View]**.
- 2 Click the **[Library]** tab, and enter the search criteria.



- 1 Set the [Wavelength Range] and [Max # of Hits].



NOTE

[Max # of Hits] is the number of spectra to display in the [UV Library Search Results] sub-window.

- 2 Set the [Library Files] parameters.



NOTE

- Select [Use All Library Files in UVLibrary Folder] to search all of the library files in the UVLibrary folder.
- Select [Use All Library Files in a Specified Folder] and specify a folder to search all of the library files in a specific folder in the UVLibrary.

- 3 Select [Prefilter] and [Enable], then click the [Index] cell and select a keyword to further filter the search results by compound name, retention time or another keyword.

3

- 3 Click  **View** (**View Mode**) in **[Method View]**.

Execute the Library Search

When the library search is executed, matching spectra are displayed in order from the highest similarity to the lowest in the [UV Library Search Results] sub-window.

The following example describes how to select a spectrum in [Spectrum View (Registered)] and perform a library search.

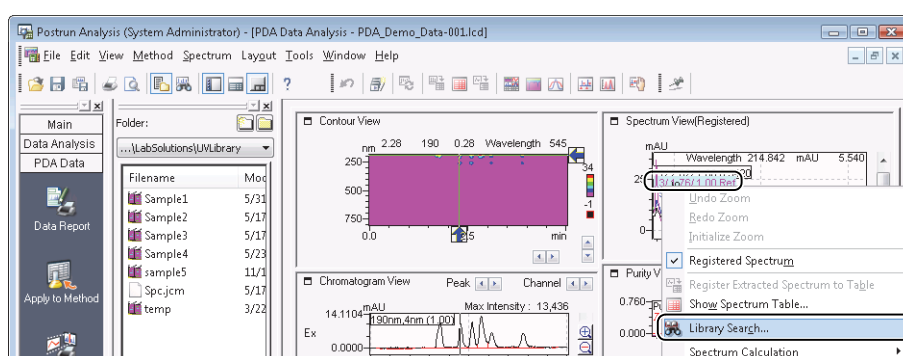


NOTE

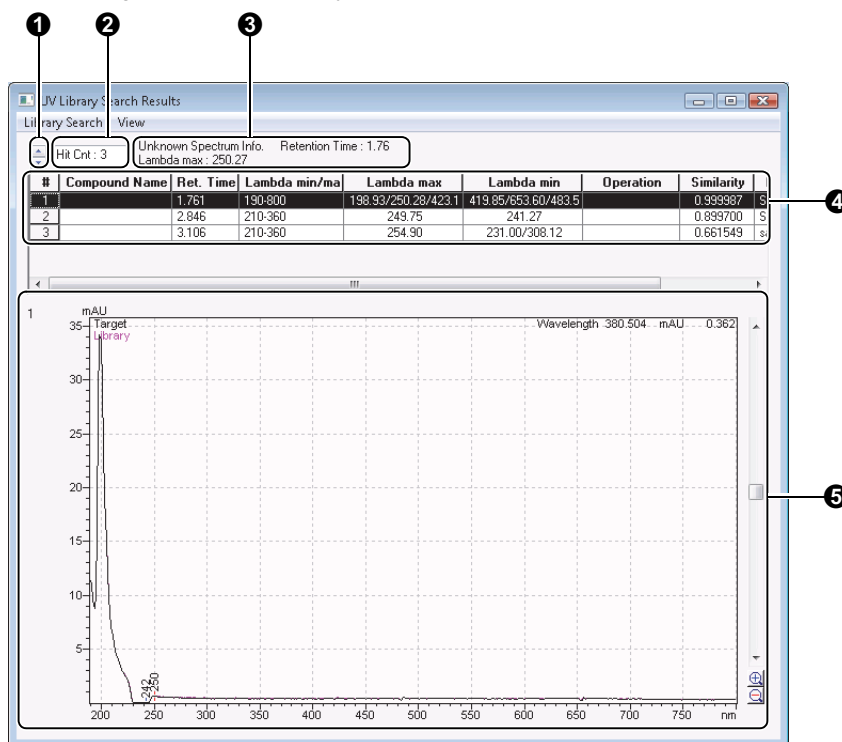
To perform a library search on the extracted spectrum, first, display the spectrum extracted from [Contour View] or [Chromatogram View] in [Spectrum View (Registered)], and execute the library search.

1

Select the spectrum in the [Spectrum View], right-click on the view, and click [Library Search].



The spectra found (hit) by the search criteria are displayed in the library search results. The following sub-window displays search results when the [Max # of Hits] is set to "3".



No.	Explanation
1	Changes the spectrum displayed in the graph. The number of graphs to display can be set at [Display Settings] on the [View] menu.
2	Determines the number of hits displayed in the search results window.
3	Displays the [Ret. Time] and [Lambda max] values for the UV spectrum of the target peak.

No.	Explanation
④	Displays a table of spectrum information that was hit (found) in the search. The spectrum information is displayed in order from the highest similarity to lowest.
⑤	Displays the searched spectra (Library) overlaying the unknown spectra (Target).

**NOTE**

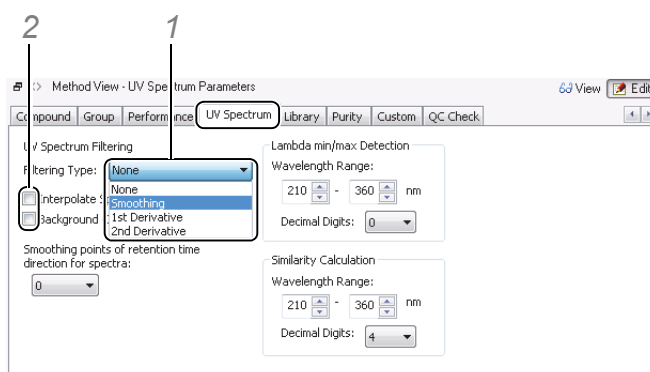
Click [Repeat Search] on the [Library Search] menu, and change the search criteria in the [Library Search] sub-window to perform the search again with new criteria.

7.5.3 Spectrum Conditions of the Search Target

Set the spectrum conditions during extraction of the UV spectrum to perform higher precision peak identification and library searches.

1 Click **Edit** (**Edit Mode**) in [Method View].

2 Click the [UV Spectrum] tab, and set the spectrum conditions.



- 1 Select [Smoothing] in the [Filtering Type] list to perform spectral smoothing.
- 2 Select [Background Compensation] to perform background compensation on spectra.

3 Click **View** (**View Mode**) in [Method View].

7.6 Peak Purity Analysis


The peak purity can be calculated and the peak shape of chromatograms at each wavelength can be compared to check whether detected peaks contain impurities.

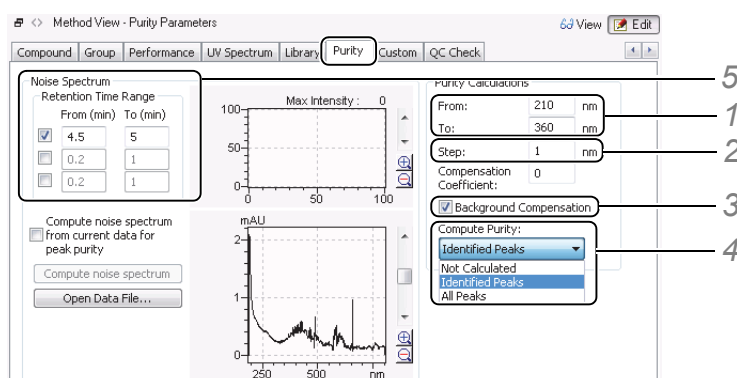
Reference

Refer to Help for details on peak purity analysis.

7.6.1 Peak Purity Calculation Parameters

This section describes how to set the calculation range and the compensation conditions based on the noise spectrum.

- 1** Click  **Edit** (Edit Mode) in [Method View].
- 2** Click the [Purity] tab, and set the conditions for the peak purity calculation.



- 1** At [From] and [To], enter the wavelength range where purity will be calculated.
- 2** At [Step], enter the wavelength interval to use for the calculation.
- 3** Select [Background Compensation].

NOTE

- Select [Background Compensation] to calculate the peak purity of components with a slow retention time or whose baseline easily drifts as in gradient acquisition.
- Insufficient peak separation causes the start and end points of the peak to overlap. Better results are obtained by not performing background compensation.

- 4** Select [Identified Peaks] from the [Compute Purity] drop-down list.

NOTE

Depending on the number of peaks and whether [All Peaks] is selected, it may take time to perform data analysis.

- 5** At [From] and [To], enter the retention time range to set as the noise spectrum. Select a time range that incorporates the retention time of the target component.

NOTE

- Display the chromatogram as a Max Plot, and verify that there are no peaks between [From] and [To], then select the noise spectrum range.
- Select [Compute noise spectrum from current data for peak purity] to compute the noise spectrum from the every data file.

3 Click View (View Mode) in [Method View].

The purity calculation is executed according to the preset conditions.

7.6.2 Displaying Calculation Results

[Purity View] has 2 sub-windows for viewing the results of the peak purity calculation, [Peak Purity] and [Peak Profile].

[Peak Purity] is used to check the peak purity based on the spectrum information of the detected peak. [Peak Profile] is used to check for impurities by comparing chromatograms at multiple wavelengths.

First, select the desired peak in [Chromatogram View] or [Contour View]. This section describes how to select peaks whose purity is to be checked in [Chromatogram View].

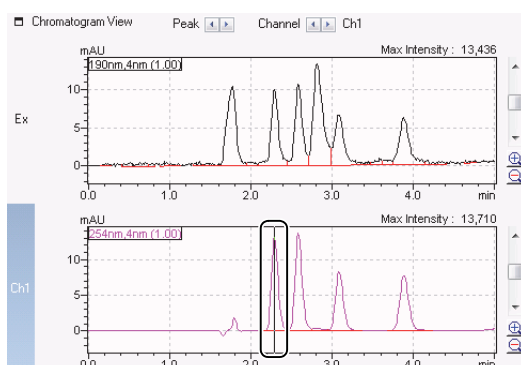
Next, check the calculation results at [Purity View]. The section describes the following 2 methods:

- *"Display Calculation Results using the 3-Point Peak Purity Method"*
- *"Display the Calculation Result using the Total Peak Purity Method"*

1 Move the extraction line in [Chromatogram View], to the peak for which purity is to be calculated.

Reference

Refer to *"Display the Spectrum of a Desired Retention Time Extracted from the Chromatogram"* P.178 for more details.

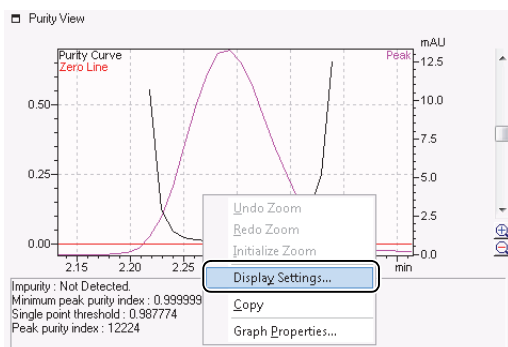


If the peak is detected, the purity of the selected peak is calculated.

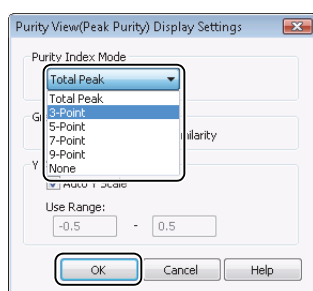
■ Display Calculation Results using the 3-Point Peak Purity Method

Peak purity is calculated based on 3 points, the upslope, peak top point and downslope.

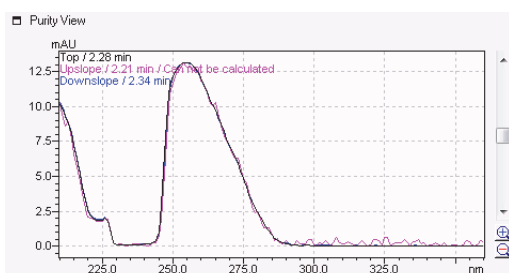
- 1 Select the [Peak Purity] tab in [Purity View] then right-click the graph and select [Display Settings].



- 2 Select [3-Point] from the [Purity Index Mode] drop-down list, and click [OK].



- 3 Confirm that the 3-point spectra method waveform and calculation results are displayed.



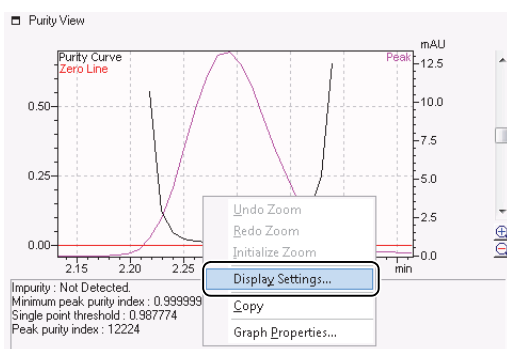
NOTE

If the spectral similarity between the peak top, the upslope and the downslope is higher than the threshold, it is an indication that the calculated peak does not contain impurities.

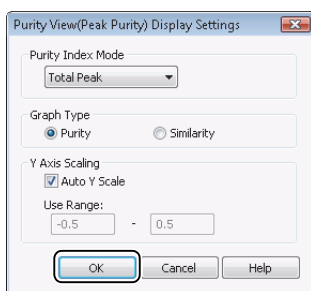
■ Display the Calculation Result using the Total Peak Purity Method

Peak purity is calculated based on all of the points from peak start to peak end, then the similarity and purity curves are displayed.

- 1** Select the [Peak Purity] tab in [Purity View] then right-click the graph and select [Display Settings].



- 2** Select [Total Peak] from the [Purity Index Mode] drop-down list, and set the [Graph Type] and [Y Axis Scaling], and click [OK].

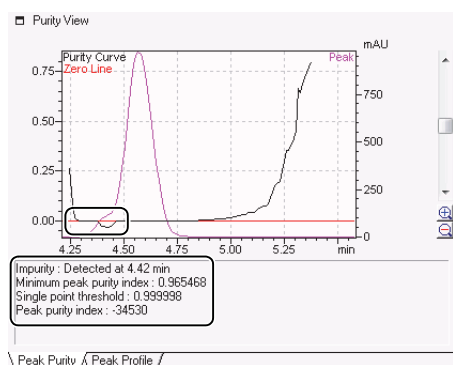


NOTE

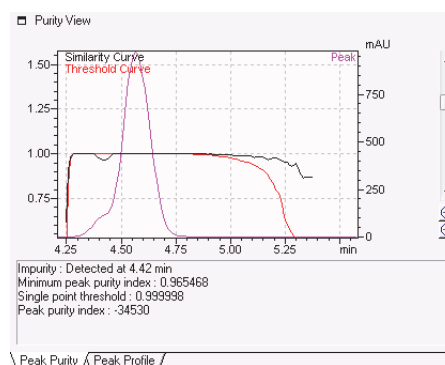
- If [Purity] is selected, the purity curve (curve obtained by subtracting the threshold curve from the similarity curve) and zero compensation line are displayed in the graph.
- If [Similarity] is selected, the similarity curve and threshold curve are displayed in the graph.
- To change the display scale of the similarity curve, deselect [Auto Y Scale] at [Y Axis Scaling], and enter a display range.
In the following example, the display range is set to 0.99 to 1.01.
- Notice in the following [Purity] graph example that impurities are detected where the purity curve is below the zero compensation line.
The negative [Peak purity index] value confirms that the sample contains impurities.

The [Purity] graph or [Similarity] graph is displayed.

Purity graph



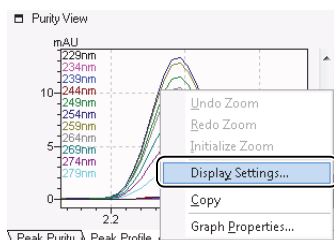
Similarity graph



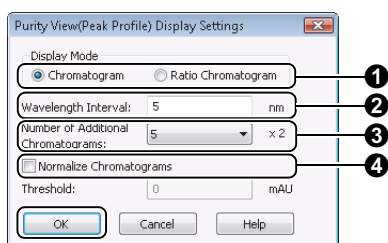
■ Examine Chromatograms using the Peak Profile

Display chromatograms at multiple wavelengths to compare peak shape.

- 1 Select the [Peak Purity] tab in [Purity View] then right-click the graph and select [Display Settings].



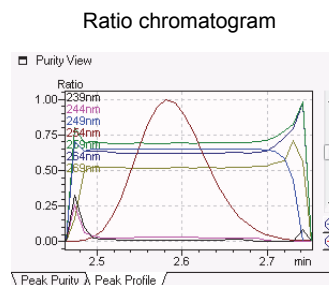
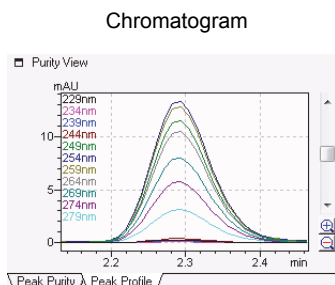
- 2 Enter the parameters in the [Display Settings] sub-window, and click [OK].



- 1 Select the [Display Mode].

No.	Explanation
①	Select [Chromatogram] to display the chromatogram based on the [Wavelength Interval] and [Number of Additional Chromatograms] parameters. Select [Ratio Chromatogram] to display the central wavelength chromatogram with the ratios between the chromatograms based on the [Wavelength Interval] and [Number of Additional Chromatograms].
②	Select how many wavelengths (nm) will separate the chromatograms displayed on the short and long sides of the center wavelength.
③	Select the number of chromatograms to display on the short and long sides of the center wavelength. Up to 5 wavelengths can be specified on each side.
④	If [Chromatogram] is selected as [Display Mode] and [Normalize Chromatograms] is selected, the intensity axis of the chromatogram is normalized.

The [Chromatogram] or [Ratio Chromatogram] is displayed.



NOTE

The center wavelength refers to the wavelength of the chromatogram extracted from the contour view or set in the Multi Chromatogram Table.

7.7 Print PDA Data Analysis Results

A report format file must be made in the [Report] window to print PDA data analysis results. This software provides several report format files to make printing easier. First-time users of this software can easily print analysis results using the pre-installed report format files. As users become more familiar with the software operations, they can edit or add report items to the pre-installed report format files, or create a new report format file and use it to print reports.

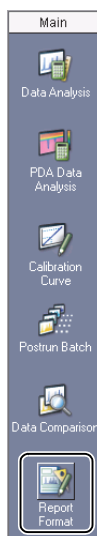
This chapter describes the following procedures.

- *"Open the [Report] Window"*
- *"Open Report Format Files"*
- *"Edit PDA Report Format"*
- *"Preview Before Printing"*
- *"Save Report Format Files"*

7.7.1 Open the [Report] Window

Open the [Report] window in either the [Realtime Analysis] program or the [Postrun Analysis] program. This section describes how to open the [Report] window in the [Postrun Analysis] program.


- 1 Click the  (Report Format) icon on the [Main] assistant bar in the [Postrun Analysis] program.

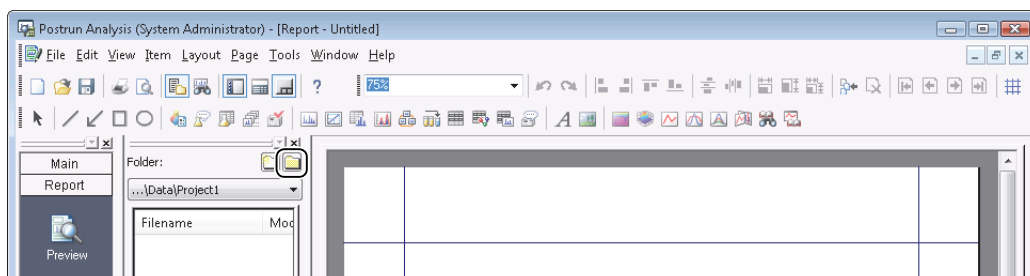


The [Report] window opens.

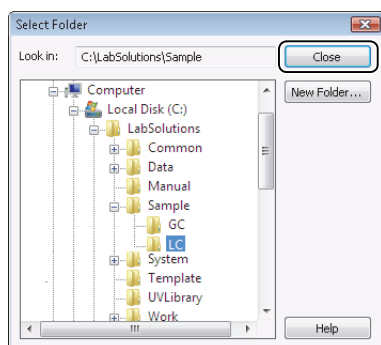
7.7.2 Open Report Format Files

Several report format files are pre-installed in the \LabSolutions\Sample\LC folder. This section describes how to open the report format file “PDA data analysis results.lcr”.

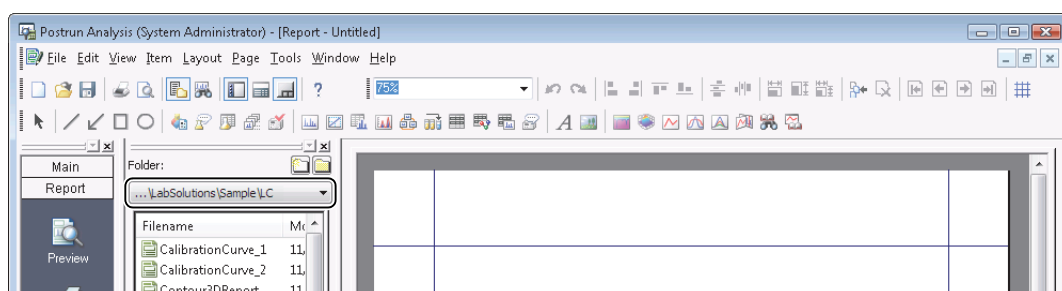
- 1 Click  (Select Folder) in the [Data Explorer] sub-window.



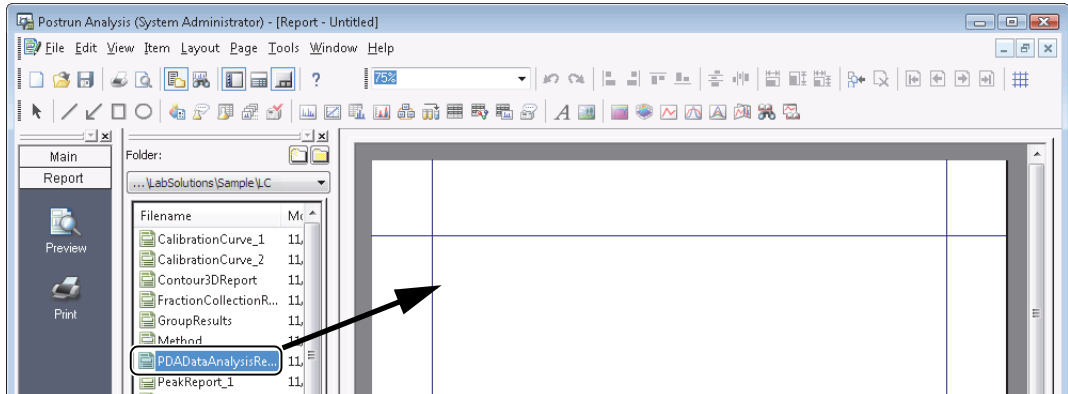
- 2 Select “\LabSolutions\Sample\LC”, and click [Close].



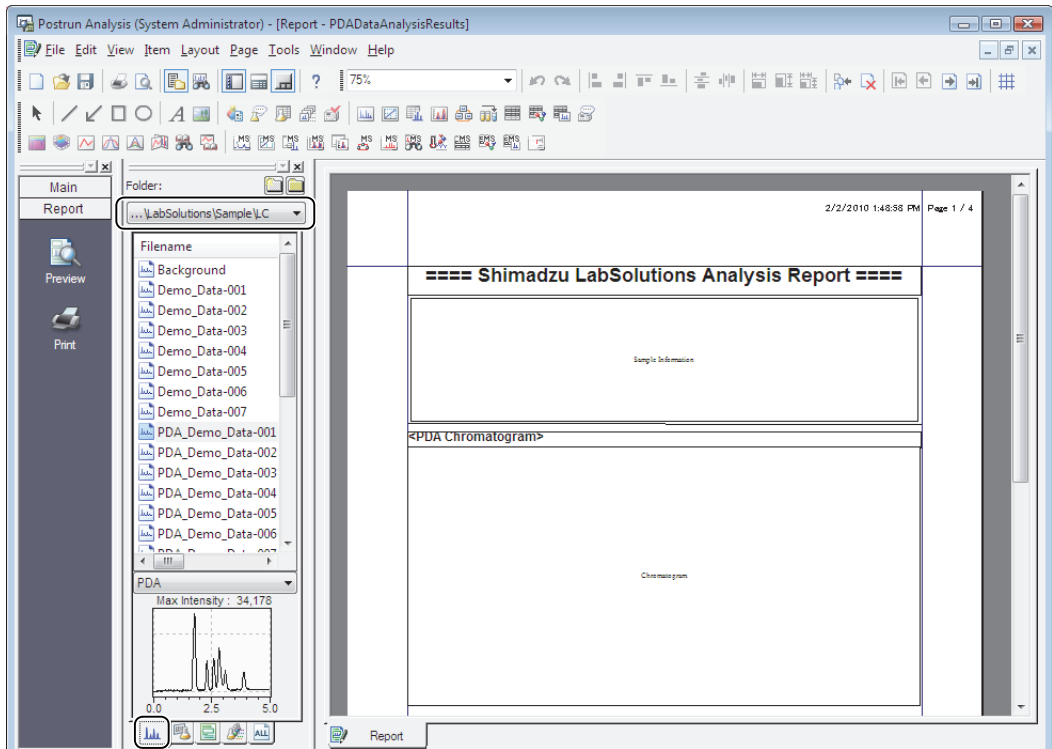
The “\LabSolutions\Sample\LC” folder is displayed in the [Data Explorer] sub-window.



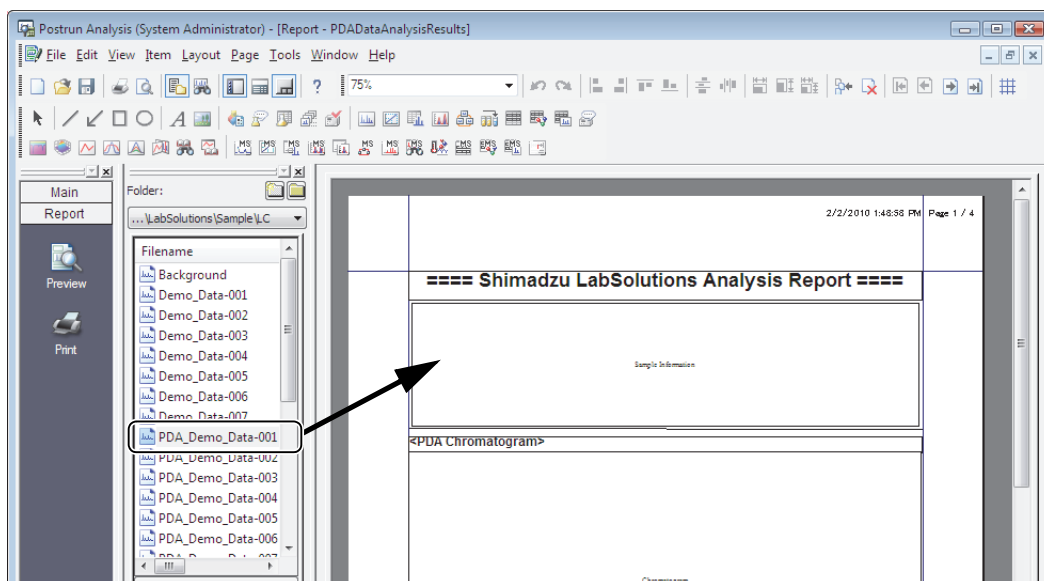
3 Drag-and-drop “PDA data analysis results.lcr” onto the [Report] window.



4 Click the (Data) tab in the [Data Explorer] sub-window, and select the appropriate data file folder.

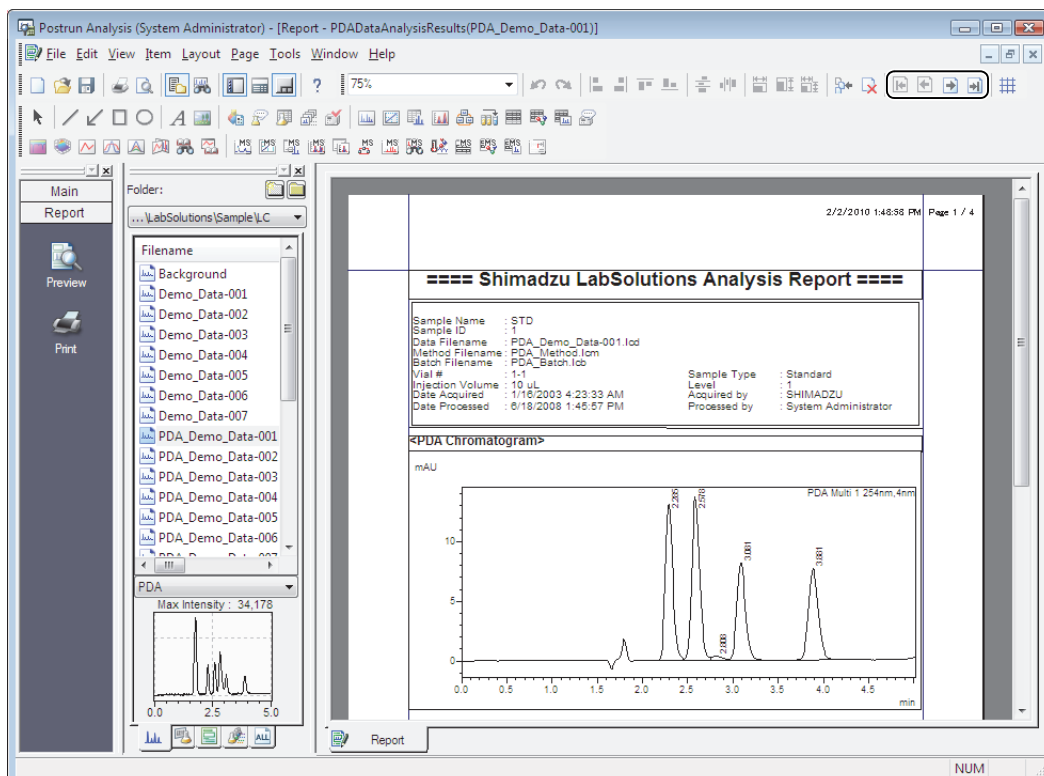


5 Drag-and-drop the data file into the report format.




The data file is loaded into the report format and displayed.

6 If the report includes multiple pages, use the icons on the toolbar to review the content of the other pages.

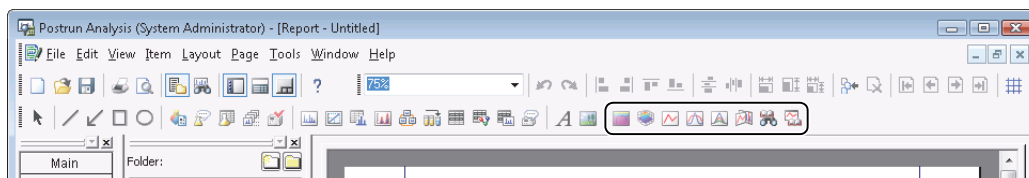










NOTE

If the desired data file is not displayed in the [Data Explorer] sub-window, click  (Select Folder), and specify the folder that contains the desired data file.

7.7.3 Edit PDA Report Format

The following 8 report items are provided for inclusions in the PDA data analysis format.



Item	Contents
 Contour Graph	Prints the contour graph and 3D graph of the data acquired by the PDA detector.
 3D Graph	Reference For details, see "Change the Display Color and Scale of the Contour View" P.210.
 UV Spectrum	Prints the information in the spectrum files and the spectra extracted from the data acquired by the PDA detector. Reference For details, see "Change the Content and Print Scale for UV Spectra" P.212.
 Peak Purity	Prints the peak purity calculation results for the data acquired by the PDA detector.
 Peak Profile	Reference For details, see "Specify the Peaks and Calculation Method to Print the Peak Purity Calculation Results" P.216.
 UV Spectrum Index	Prints the identified peak information and its spectrum.
 UV Library Search	Prints the library search results for the data acquired by the PDA detector. Reference For details, see "Change the Content and Print Scale for Library Search Results" P.214.
 UV Library	Prints a list of the spectrum information registered to the UV spectrum library.

This section describes how to edit items in the report format file opened at ["7.7.2 Open Report Format Files"](#).

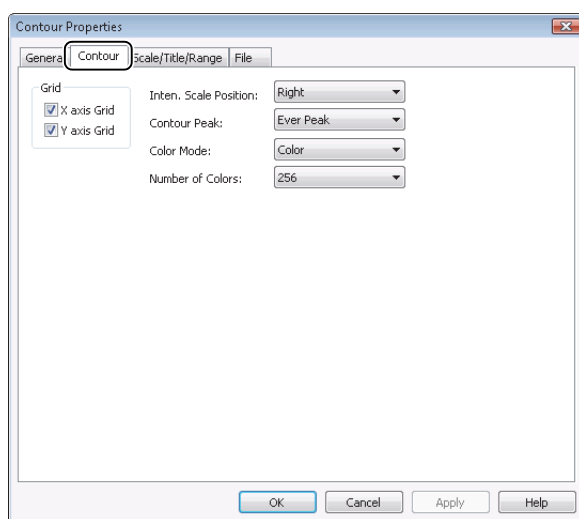
Change the Display Color and Scale of the Contour View

Use the pre-installed report format file "Contour3DReport.lsr" to print contour views. Refer to ["7.7.2 Open Report Format Files"](#) and open "Contour3DReport.lsr".

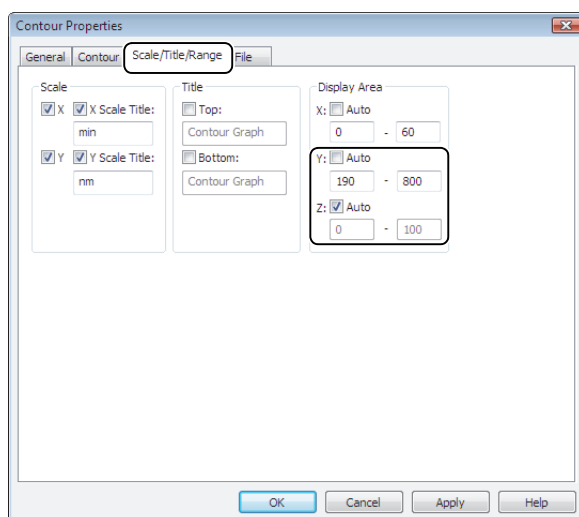
1 Double-click the [Contour Graph] item.

The [Contour Properties] sub-window is displayed.

2 Click the [Contour] tab, and set the [Inten. Scale Position], [Color Mode], and [Number of Colors] parameters.



3 Click the [Scale/Title/Range] tab, then under the [Display Area] deselect [Auto] for the X-axis (time), Y-axis (wavelength) and X-axis (intensity). Enter the desired scale for each.



4 Click [OK].

Reference

For details, see ["7.7.4 Preview Before Printing" P.218.](#)

Change the Display Scale of 3D Graphs

Use the pre-installed report format file "Contour3DReport.lsr" to print 3D graphs. Refer to ["7.7.2 Open Report Format Files"](#) to open "Contour3DReport.lsr".

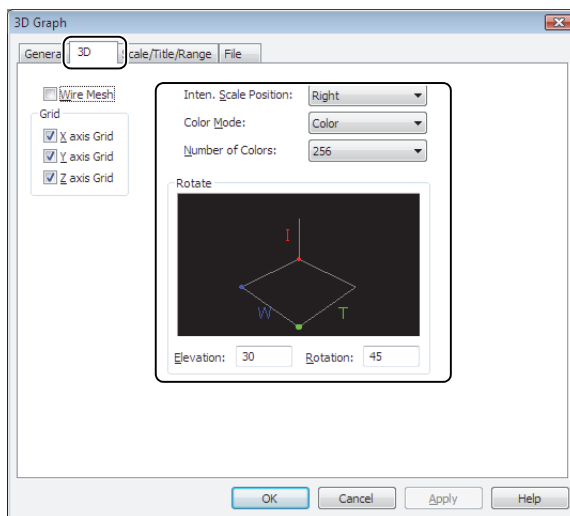
1 Double-click the [3D Graph] item.



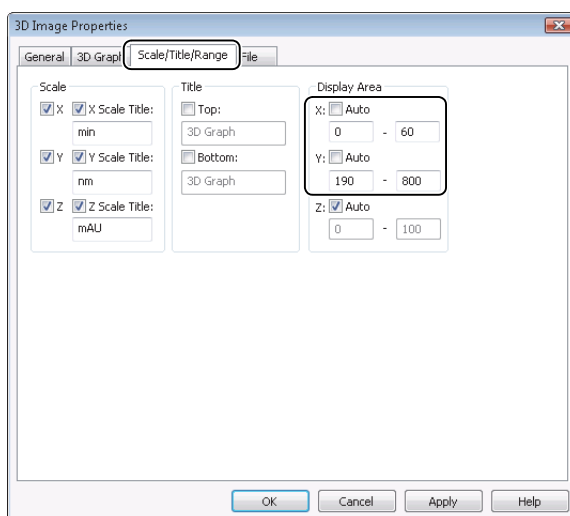
NOTE

The [3D Graph] item is located on the second page of "Contour3DReport.lsr".

2 Click the [3D] tab, and set the [Inten. Scale Position], [Color Mode], [Number of Colors], and [Rotate] parameters.



3 Click the [Scale/Title/Range] tab and under the [Display Area], deselect [Auto] for the X-axis (time), Y-axis (wavelength) and Z-axis (intensity). Enter the desired scale for each.



4 Click [OK].



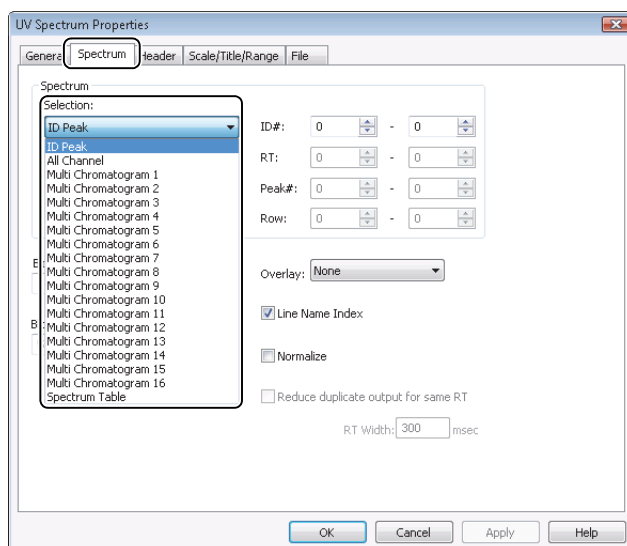
Reference

For details, see ["7.7.4 Preview Before Printing" P.218.](#)

Change the Content and Print Scale for UV Spectra

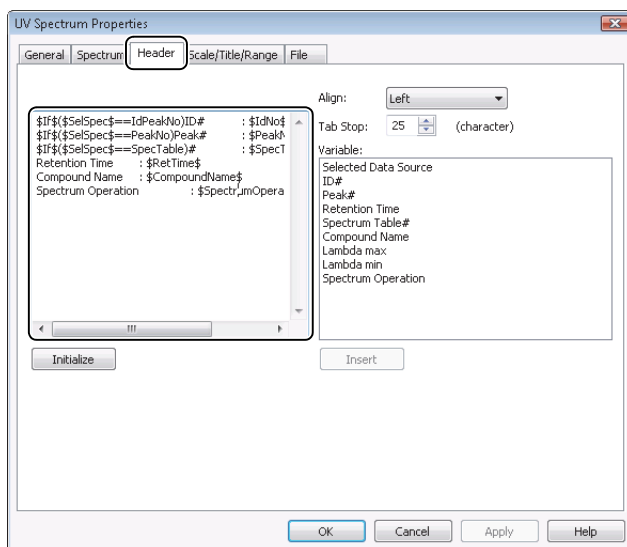
Use the pre-installed report format file “PDADDataAnalysisResults.Isr” to print UV spectra. Refer to [“7.7.2 Open Report Format Files”](#) to open “PDADDataAnalysisResults.Isr”.

- 1 Double-click the [UV Spectrum] item.
- 2 Click the [Spectrum] tab, and select the spectrum from the [Selection] list.

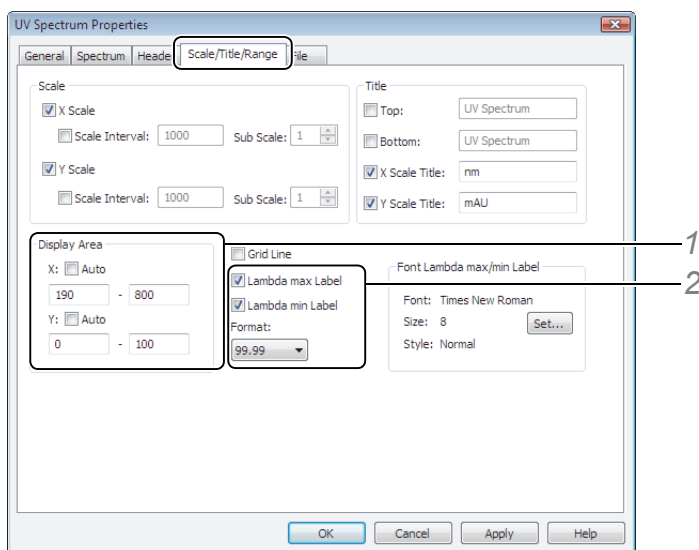


Parameter	Explanation
ID Peak	Selects the spectra to print by entering the ID#s of the compounds in the Compound Table. The spectra of all identified peaks are printed if [0]-[0] is entered.
All Channel	Select the retention time range at [RT]. The spectra of all detected peaks are printed if [0]-[0] is entered. If multiple peaks are detected, the printed spectra can be easily checked by selecting [Reduce duplicate output for same RT].
Multi Chromatogram	Sets the number of the peak at [Peak #]. The spectra of all detected peaks are printed if [0]-[0] is entered.
Spectrum Table	Sets the row No. of the table at [Row]. All of the spectra registered in the Spectrum Table are printed if [0]-[0] is entered.

3 Click the [Header] tab, and edit the items to display in the report.



4 Click the [Scale/Title/Range] tab.



- 1 Deselect [Auto] for the X-axis (wavelength) and Y-axis (intensity) in the [Display Area], and enter the desired scale.
- 2 To output reports of lambda max or lambda min spectrum, select [Lambda max Label] or [Lambda min Label], and click [Format].

5 Click [OK].

Reference

Refer to "7.7.4 Preview Before Printing" P.218 for details.

Change the Content and Print Scale for Library Search Results

Use the pre-installed report format file "PDADDataAnalysisResults.lsr" to print library search results. Refer to "7.7.2 Open Report Format Files" to open "PDADDataAnalysisResults.lsr".



NOTE

Data processing parameter changes on the [Library Search] tab for the data file are not printed even if the library search results are printed. Add the [Method] item to print the settings made on the [Library Search] tab.

1

Double-click the [UV Library Search] item.



NOTE

The [UV Library Search] item is located on the second page of "PDADDataAnalysisResults.lsr".

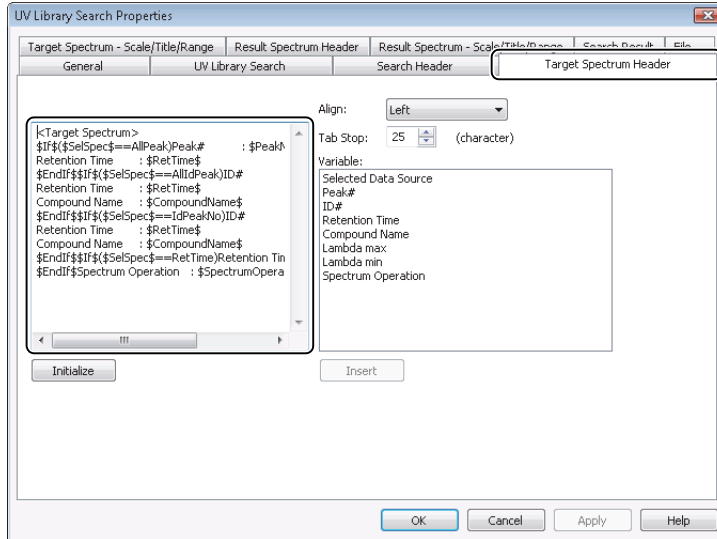
2

Click the [UV Library Search] tab.

- 1 Select the searched peaks to display in the [Selection] list.
- 2 Enter the number of hits to display at [# of Hits].
- 3 Select the target spectrum print method at [Display target spectrum].

3 Click each of the [Search Header], [Result Spectrum Header], and [Target Spectrum Header] tabs, and edit the header information to display in the report.

The [Target Spectrum Header] tab is shown in the following example.

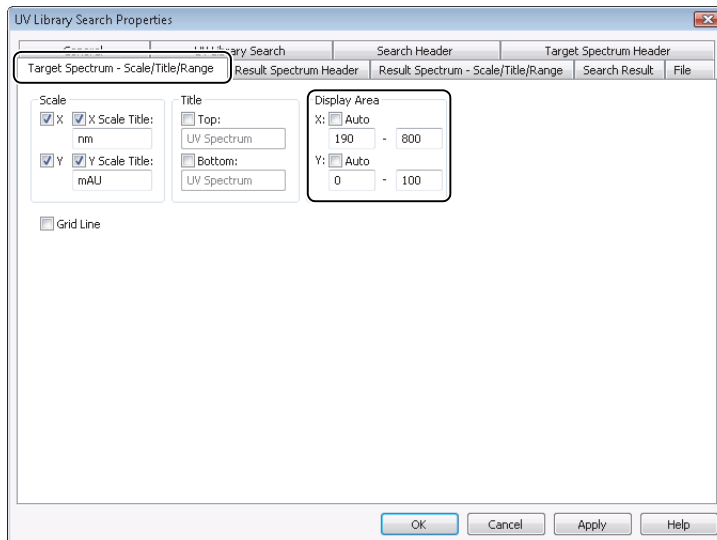


Reference

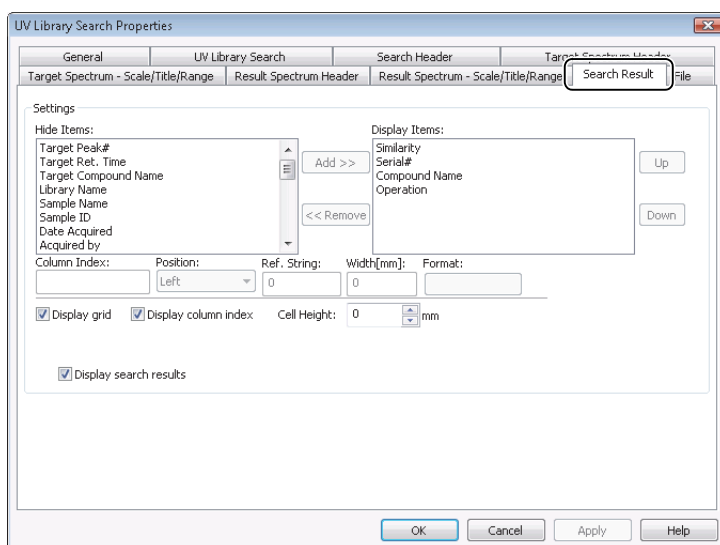
Refer to "8.5.11 Edit Calibration Curve Information" P.247 for more details.

4 Click each of the [Result Spectrum - Scale/Title/Range], and [Target Spectrum - Scale/Title/Range] tabs and under [Display Area], deselect [Auto] for X-axis (wavelength) and Y-axis (intensity). Then, enter the desired scale.

The [Target Spectrum - Scale/Title/Range] tab is shown in the following example.



- 5** Click the [Search Result] tab, and select the table information to be displayed for each of the spectra hit (found) in the search.



- 6** Click [OK].

Reference

Refer to ["7.7.4 Preview Before Printing" P.218](#) for details.

■ Specify the Peaks and Calculation Method to Print the Peak Purity Calculation Results

Use the pre-installed report format file "PDADDataAnalysisResults.lsr" to print peak purity calculation results. Refer to ["7.7.2 Open Report Format Files"](#) to open "PDADDataAnalysisResults.lsr".

NOTE

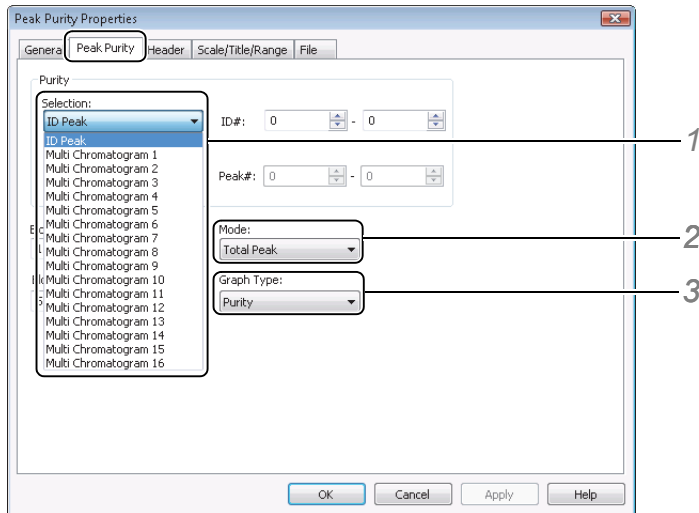
Data processing parameter changes made on the [Purity] tab for the data file are not printed even if the peak purity calculation results are printed. Add the [Method] item to print the settings made on the [Purity] tab.

- 1** Double-click the [Peak Purity] item.

NOTE

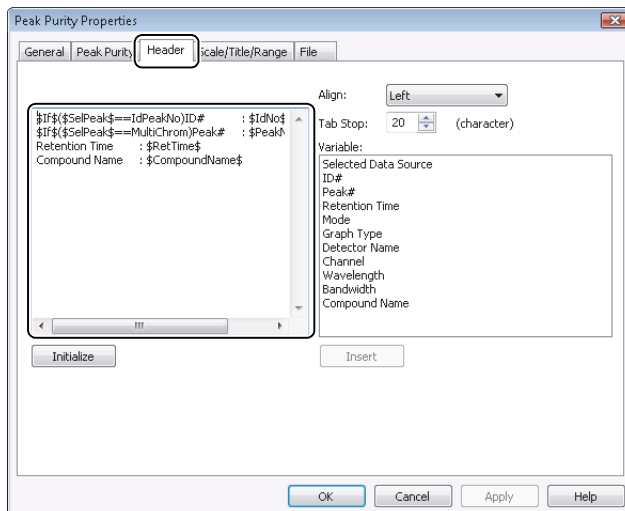
The [Peak Purity] item is located on the third page of "PDADDataAnalysisResults.lsr".

2 Click the [Peak Purity] tab.



- 1 Select the peaks to display in the [Selection] list.
If [ID Peak] is selected, select the calculation results to print by entering the ID#s of the compounds in the Compound Table. The calculation results of all identified peaks are printed if [0]-[0] is entered.
If [Multi Chrom] is selected, select the number of the peak at [Peak #]. The calculation results of all detected peaks are printed if [0]-[0] is entered.
- 2 Select the purity calculation mode in the [Mode] list.
- 3 Select the display graph in the [Graph Type] list.

3 Click the [Header] tab, and edit the items to display in the report.



Reference

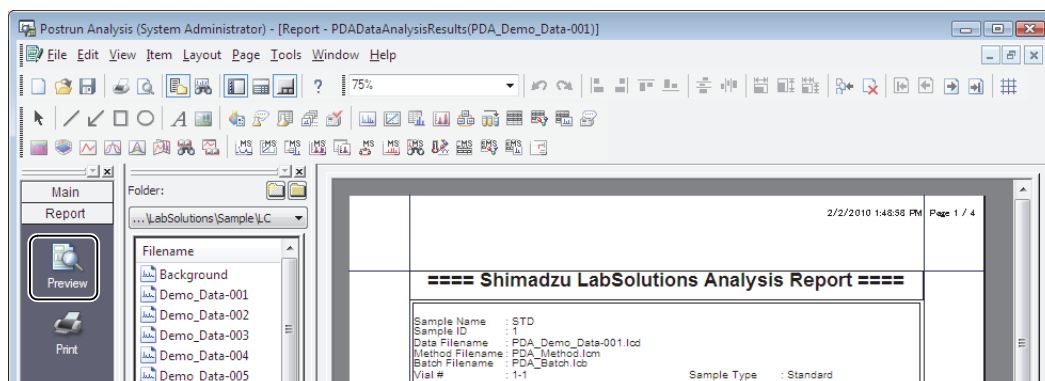
Refer to ["8.5.11 Edit Calibration Curve Information" P.247](#) for details.

4 Click [OK].

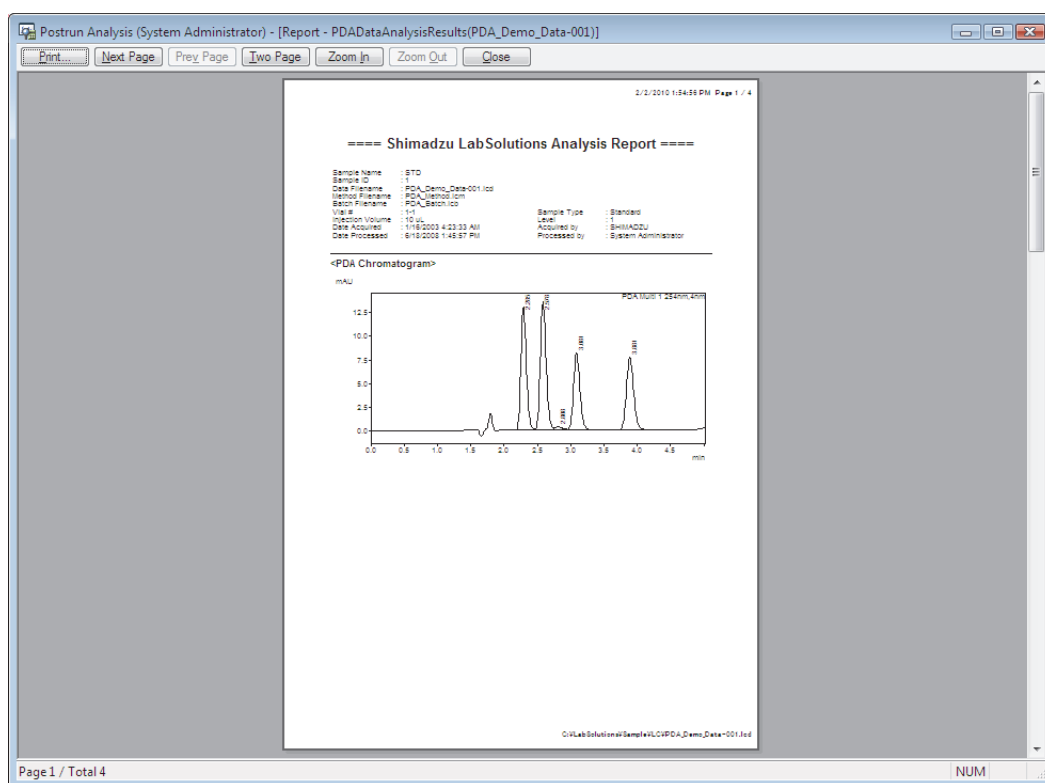
7.7.4 Preview Before Printing

Preview the print details set in "7.7.3 Edit PDA Report Format" before printing the report.

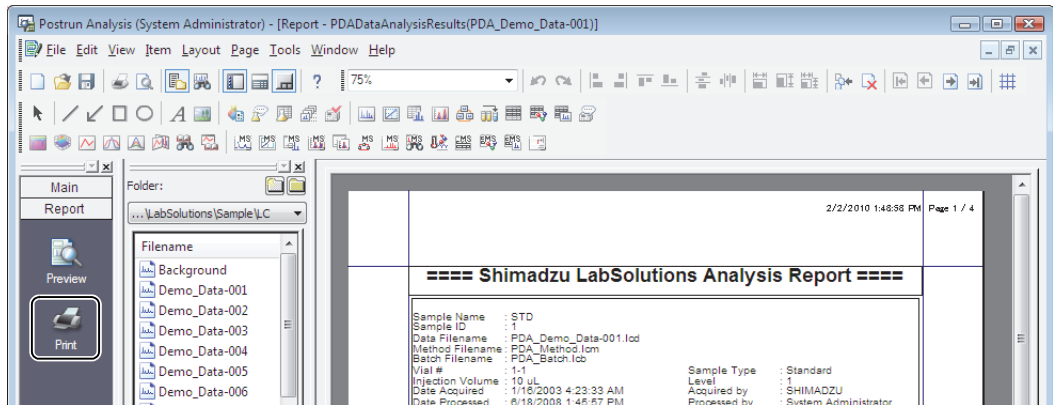
- 1 Click the  (Preview) icon on the [Report] assistant bar.



- 2 Check the report in the preview sub-window, and click [Close].



3 Click the (Print) icon on the [Report] assistant bar.

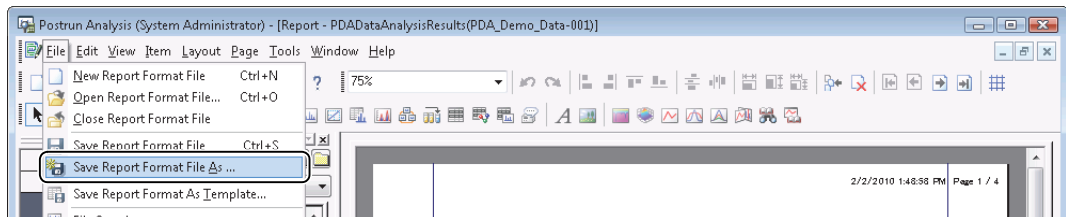


The report is printed.

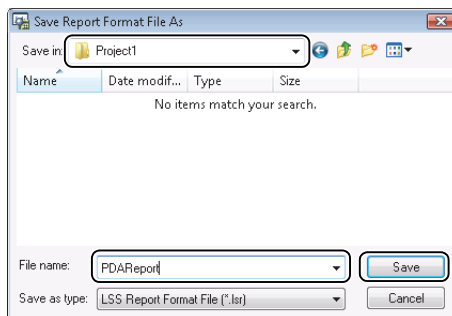
7.7.5 Save Report Format Files

Once a report format is complete, save the report format file under a new name.

1 Click [Save Report Format File As] on the [File] menu.



2 Set [Save in], enter the file name, and click [Save].



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8

Report Function

This chapter describes how to use the report function to print chromatograms and quantitative results. Use the report format function, to combine report items, such as sample information, chromatograms and quantitative results, to create reports in various formats.

8.1 Print Reports in Batch Processing

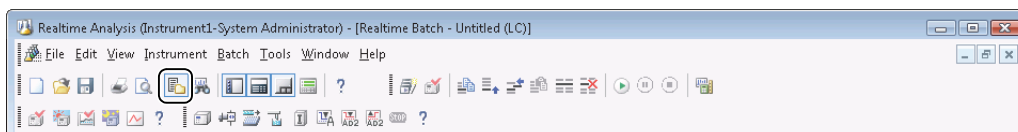
This section describes how to use the Batch Table to print reports in realtime batch.

Reference

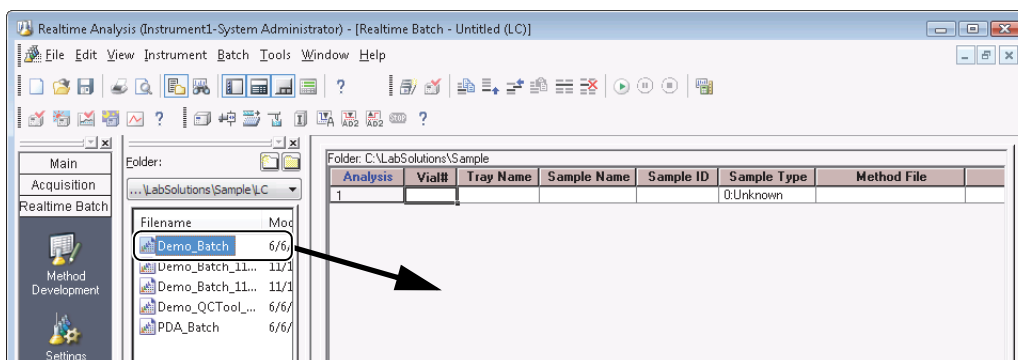
Refer to *"4.2 Create Batch Tables" P.63* for details on creating a new Batch Table.

1 Click the  (Realtime Batch) icon on the [Main] assistant bar in the [Realtime Analysis] program.

2 Click  (Toggle Data Explorer) on the toolbar.



3 In the [Data Explorer] sub-window, drag-and-drop the target batch file onto the Batch Table.

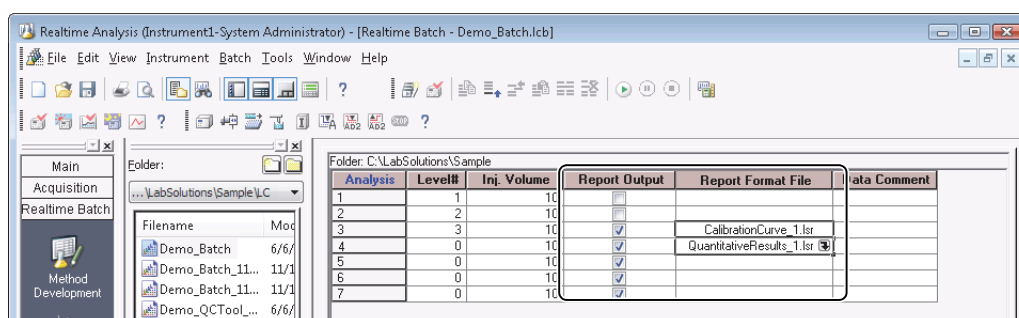


4 Select the [Report Output] cell in the desired rows, and select the [Report Format File].

- If a new report format file has not been created, select an installed report format file in the [Report Format File] cell.
- If a report format file has been created, select that report format file in the [Report Format File] cell.
- If the [Report Format File] cell is left blank, the default report format file "Default.lsr" is used to print the report.

Reference

- Refer to ["8.3.1 Installed Report Format Files" P.230](#) for details on pre-installed report format files.
- Refer to ["8.1.1 Change the Default Report Format File" P.222](#) for details on the default report format file.



5 Click the (Start Realtime Batch) icon on the [Realtime Batch] assistant bar.

The report is automatically printed when data acquisition for the selected row is complete.

NOTE

Set the Batch Table in the same way in the [Postrun Batch] window, to automatically print reports in postrun batch.

Reference

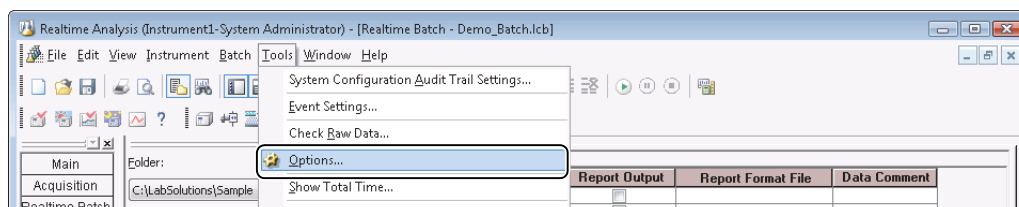
Refer to ["4.4.4 Print a Summary Report" P.89](#) for details on outputting summary reports.

8.1.1 Change the Default Report Format File

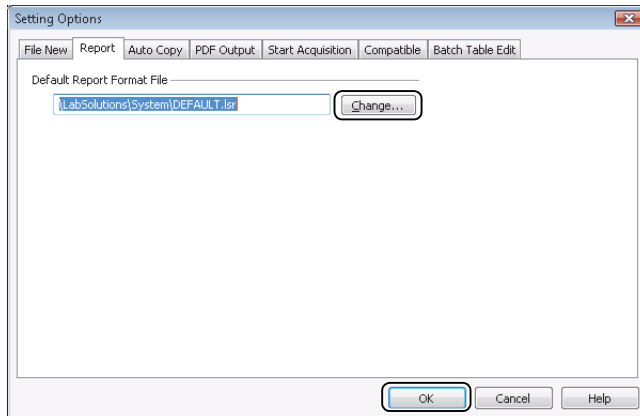
When [Report Output] is selected for single run or realtime batch, reports are printed in a pre-determined default report format even if a report format file is not set.

This section describes how to change the default report format file in the [Realtime Batch] window.

1 Click [Options] on the [Tools] menu in the [Realtime Batch] window.



2 Click [Change] on the [Report] tab, set the report file to change, and click [OK].



NOTE

- Do not delete or move the default report format file.
- If the [Report Format File] cell is left blank and [Report Output] is selected, reports are printed in the report format saved in each data file.

Reference

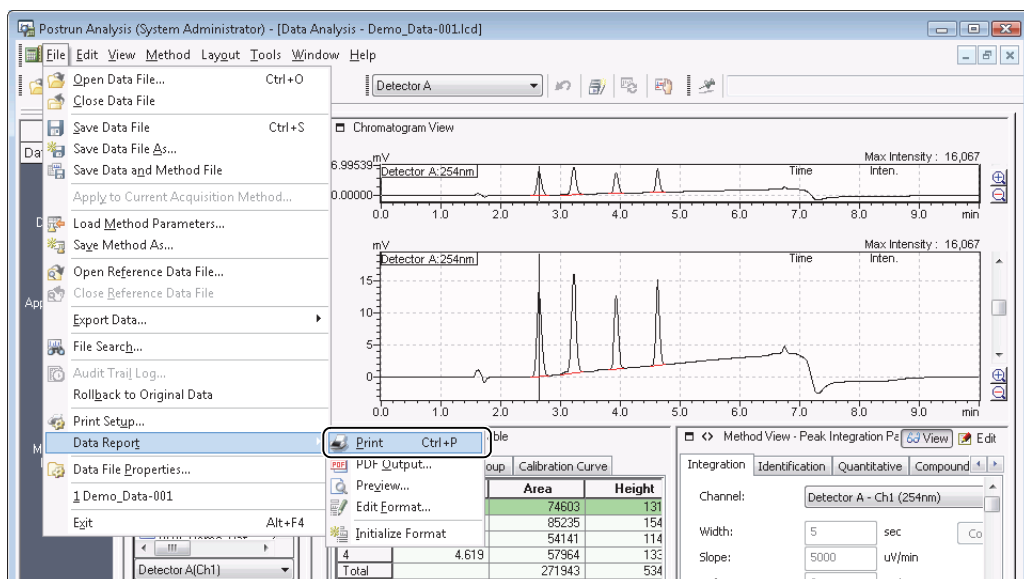
Refer to "8.2 Print Data Processing Results" P.223 for details on the report format saved in each data file.

8.2 Print Data Processing Results

8

This section describes how to print reports from data files in the [Data Analysis] window or [PDA Data Analysis] window.

1 Open the data file in the [Data Analysis] window or [PDA Data Analysis] window, select [Data Report] on the [File] menu, and click [Print].



The report is printed.



NOTE

- If a report format file was not specified at the time of data acquisition, the default report format file [Default.lsr] is used to print the report.
- Select [Data Report] on the [File] menu, and click [Preview] to check the printed details. The preview sub-window opens.
- Select [Data Report] on the [File] menu, and click [Edit Format] to change the report format. The report format in the data file is edited.



Reference

Refer to "[8.4 Create a Report Format File](#)" P.232 for details on pasting new items to reports.

8.3 Edit Report Format Files


Sample report format files are installed in the \LabSolutions\Sample\LC (or \LabSolutions\Sample\GC) folder. First-time users should use these report format files as a base to make new report format files.

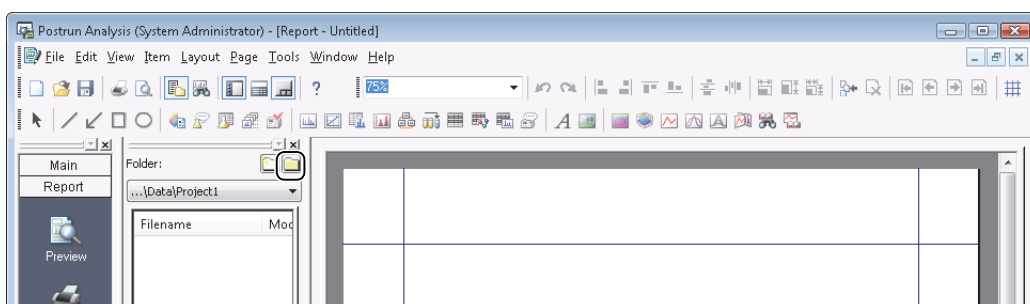
This section describes how to open the pre-installed report format file "peak report_1.lsr" in the [Report] window, and display the compound name in the peak top comment of the chromatogram.

Reference

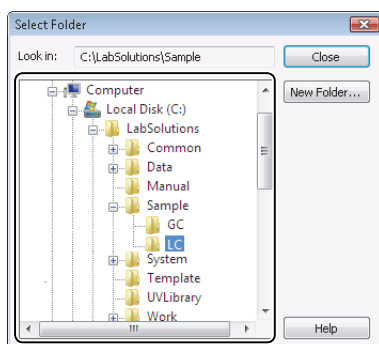
Refer to ["8.3.1 Installed Report Format Files" P.230](#) for details on pre-installed report format files.

- 1 Click the  (Report Format) icon on the [Main] assistant bar.
The [Report] window opens.

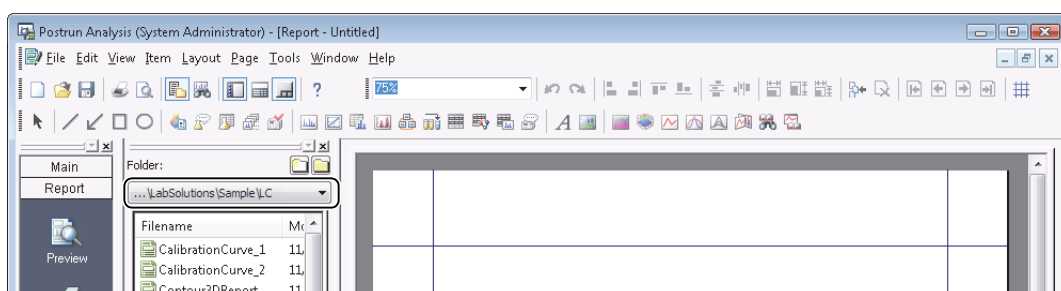
- 2 Click  (Select Folder) in the [Data Explorer] sub-window.



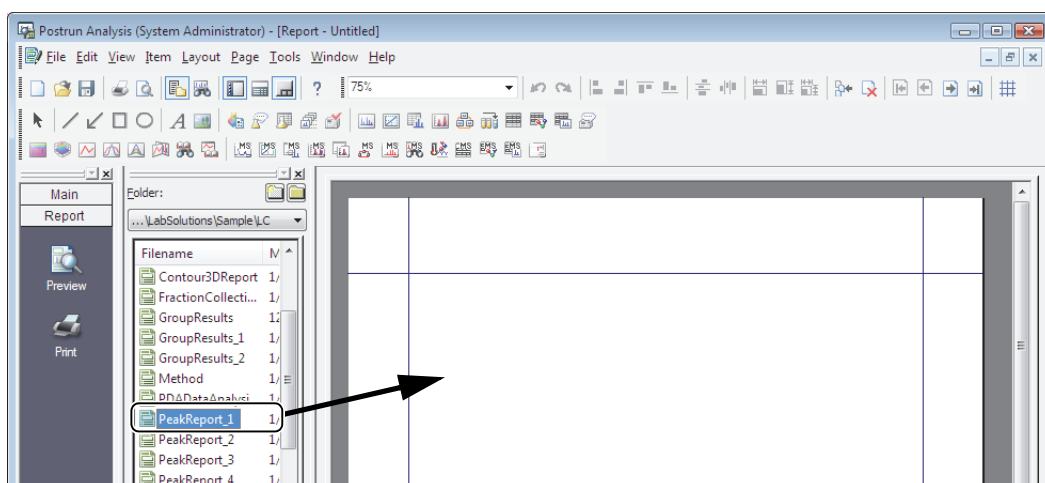
- 3 Select "\LabSolutions\Sample\LC" (or "\LabSolutions\Sample\GC"), and click [Close].




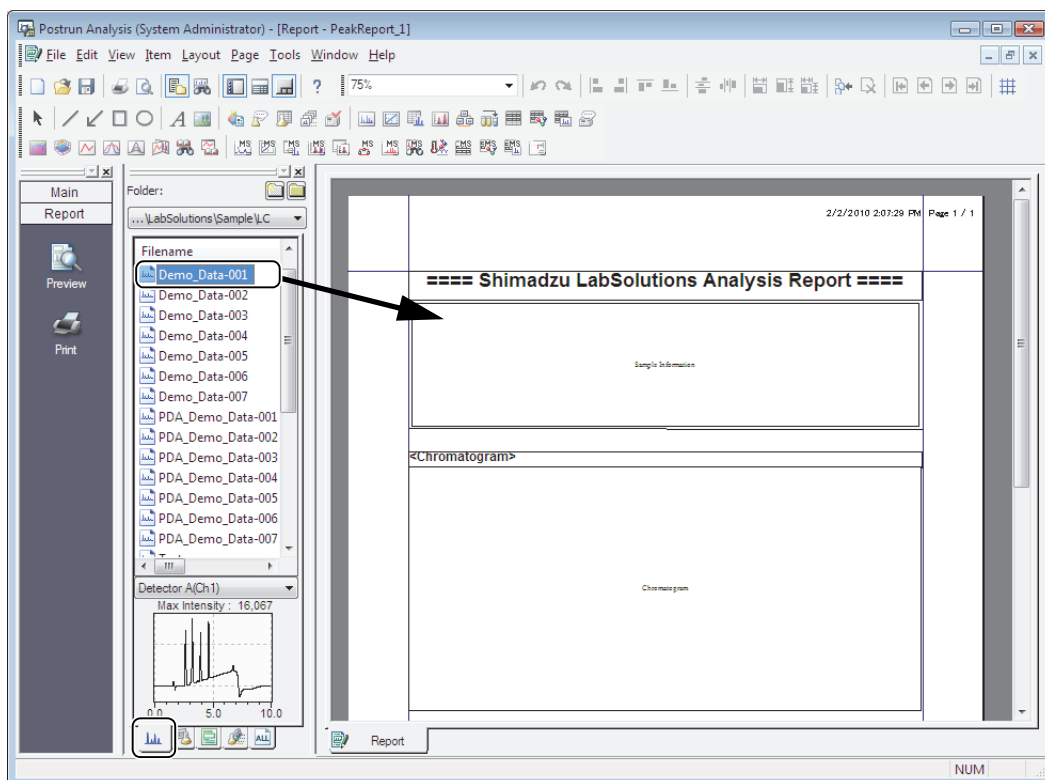
The contents of the "\LabSolutions\Sample\LC" (or "\LabSolutions\Sample\GC") [Folder] is displayed in the [Data Explorer] sub-window.



- 4** Drag-and-drop “peak report_1.lcr” from the [Data Explorer] sub-window onto the [Report] window.



- 5** Click the  (Data) tab at the bottom of the [Data Explorer] sub-window, and drag-and-drop the data file.



The contents of the data file is displayed in the [Report] window.

The screenshot displays the Postrun Analysis software window titled "Postrun Analysis (System Administrator) - [Report - PeakReport_1(Demo_Data-001)]". The interface includes a menu bar (File, Edit, View, Item, Layout, Page, Tools, Window, Help), a toolbar, and a sidebar with "Main", "Report", "Preview", and "Print" options. The "Report" window is active, showing a "Shimadzu LabSolutions Analysis Report" for "Demo_Data-001".

The report details include:

- Sample Name: STD
- Sample ID: 1
- Data Filename: Demo_Data-001.lod
- Method Filename: Demo_Method.lom
- Batch Filename: Demo_Batch.lob
- Injection Volume: 10 uL
- Date Acquired: 1/16/2003 5:26:02 AM
- Date Processed: 6/18/2008 1:49:47 PM
- Sample Type: Standard
- Level: 1
- Acquired by: SHIMADZU
- Processed by: System Administrator

The chromatogram, titled "<Chromatogram>", shows a plot of mV versus time (min) from 0.0 to 10.0. The y-axis ranges from 0 to 15. Several peaks are labeled with their retention times: 2.100, 3.200, 3.600, and 4.100. The detector is identified as "Detector A 254nm". A small inset chromatogram in the sidebar shows the same data with a "Max Intensity: 16.067".

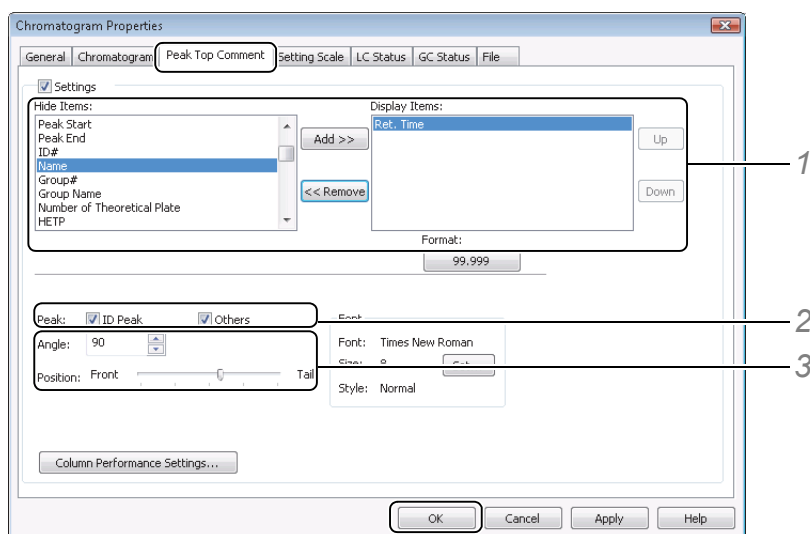
NOTE

If the data file is not displayed in the [Data Explorer] sub-window, click (Select Folder), and specify the folder that contains the desired data file.

6 Double-click the chromatogram item.

The [LC/PDA Chromatogram Properties] sub-window opens.

- 7** Click the **[Peak Top Comment]** tab, enter the **[Peak Top Comment]** tab parameters, and click **[OK]**.



- 1 Select **[Name]** in the **[Hide Items]** box, and click **[Add]**.
[Name] is displayed in the **[Display Items]** box.

**NOTE**

Click **[Format]** to open the **[Format Settings]** sub-window to edit the number of display digits and rounding method. Refer to ["8.5.9 Edit the Numeric Value Format in the Quantitative Results Table" P.245](#) for details.

- 2 Select **[ID Peak]** and **[Others]** to display the peak top comment on all detected peaks.
- 3 Enter the **[Angle]** or **[Position]** to change the angle or position of the peak top comment.

**NOTE**

The default angle is "90". Increase the value to rotate the comment counterclockwise from the start of the text string.

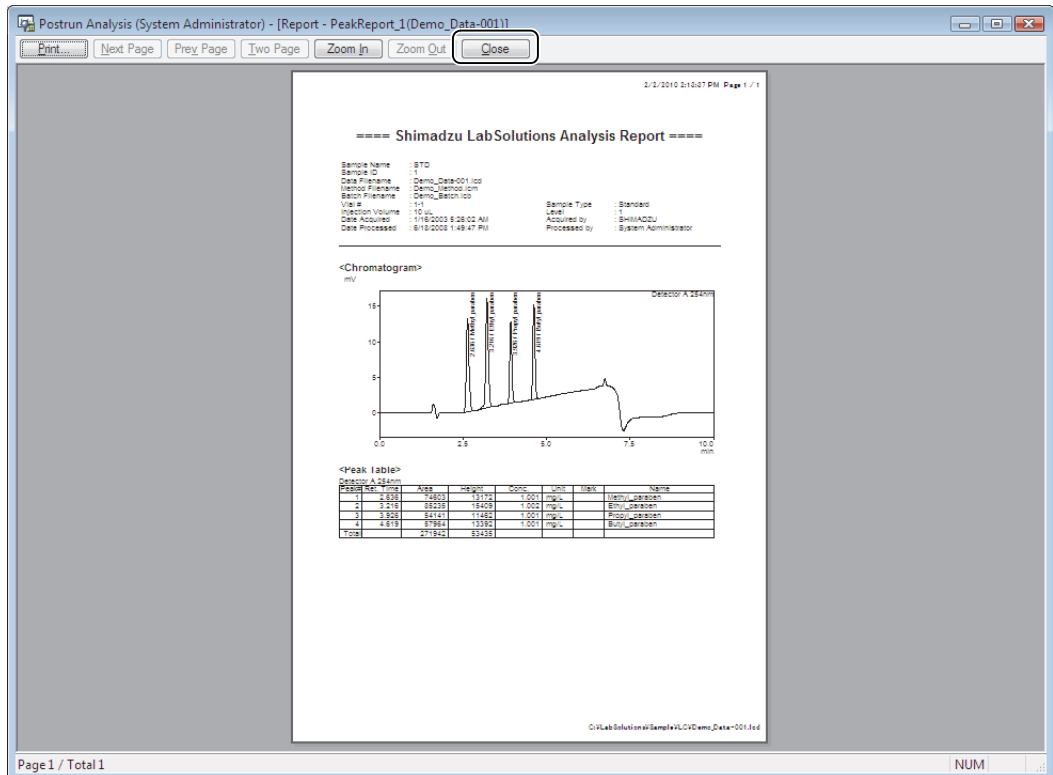
Reference

Refer to ["8.4 Create a Report Format File" P.232](#) for details on adding items to the report format. Refer to ["8.5 Edit Report Items" P.237](#) or ["7.7.3 Edit PDA Report Format" P.209](#) to edit other report format items.

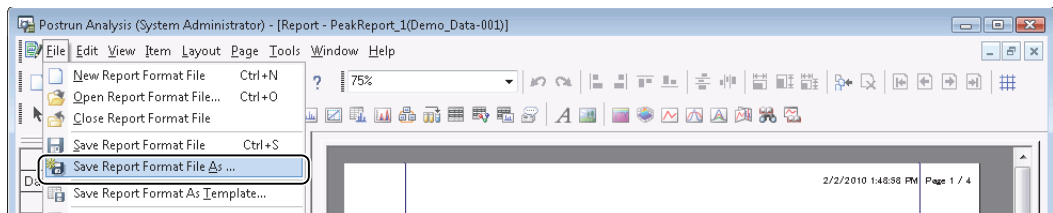
8

- Click the  **(Preview)** icon on the **[Report]** assistant bar.

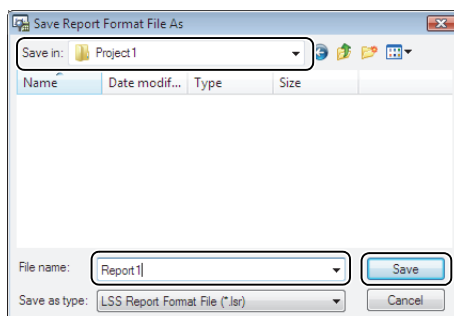
9 Preview the report, and click [Close].



10 Click [Save Report Format File As] on the [File] menu.



11 Enter a file name at [Save in], and click [Save].



8.3.1 Installed Report Format Files

The following report format files are installed.

Pre-installed report format files are saved to the \LabSolutions\Sample\LC (\LabSolutions\Sample\GC) folder.

Report Format File	Contents
Method.lsr	This file is used to print all instrument parameters and data processing parameters set in the method file.
CalibrationCurveReport_1.lsr	This file is used to print a calibration curve graph and calibration curve information.
CalibrationCurveReport_2.lsr	This file is used to print chromatograms, sample information, quantitative results, and calibration curve information.
CalibrationCurveReport_3.lsr	This file is used to print two blocks of calibration curve graph and rhe list.
QuantitativeResults_1.lsr	This file is used to print sample information, chromatograms, and quantitative results. (This is a basic report format file.)
QuantitativeResults_2.lsr	This file is used to print vertical stack display, sample information and quantitative results of chromatograms acquired by detector1 and detector2.
QuantitativeResults_3.lsr	This file is used to print horizontal stack display, sample information and quantitative results of chromatograms acquired by detector1 and detectorB.
QuantitativeResults_4.lsr	This file is used to print the chromatogram and quantitative results of detector1 on the first page, and the chromatogram and quantitative results of detector2 on the second page.
QuantitativeResults_5.lsr	This file is used to print the all chromatogram (overlay) and the quantitative results in landscape page.
PeakReport_1.lsr	This file is used to print sample information, chromatograms, and peak reports. (This is a basic report format file.)
PeakReport_2.lsr	This file is used to print chromatograms in landscape orientation.
PeakReport_3.lsr	This file is used to print basic method information in addition to the content of the basic format.
PeakReport_4.lsr	This file is used to print the chromatogram and the peak report in landscape page.
PeakReport_5.lsr	This file is used to print the divided chromatogram and the peak report.
PeakReport_CalibrationCurve.lsr	This file is used to print calibration curve information in addition to the content of the basic format.
SummaryReport_1.lsr	This file is used to print a summary of chromatograms and peak reports of multiple data.
SummaryReport_2.lsr	This file is used to print the concentration, area and height of multiple data by individual compound.
SummaryReport_3.lsr	This file is used to print the chromatograms and the statistical calculation results of the concentration, area and height of multiple data.
SummaryReport_4.lsr	This file is used to print the chromatogram(Landscape), and the quantitative summary report for each compound.
SummaryReport_5.lsr	This file is used to print the concentration summary report, the area summary report and the height summary report in landscape page.
SummaryReport_6.lsr	This file is used to print the chromatogram(overlay), and the quantitative summary report for each compound.
GroupResults_1.lsr	This file is used to print chromatograms and grouping results.

Report Format File	Contents
GroupResults_2.lsr	This file is used to print chromatograms, grouping results and group calibration curve.
BatchTable.lcr	This file is used to print the batch table in landscape page.
FractionCollectionReport.lsr(*1)	This file is used to print chromatograms and fraction collection results.
Contour3DReport.lsr(*1)	This file is used to print contour views and 3D graphs of PDA data.
PDADataAnalysisResults.lsr(*1)	This file is used to print chromatograms and PDA data analysis results (UV spectra, library search and peak purity).
GCMethodShort.lcr(*2)	This file is used to print the chromatogram and the peak report with general method parameters.
GCConfiguraton.lcr(*2)	This file is used to print the GC system configuration.

*1:\LabSolutions\Sample\LC folder only

*2:\LabSolutions\Sample\GC folder only

8.4 Create a Report Format File

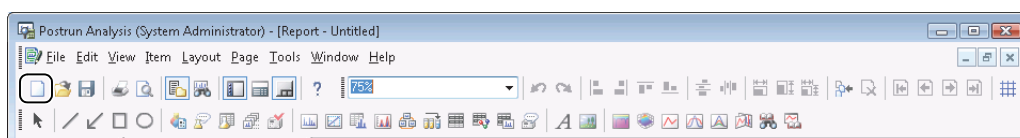
This section describes an example of how to make a new report format file in the [Report] window.

Reference

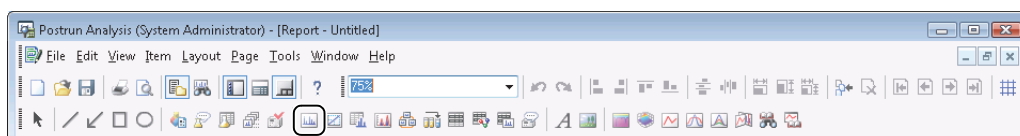
Refer to "8.5 Edit Report Items" P.237 for details.

1 Click the  (Report Format) icon on the [Main] assistant bar.

2 Click  (New) on the toolbar.



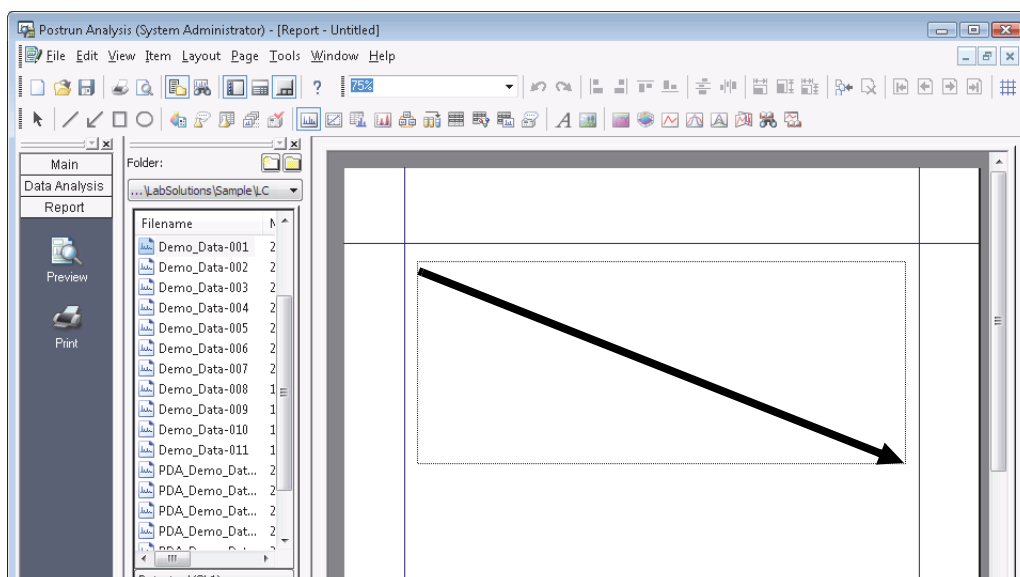
3 Click  (Chromatogram) on the toolbar.



Reference

Refer to "8.4.1 Types of Report Items" P.236 for details on each toolbar item.

4 Drag the cursor on the format to specify a range for the chromatogram.




- 5** In the [LC/PDA Chromatogram Properties] sub-window, correct the display position and edit the display items, and click [OK].

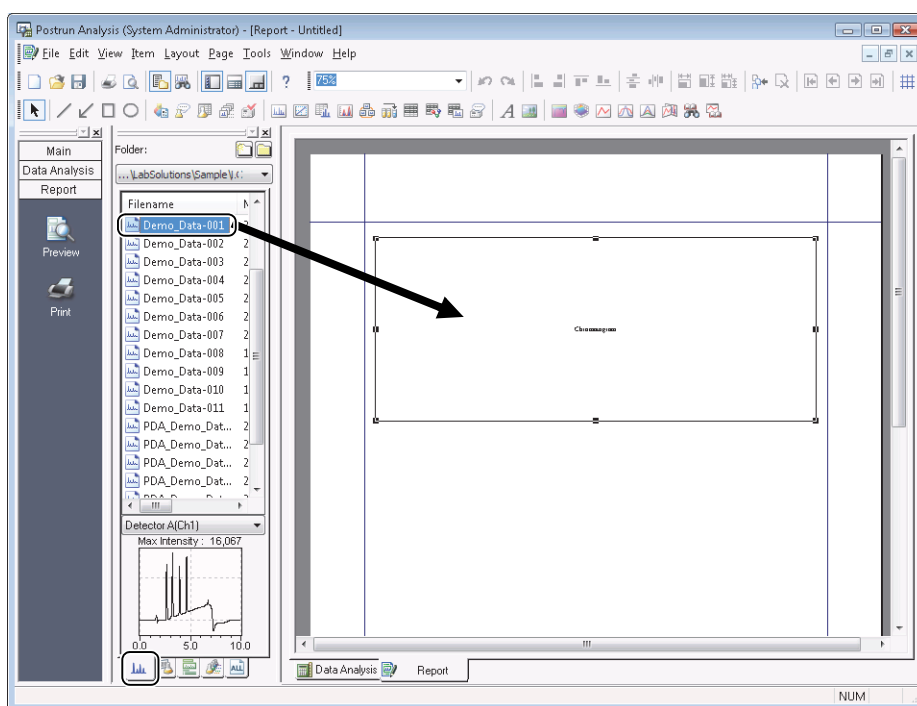
**NOTE**

Double-click inside the item frame to open the [LC/PDA Chromatogram Properties] sub-window.

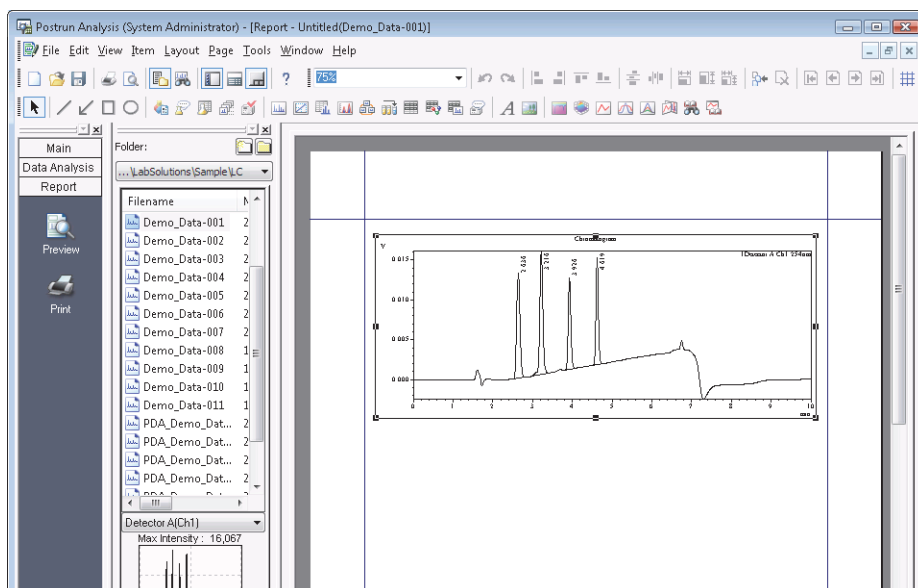
**Reference**

Refer to "8.5.1 Change the Chromatogram Properties" P.237 or "8.5.2 Chromatogram Display Scale" P.238 for details on editing the chromatogram display.


- 6** Click the  (Data) tab at the bottom of the [Data Explorer] sub-window and drag-and-drop the target data file onto the report format to examine the print details of a report format file.



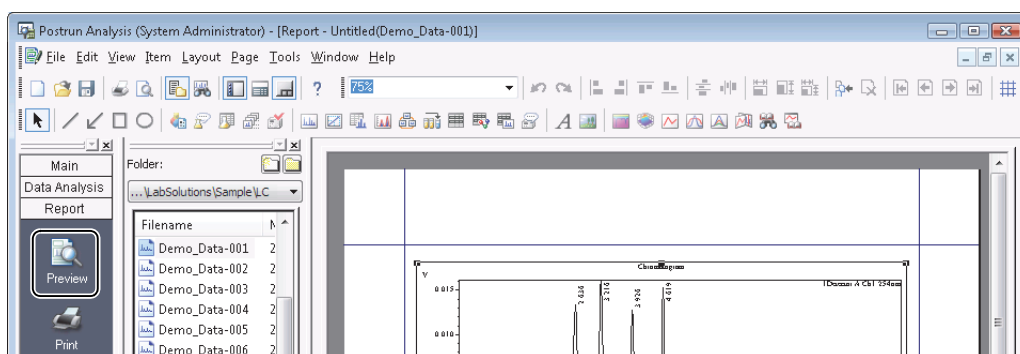
The chromatogram information of the data file is displayed in the [Report] window.



NOTE

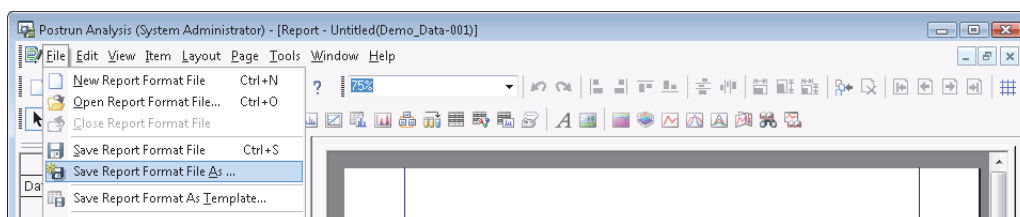
- Right-click on an item and click [Delete] to remove the item.
- Drag-and-drop the data file to a specific item with the [Shift] key held down to load data only to that item.
- If the data file is not displayed in the [Data Explorer] sub-window, click  (Select Folder), and specify the folder containing the desired data file.

7 Click the (Preview) icon on the [Report] assistant bar.

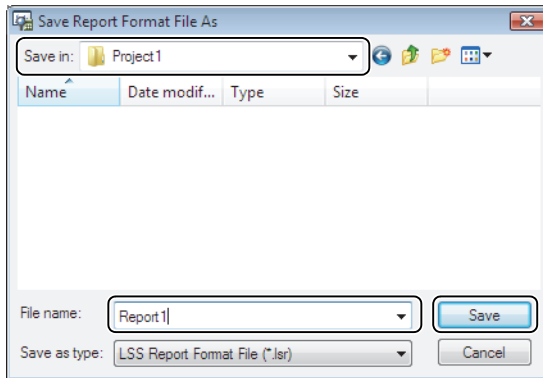


8 Examine the report in the preview sub-window, and click [Close].

9 Click [Save Report Format File As] on the [File] menu.

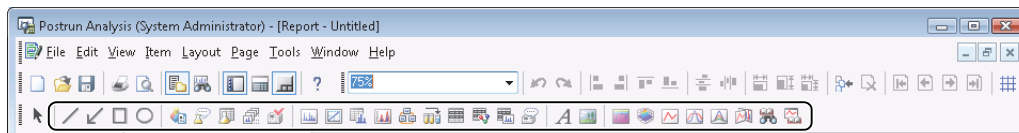




























10

 Specify a folder at [Save in], enter a [File Name], and click [Save].

8.4.1 Types of Report Items

Items, such as chromatograms and quantitative result information, can be added to the report format using the icons on the toolbar. The following report items are available.



Item	Content
 Figure	Use these icons to add a Line, Arrow, Rectangle or Ellipse to the report format.
 Text	Use this icon to add a text box to the report format.
 Picture	Use this icon to add bitmaps or other image files to the report format.
 System Configuration	Use this icon to add the instrument configuration at the time of data acquisition to the report format.
 Sample Information	Use this icon to add sample information to the report format.
 Method	Use this icon to add method file information, such as the instrument and data processing parameters to the report format.
 Batch Table	Use this icon to add the Batch Table and batch file settings to the report format.
 System Check	Use this icon to add the system check results saved in data files to the report format.
 Chromatogram	Use this icon to add chromatograms and instrument status information to the report format.
 Calibration Curve	Use this icon to add the calibration curve graph and information to the report format.
 Peak Table	Use this icon to add a table of the retention times and area values of detected peaks to the report format.
 Quantitative Results	Use this icon to add a table of the quantitative results of identified peaks to the report format.
 Group Results	Use this icon to add a table of the quantitative results for grouped compounds to the report format.
 Fraction Collection Report	Use this icon to add a table of the fraction collection status to the report format.
 Summary (Concentration)	Use this icon to add a summary of the chromatograms, statistical concentration results, areas and heights for multiple data acquisitions to the report format.
 Summary (Compound)	Use this icon to add a summary of the concentrations, areas and heights of multiple data by individual compound to the report format.
 Summary (Data)	Use this icon to add a summary of the chromatograms and Peak Tables for multiple data to the report format.
 Status Information	Use this icon to add contour graphs of PDA data to the report format.
 Contour Graph	Use this icon to add 3D graphs of PDA data to the report format.
 3D Graph	Use this item to add PDA spectra and spectra information to the report format.
 UV Spectrum	Use this icon to add the PDA peak purity results to the report format.
 Peak Purity	Use this icon to add the PDA peak profile information to the report format.
 Peak Profile	Use this icon to add PDA chromatograms and spectra for detected peaks to the report format.
 UV Spectrum Index	Use this icon to add UV Library Search results to the report format.
 UV Library Search	Use this icon to add a list of the spectra in the library file to the report format.
 UV Library	Use these icons to add a Line, Arrow, Rectangle or Ellipse to the report format.

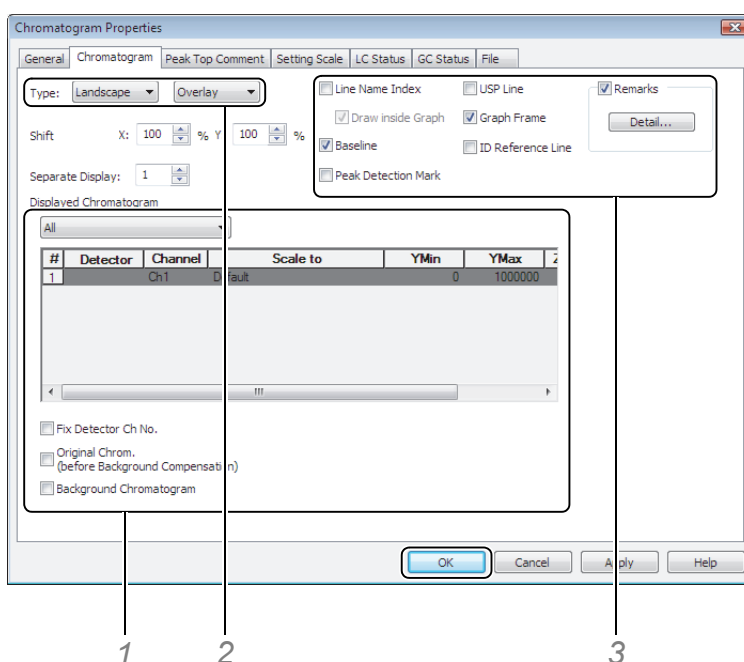
8.5 Edit Report Items

This section describes how to edit properties for each report item.

8.5.1 Change the Chromatogram Properties

The following section describes how to set the chromatogram display properties on the [Chromatogram] tab of the [Chromatogram Properties] sub-window.

- 1 Click the [Chromatogram] tab.
- 2 Enter the properties on the [Chromatogram] tab, and click [OK].



- 1 Select each of the checkboxes to print the [Baseline] and [Peak Detection Mark].
- 2 Click [Portrait] and [Overlay] in the [Type] list to draw chromatograms overlaid in a portrait orientation.
Click [Landscape] and [Separate] in the [Type] list to draw chromatograms overlaid in a landscape orientation.
- 3 Click [All] in the [Displayed Chromatogram] list.



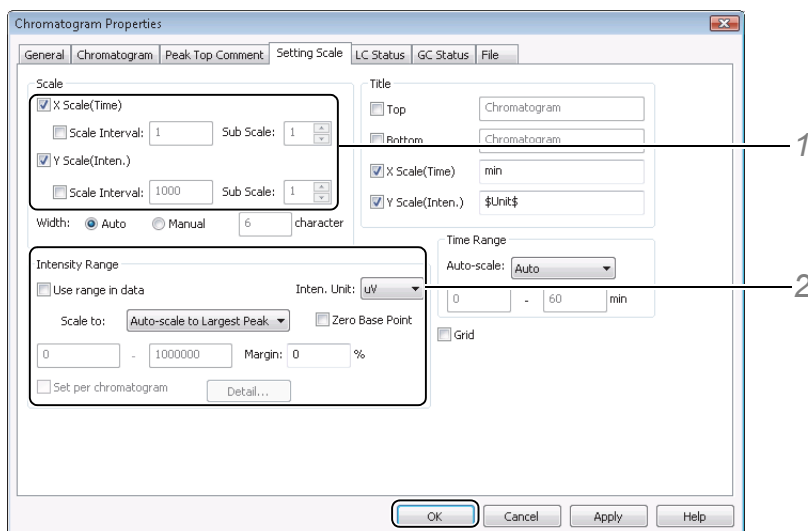
NOTE

- When [Select Chromatogram] in the [Displayed Chromatogram] list is selected and select the detector in [Detector], all of the channels set by that detector are displayed.
- When [No Chromatogram] is selected in the [Displayed Chromatogram] list, chromatograms are not displayed. Use this parameter to display only the instrument status.

8.5.2 Chromatogram Display Scale

Set the chromatogram display scale and scale interval on the [Setting Scale] tab in the [Chromatogram Properties] sub-window.

- 1 Click the [Setting Scale] tab.
- 2 Enter the properties on the [Setting Scale] tab, and click [OK].



- 1 Select [Scale Interval], and set the interval at [Scale Interval] and [Sub Scale] to display the scale on the intensity axis (Y-axis) and time axis (X-axis).
- 2 Deselect [Use range in data], and select the display unit and reference peak at [Inten. Unit] and [Scale to] to set the chromatogram intensity axis (Y-axis).

NOTE

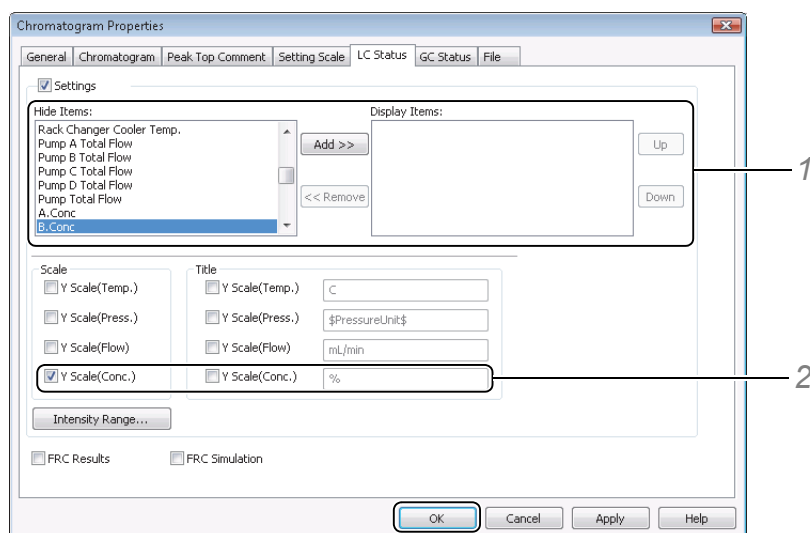
- The default setting is [Use range in data], and the intensity unit and intensity axis range saved in data files are used.
- If [Zero Base Point] is selected and a setting other than [User Defined] is selected at [Scale to], chromatograms are auto-scaled and displayed on the intensity axis of 0 V or more.
- Set the upper/lower width (margin) of the intensity axis at [Margin] when chromatogram displays are auto-scaled.
- If the intensity axis is unique for each chromatogram, for example, because the peak height of obtained by data acquisition differs for each detection channel, select [Set per Chromatogram] and enter the upper limit and lower limit values for each chromatogram.

8.5.3 Display the LC Instrument Status and Gradient Curve

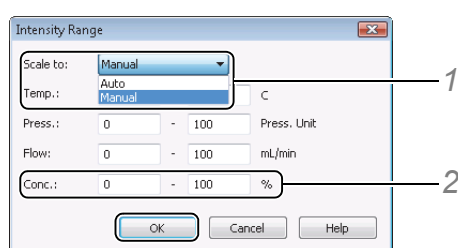
Use the [LC Status] tab of the [Chromatogram Properties] sub-window to overlay the instrument status information and gradient curve on chromatograms.

This section describes how to overlay the gradient curve for pump B (B.Conc%) on a chromatogram.

- 1 Click the [LC Status] tab.
- 2 Enter the [LC Status] tab parameters, and click [OK].



- 1 Select [B.Conc] in the [Hide Items] box, and click [Add].
[B.Conc] is added to the [Display Items] box.
 - 2 Select [Y Scale (Conc.)] at [Scale] and [Title].
- 3 Click [Intensity Range] to set the intensity axis range.



- 1 Click [Manual] in the [Scale to] list.
- 2 Enter the upper limit and lower limits at [Conc].
- 3 Click [OK].

- 4 Check the edited details, and click [OK].

8.5.4 Display the GC Instrument Status and Column Oven Temperature

To draw the instrument status information and column oven monitor temperature overlaid on chromatograms, set this on the [GC Status] tab in the [Chromatogram Properties] sub-window.

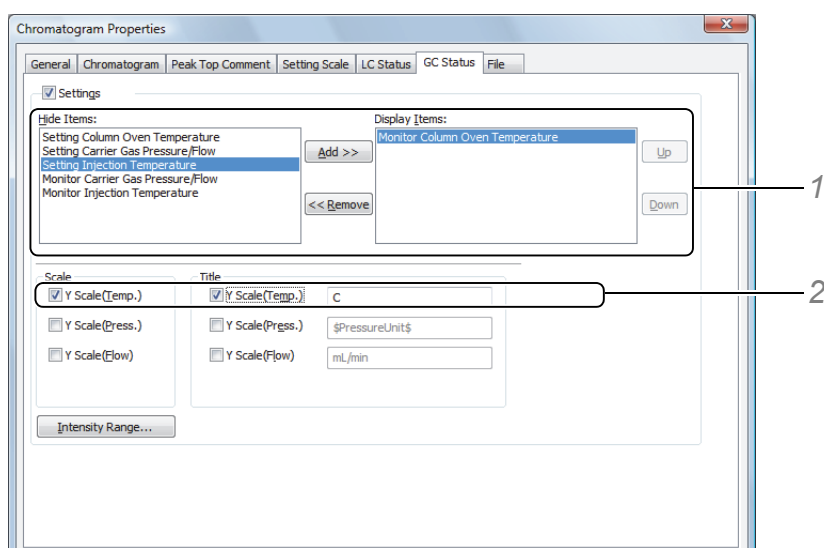
This section describes how to draw the column oven monitor temperature overlaid on chromatograms.

NOTE

- If [Save the Status Monitor] is selected in the [Properties] sub-window for the GC in the [System Configuration] sub-window, the monitor temperature can be displayed overlaid by performing data acquisition. The monitor temperature can be displayed only for the data file that retains monitor values.
- With the GC other than GC-2010 and GC-2014, status monitor values cannot be retained.

1 Click the [GC Status] tab.

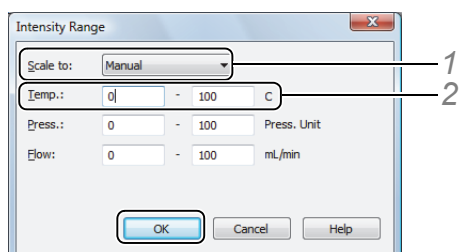
2 Set the [GC Status] tab.



1 Select [Monitor Column Oven Temperature] in the [Hide Items] list, and click [Add].
[Monitor Column Oven Temperature] is added to the [Display Item] list.

2 Select [Y Scale (Temp.)] at [Scale] and [Title].

3 Click [Intensity Range] to set the intensity axis range.



1 Select [Manual] in the [Scale to] list.

2 Enter the upper limit and lower limits at [Temp.].

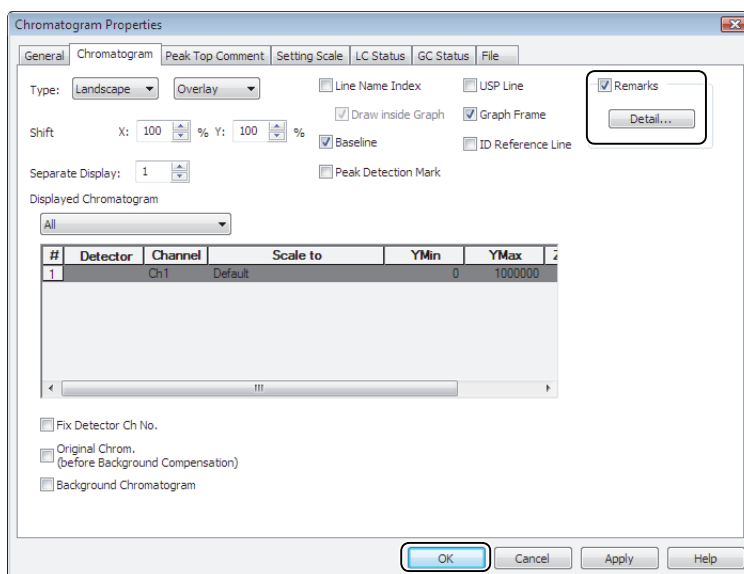
3 Click [OK].

4 Check the edited details, and click [OK].

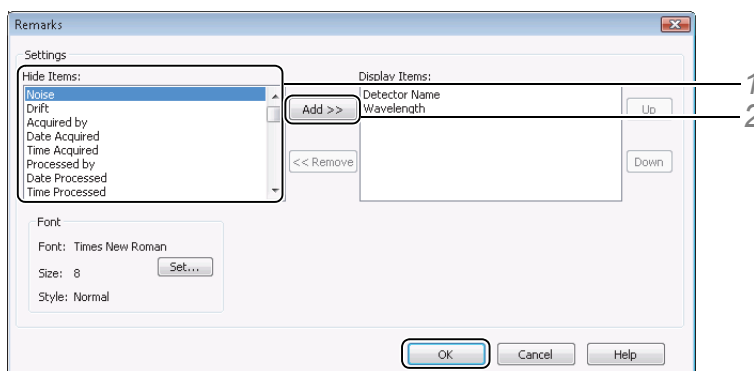
8.5.5 Edit Sample Information Display

Click [Remarks] on the [Chromatogram] tab of the [Chromatogram Properties] sub-window, and select the desired remark to display sample information in the chromatogram remarks section.

- 1 Click the [Chromatogram] tab, select [Remarks], and click [Detail].



- 2 Select the display item in the [Remarks] sub-window, and click [OK].

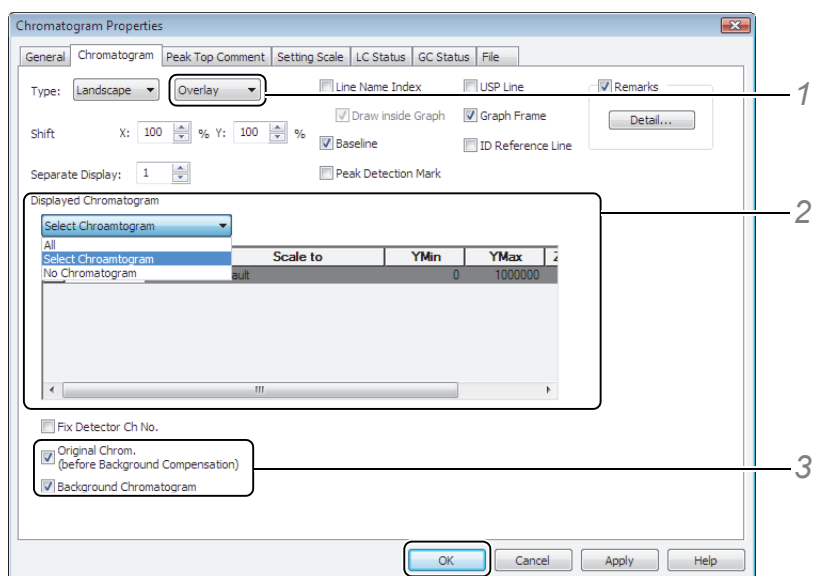


- 1 Select the items to print in the [Hide Items] box.
- 2 Click [Add].
The added items are displayed in the [Display Items] box.

8.5.6 Display the Background File

Use the [Chromatogram] tab in the [Chromatogram Properties] sub-window to overlay the background data or the chromatograms before background compensation.

- 1 Click the [Chromatogram] tab.
- 2 Enter the [Chromatogram] tab parameters, and click [OK].

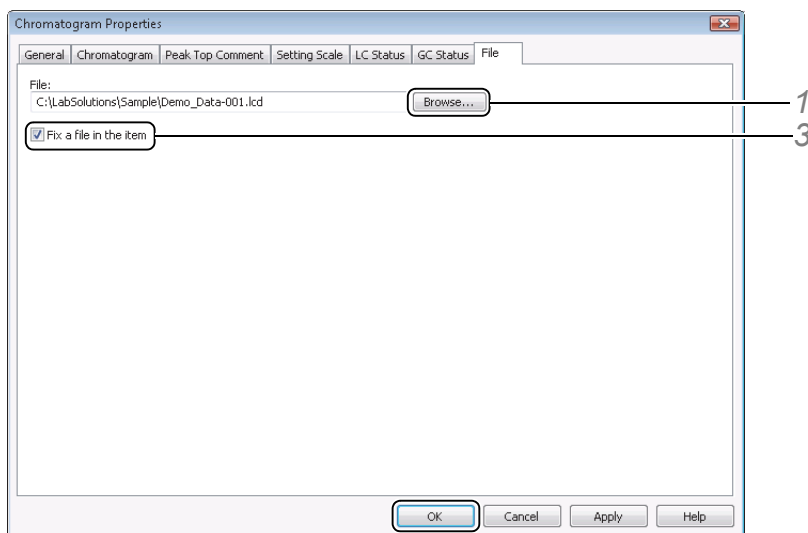


- 1 Click [Overlay] in the [Type] list.
- 2 Select the chromatograms to be overlaid at [Displayed Chromatogram].
- 3 Select [Original Chrom. (before Background Compensation)] and [Background Chromatogram].

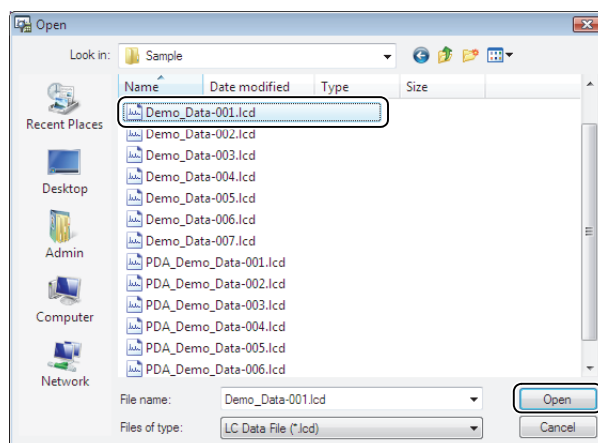
8.5.7 Attach a Specific Chromatogram to the Report Format

Enter a file on the [File] tab of the [Chromatogram Properties] sub-window to attach a specific (reference) chromatogram to the report format and cause the same chromatogram to be printed each time the report format is used to print data.

- 1 Click the [File] tab.
- 2 Select the [File] tab parameters, and click [OK].



- 1 Click [Browse] and select the desired data file, and click [Open].



- 2 Select [Fix file in the item].

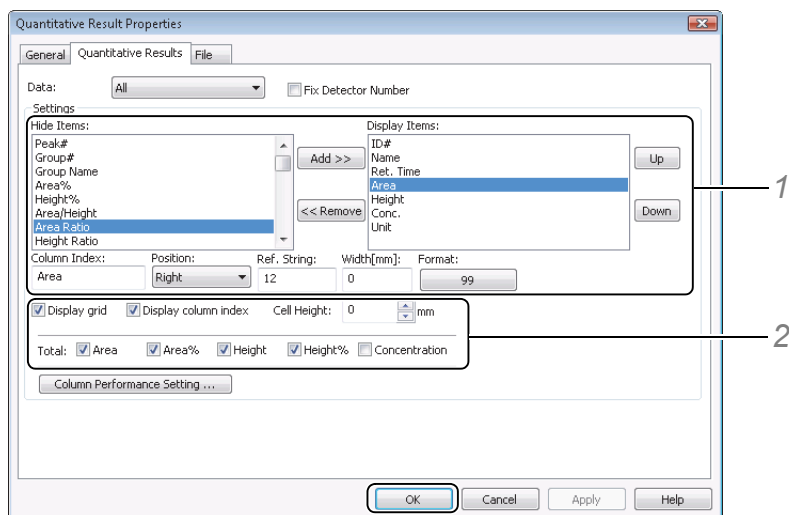


NOTE

Select [Fix file in the item] to print the chromatogram selected in [File] each time the report format is used. This selected chromatogram is printed even if a different data file is loaded in the [Report] window.

8.5.8 Edit the Quantitative Results Table

- 1 Click the [Quantitative Results] tab.
- 2 Set the [Quantitative Results] tab parameters, and click [OK].



- 1 Select items to print in the [Hide Items] box, and click [Add].
The added items are displayed in the [Display Items] box.
- 2 Select the desired items to display statistical calculation results and the grid.

NOTE

When displayed items include column performance parameters (e.g. number of theoretical plates and tailing factor), all values calculated by the various pharmacopoeia methods (JP, USP, etc.) specified in the data processing parameters are displayed.

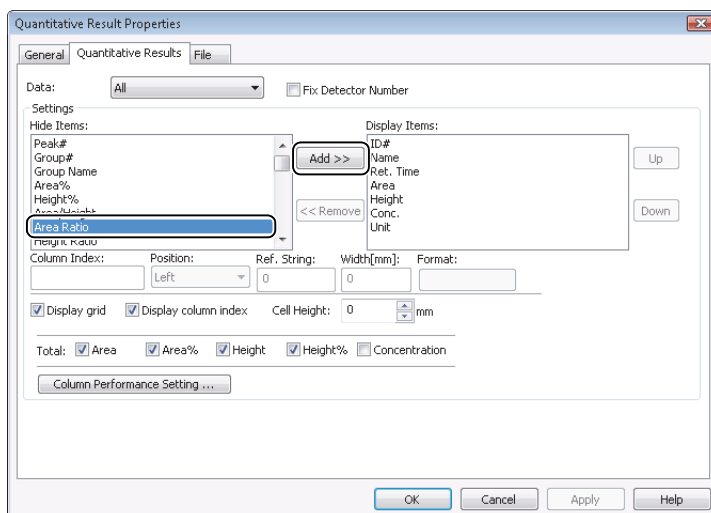
To filter the reported calculation results in the Quantitative Results Table, click the [Column Performance Settings] button, select [Display only selected calc. method] in the [Display Settings for Column Performance Results] sub-window that is displayed, and specify the calculation results to display.

8.5.9 Edit the Numeric Value Format in the Quantitative Results Table

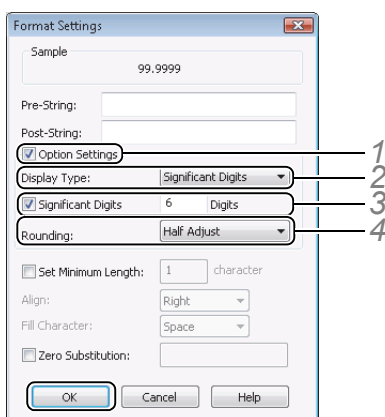
It is possible to set the rounding method and the display parameters for the numeric data.

This section describes the procedure for changing the numeric format of [Area Ratio].

- 1 Click the [Quantitative Results] tab.
- 2 Select [Area Ratio] in the [Hide Items] box, and click [Add].
[Area Ratio] is displayed in the [Display Items] box.



- 3 Select [Area Ratio] in the [Display Items] box, and click the [99.9999] format.
- 4 Make the appropriate settings in the [Format Settings] sub-window, and click [OK].



- 1 Select [Option Settings].
- 2 Click [Significant Digits] at [Display Type].
- 3 Select [Significant Digits], and enter "6".
- 4 Click [Half Adjust] at [Rounding].

NOTE

By default, [Option Settings] is deselected and the display format and rounding method set in the [Data Processing Setting] sub-window for [System Settings] in [Administration Tools] are used.

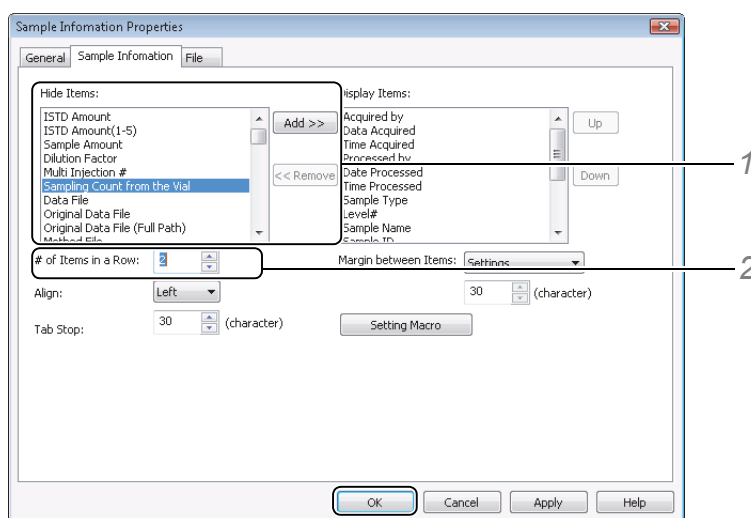
- 5 Check the edited details, and click [OK].

8.5.10 Edit Sample Information

Use the [Sample Information] tab of the [Sample Information Properties] sub-window to select the sample information to include in the report format.

The following section describes how to display the repeat injection count of the same vial number set in the batch file.

- 1 Click the [Sample Information] tab.
- 2 Set the [Sample Information] tab parameters, and click [OK].



- 1 Select [Sampling Count from the Vial] in the [Hide Items] box, and click [Add].
[Sampling Count from the Vial] is displayed in the [Display Items] box.
- 2 To display 2 sample information items in a row, enter "2" at [# of Items in a Row].



NOTE

Click [Setting Macro] on the [Sample Information] tab and create a method using macros to display sample information. Select the information to be displayed and the position in the macros sub-window. Once macros have been used to set the [Sample Information] tab parameters, the original table format sub-window cannot be displayed.

8.5.11 Edit Calibration Curve Information

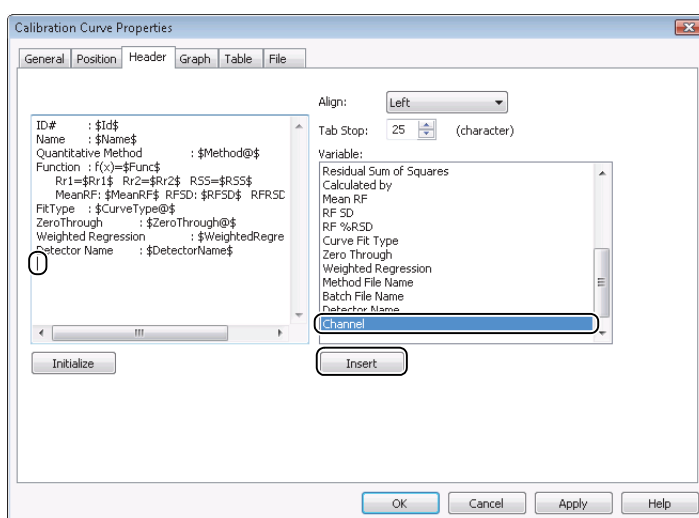
Use the [Header] tab in the [Calibration Curve Properties] sub-window to edit calibration curve information such as, calibration curve expressions and quantitative calculation methods.

Macros are provided for each of the [Header] tab items. These macros can be edited to determine display items and positions in reports.

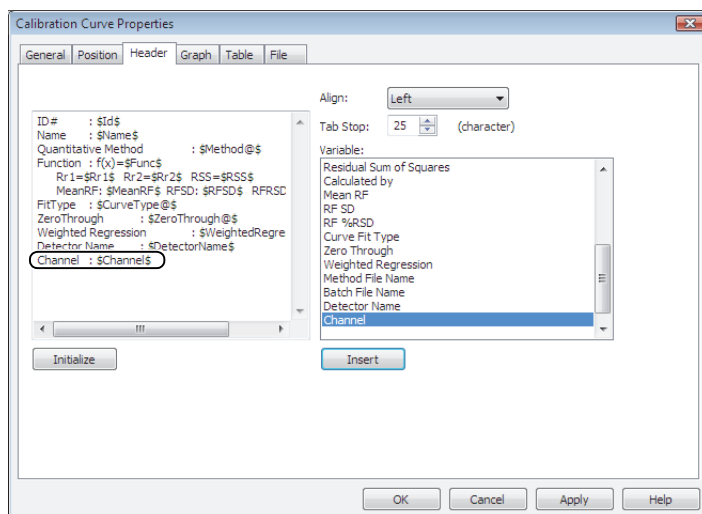
This section describes how to edit the [Channel] macro to print the channel.

- 1** Click the [Header] tab.
- 2** Place the cursor in the position where the new information is to be added in the display area to the left, select [Channel] in the [Variable] list, and click [Insert].

[\$Channel\$] is added to the text display area.

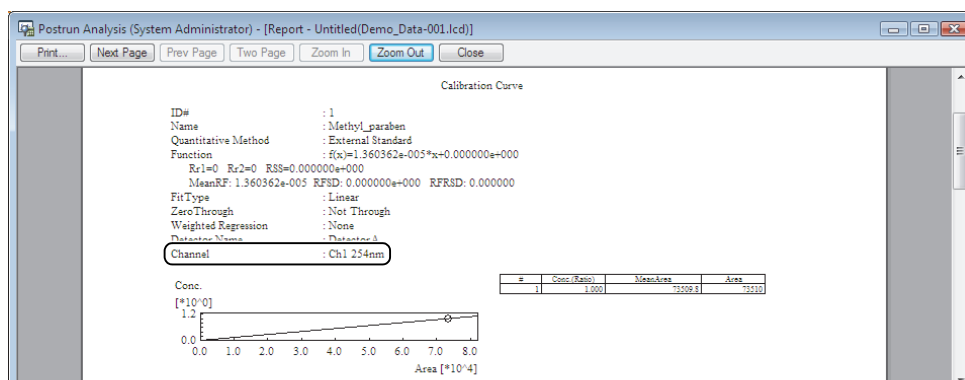


3 Prefix the additional macro [\$Channel\$] with “Channel:”.



NOTE

- Tabs can be inserted by pressing the [Ctrl] and [I] keys at the same time. The tab interval is the number of characters set at [Tab Stop].
- Click [Initialize] to restore the default settings.
- Use the [Position] tab to change the display position of the calibration curve graph and table.
- [Channel] is displayed as follows:



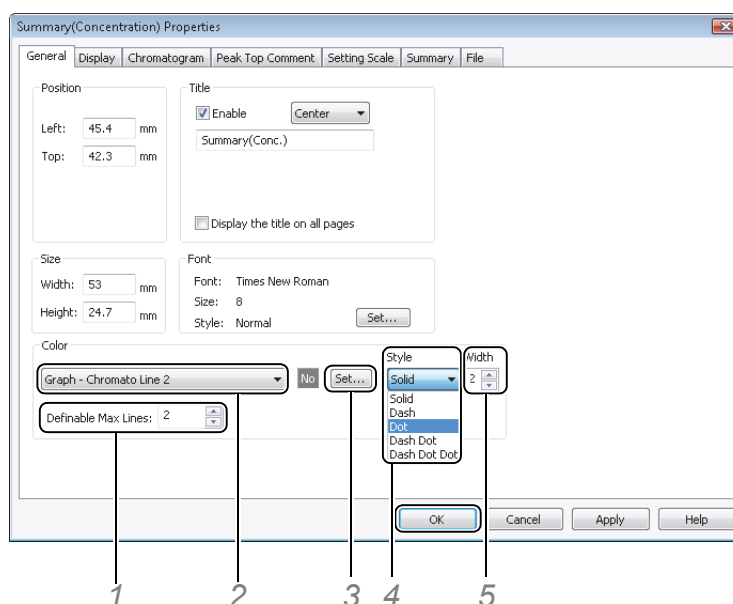
4 Check the edited details, and click [OK].

8.5.12 Change the Color and Line Width of Overlaid Chromatograms

Select the number of lines, line color and line width for overlaid chromatograms on the [General] tab in the [Summary (Concentration) Properties] sub-window.

This section describes how to change the color, line type and line width of overlaid chromatograms.

- 1 Click the [General] tab.
- 2 Set the [General] tab parameters, and click [OK].



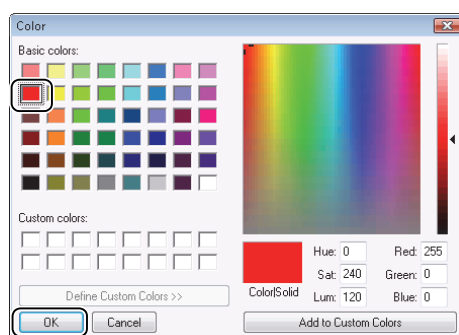
- 1 Enter "2" at [Definable Max Lines].



NOTE

When "2" is set to [Definable Max Lines], [Graph - Chromato Line 2] is added to the [Color] list. Values higher than 2 for [Definable Max Lines] add additional chromatograms to the color list.

- 2 Select [Graph - Chromato Line 2] in the [Color] list.
- 3 Click [Set], select red in the [Color] sub-window, and click [OK].



- 4 Click [Dot] in the [Style] list.
- 5 Set [Width] to "2".



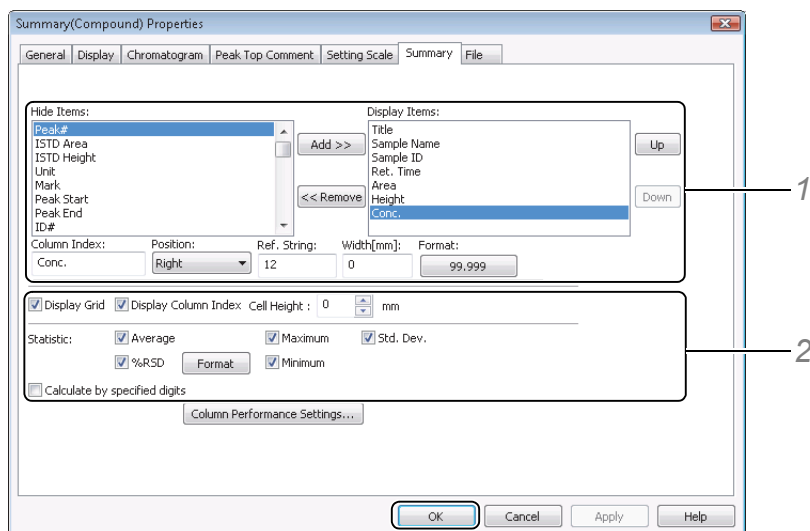
NOTE

In addition to chromatograms, statistical results can also be output with the [Summary (Concentration)] item. Select the summary data (area, height and concentration) and the statistical items to display on the [Summary] tab to display the statistical calculation results of multiple data.

8.5.13 Edit the Statistical Results Table

Items such as statistical results can be displayed by adding them to the [Display Items] box on the [Summary] tab in [Summary (Compound) Properties].

- 1 Click the [Summary] tab.
- 2 Set the [Summary] tab parameters, and click [OK].



- 1 Select the items to be displayed in the report in the [Hide Items] box, and click [Add]. The added items are displayed in the [Display Items] box.
- 2 Select the respective items to display the statistical results and the grid in the table.

NOTE

- If [Calculate by specified digits] is selected, statistical calculation is performed using the number of digits set in the [Format Settings] sub-window.
- If the number of theoretical plates and tailing factor display items are selected, all values calculated by the formulas (JP method and USP method) specified in the data processing parameters are displayed.

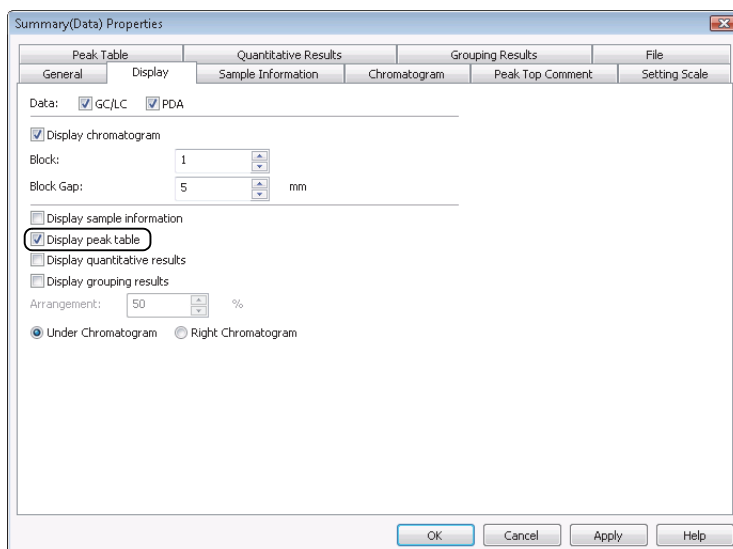
Click the [Column Performance Settings] button, and select [Display only selected calc. method] in the [Display Settings for Column Performance Results] sub-window to select calculation results to display in the Quantitative Results Table.

8.5.14 Edit the Measurement Results Table

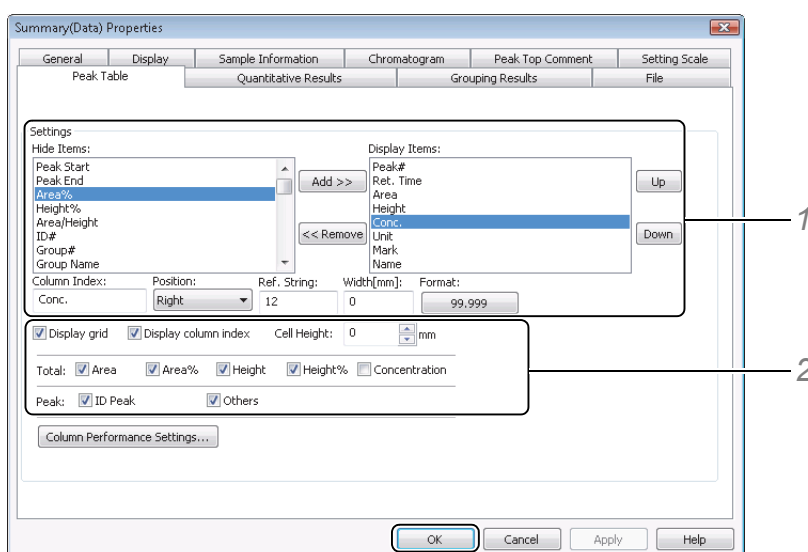
Use the [Summary (Data)] item to display one of three tables, the Peak Table, Quantitative Results Table and Grouping Results Table.

This section describes how to use the [Summary (Data)] item to edit the Peak Table display items.

- 1 Click the [Display] tab.
- 2 Select [Display peak table].



- 3 Click the [Peak Table] tab.
- 4 Set the [Peak Table] tab parameters, and click [OK].



- 1 Select the desired items in the [Hide Items] box, and click [Add].
The added items are displayed in the [Display Items] box.
- 2 Select the respective items to display the total values and grids.

NOTE

- If the number of theoretical plates and tailing factor display items are selected, all values calculated by the formulas (JP method and USP method) specified in the data processing parameters are displayed.

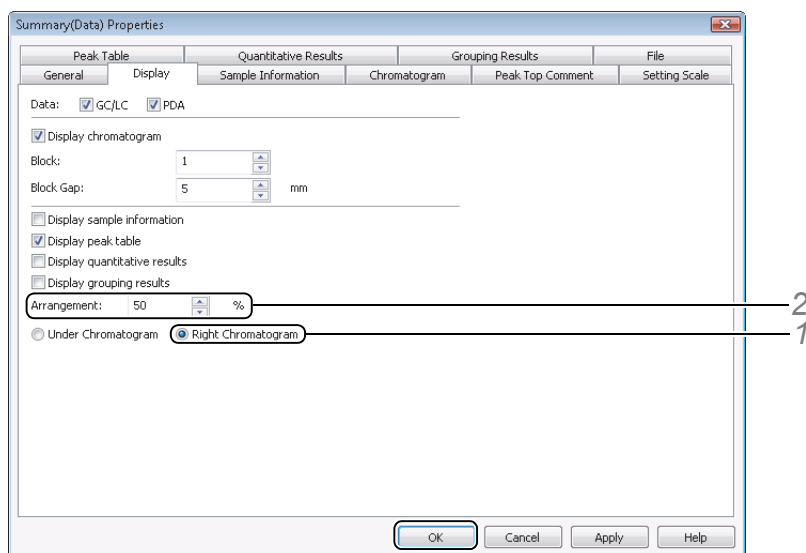
Click the [Column Performance Settings] button, and select [Display only selected calc. method] in the [Display Settings for Column Performance Results] sub-window to select the calculation results to display in the Quantitative Results Table.

8.5.15 Change the Display of Chromatograms and Results Tables

Use the [Display] tab in the [Summary (Data) Properties] sub-window to change the horizontal and vertical chromatogram display and table information to display.

1 Click the [Display] tab.

2 Set the [Display] tab parameters, and click [OK].



- 1 Click [Right Chromatogram] to display the table on the right side of the chromatogram.
- 2 Change [Arrangement] to change the display aspect ratio of chromatograms and tables.

8.6 Report Layout


Functions for editing the positions of report items include position and size adjustment, header/footer setting and the ability to add, move or delete pages.

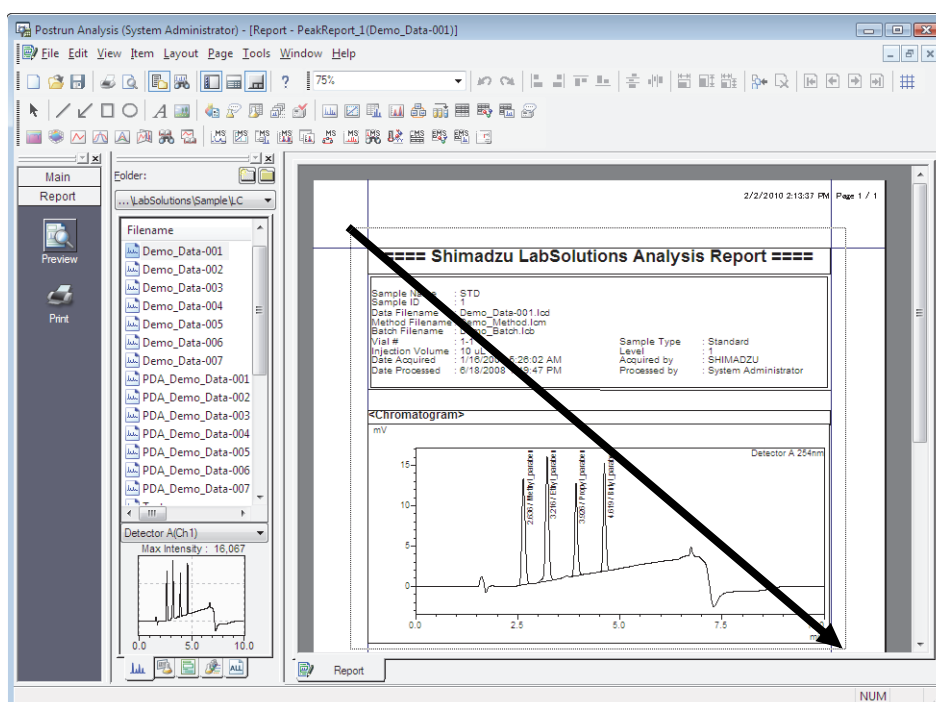
8.6.1 Change the Item Position and Number of Pages

If a report format includes multiple items, the layout icons are enabled in the toolbar so that the items can be repositioned.

Pages can be added to and deleted from the report format.

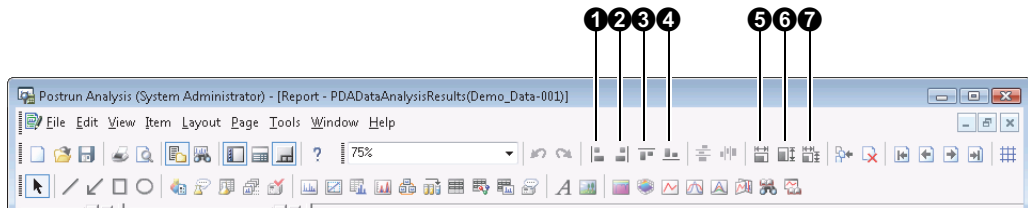
■ Re-Position Items

- 1 Click  (Pointer) on the toolbar.
- 2 Drag the point so that it encloses the items to be re-positioned.



3

Click each of the items on the [Report] toolbar, and adjust the position of items.

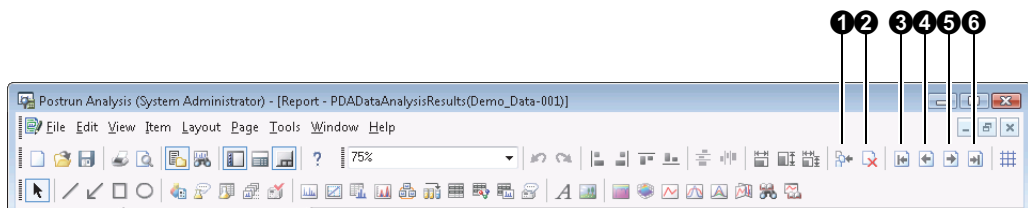


No.	Explanation
①	Aligns items to the left edge of the left most item.
②	Aligns items to the right edge of the right most item.
③	Aligns items to the top edge of the topmost item.
④	Aligns items to the bottom edge of the bottommost item.
⑤	Aligns the width of each item to the longest horizontal item.
⑥	Aligns the height of each item to the longest vertical item.
⑦	Aligns the width and height of each item to the longest horizontal and vertical item.

**NOTE**

- Some of the layout icons are disabled if only one item is selected.
- Drag the frame of the report item to resize that item.

■ Add or Delete Report Pages



No.	Explanation
①	Inserts a page after the currently displayed page.
②	Deletes the currently displayed page.
③	Displays the first page.
④	Displays the previous page.
⑤	Displays the next page.
⑥	Displays the last page.

**NOTE**

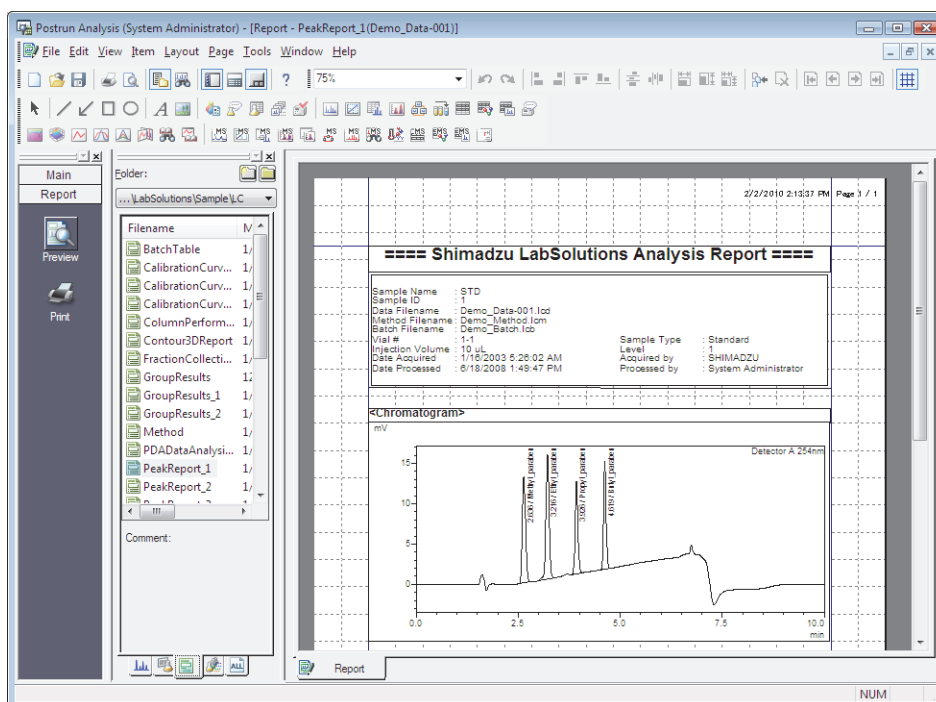
All icons except the [Insert (Page)] icon (①) are disabled if there is only one page.

8.6.2 Use the Grid

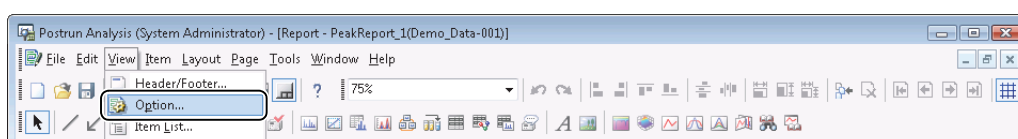
Use the grid to adjust the positions of report items.

This section describes how to display the grid in the [Report] window.

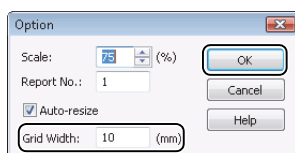
- 1 Display the report format file on the [Report] window, and click  (Toggle Grid) on the toolbar.



- 2 To adjust the interval of the displayed grid, click [Option] on the [View] menu.



- 3 Enter [Grid Width], and click [OK].

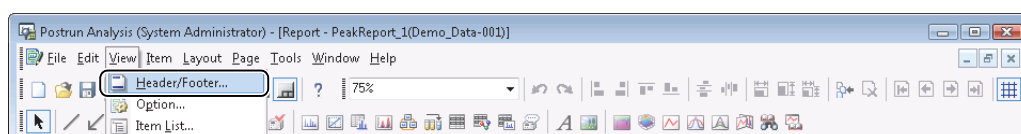


The grid is displayed at that interval.

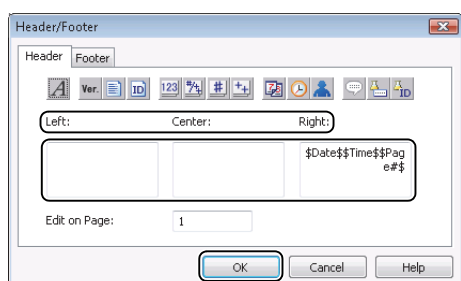
8.6.3 Headers and Footers

This section describes how to display information such as, print date, page number in the header or footer of the report format.

- 1 Display the report format file on the [Report] window, and click [Header/Footer] on the [View] menu.



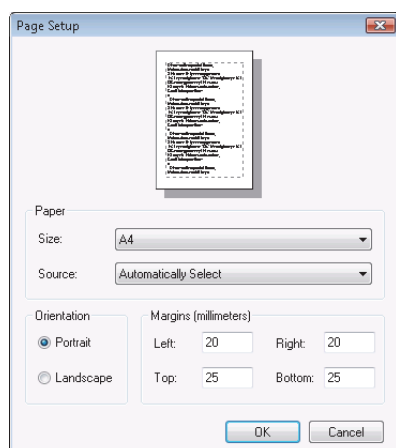
- 2 Select the [Header] or [Footer] tab and select the information to be displayed in the [Left], [Center], and [Right] sections.



- 3 Click [OK].
The settings are displayed in the report header or footer.

8.6.4 Paper Size and Margin

Click [Page Setup] on the [File] menu in the [Report] window. The [Page Setup] sub-window is displayed. Select the paper size, paper source, orientation (portrait or landscape), and margins of the report.



8.7 Other Reports

Exclusive reports can also be output from the following sub-windows.

Window/Sub-Window	Explanation (Operation Method)
Data Acquisition	The contents of the displayed method file are loaded to a system exclusive report format and output. ([Print Method File] on the [File] menu)
System Configuration	The current system configuration information is loaded to a system exclusive report format and output. ([Print] button)
Realtime Batch Postrun Batch	The contents of the Batch Table are loaded to a system exclusive report format and output. Edit the report format to match specific display items. ([Print Batch Table] on the [File] menu)
Data Analysis PDA Data Analysis Calibration Curve Data Comparison UV Library Editor Quant Browser	The contents of files loaded to each window can be loaded to a system exclusive report format and output.
Spectrum Index	The PDA chromatograms and spectra for detected peaks are loaded to a system exclusive report format and output. ([Print Spectrum Index] on the [File] menu in the [PDA Data Analysis] window)
Spectrum Table	Spectrum information registered to the Spectrum Table is output.
UV Library Search Results	The UV library search results are loaded to an exclusive report format and output. Edit the report format to match the settings made in the data processing parameters. ([Print] on the [Library Search] menu)
Audit Trail Log	If the audit trail log is activated, the log contents are output in a fixed format. ([Print] button)
Log Browser	Each log displayed in the log browser is output in a fixed format.
Show Check Result	Results of the program or raw data check are output in a fixed format.
System Check Results	The system check results are output in a fixed format. ([Print] button)

9

Quant Browser

Use the [Quant Browser] window to edit a method file and then perform quantitative calculation on multiple data.

This chapter describes how to edit the quantitative results for multiple data files, and perform collective postrun analysis on multiple data files.

9.1 [Quant Browser] Window

The [Quant Browser] window is comprised of the following views:

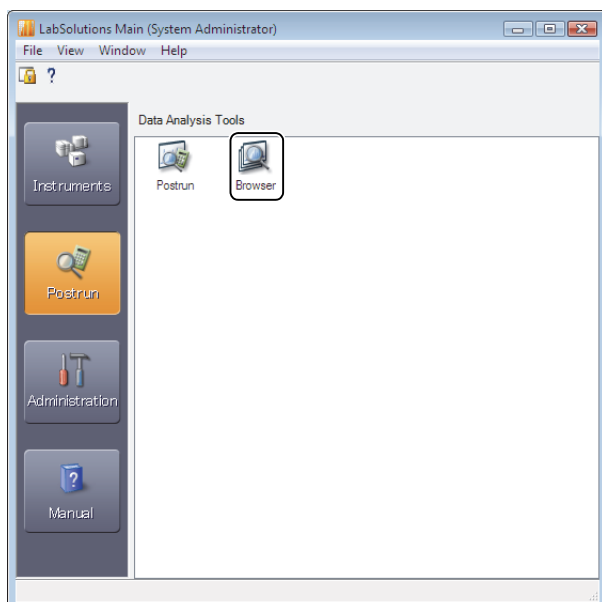
- [Quantitative Results View] - displays the quantitative calculation results
- [Method View] - displays the method file parameters
- [Chromatogram View] - displays the chromatograms and sample information
- [Calibration Curve/Spectrum View] - displays the calibration curves and spectra

9.1.1 Open the [Quant Browser] Window

1

Select the  icon on the [LabSolutions Main] icon bar, and double-click the  icon.

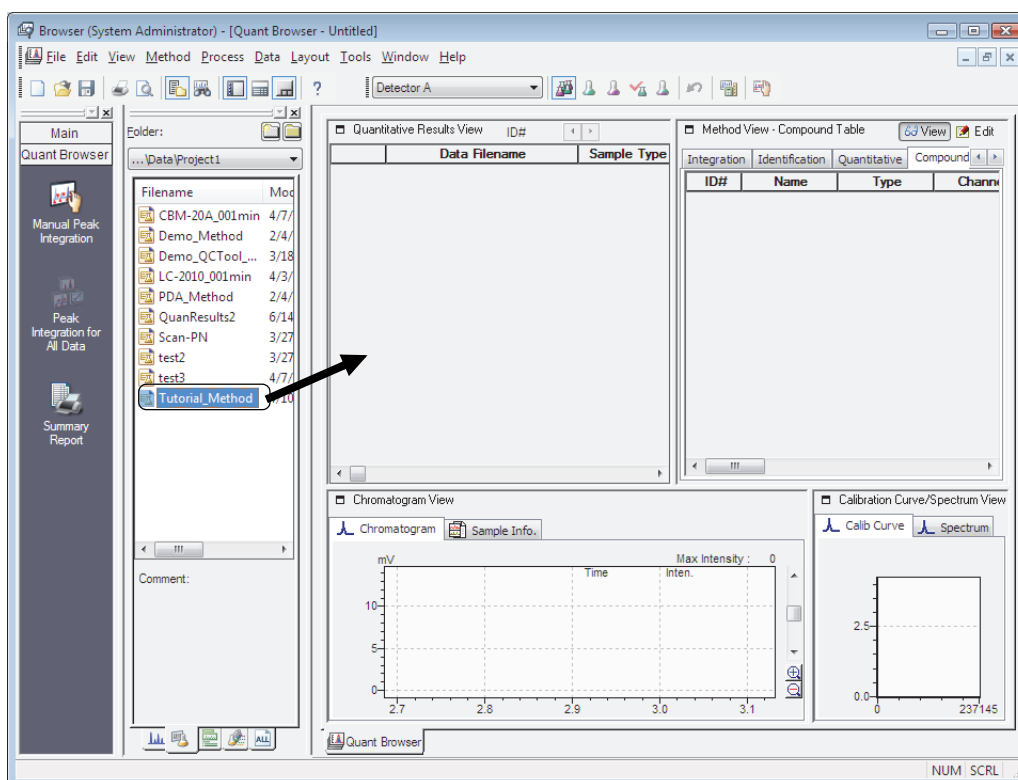
The [Browser] program opens.



- 2** Click the  (Quant Browser) icon on the [Main] assistant bar in the [Browser] program.



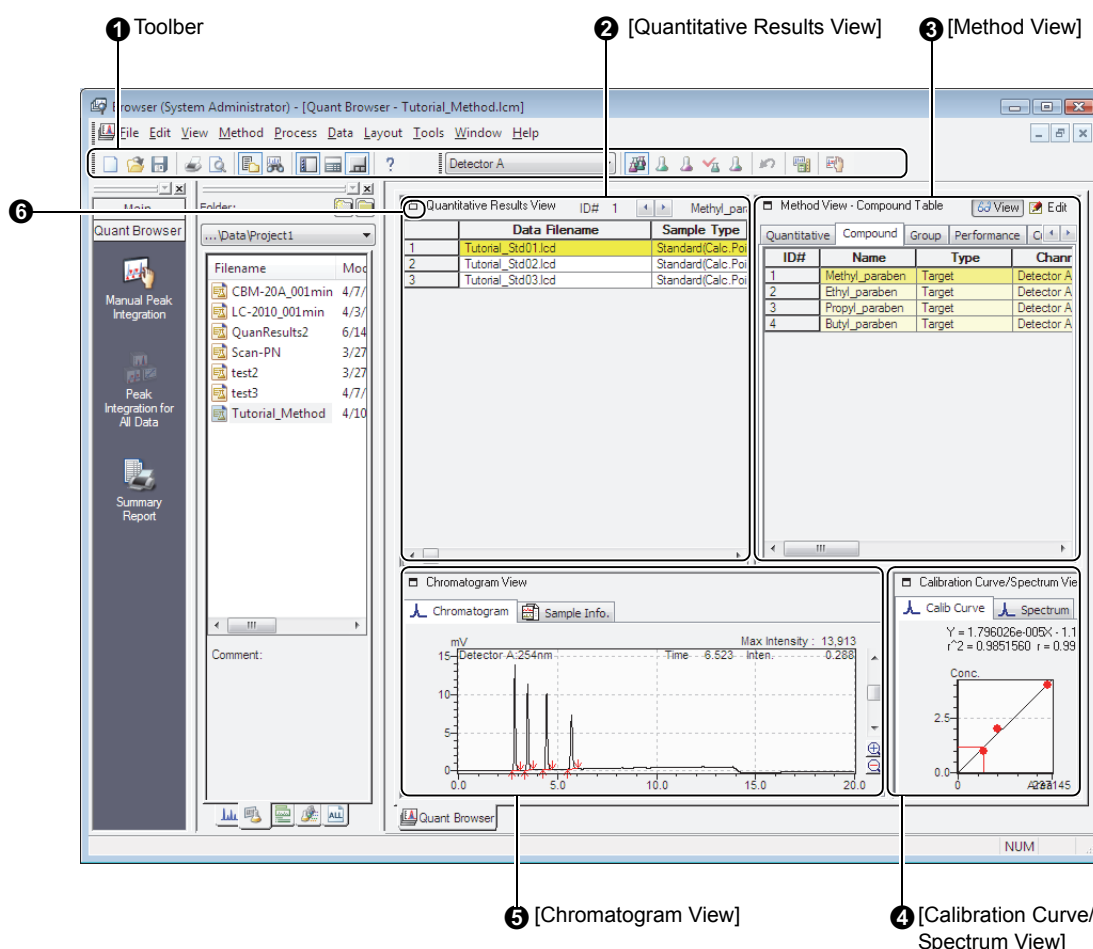
- 3** Drag-and-drop the method file from the [Data Explorer] sub-window onto the [Quant Browser] window.



The contents of the method file are displayed in the [Quant Browser] window.

9.1.2 [Quant Browser] Window Description

This section describes how to view and use the [Quant Browser] window.



No.	Explanation
1	Displays the [Standard] and [Quant Browser] toolbars.
2	Displays the quantitative calculation results of compounds selected on the [Compound] tab in [Method View]. Click to change the ID # and the displayed compound.
3	Displays the data processing parameters in the method file. Click (Edit Mode) to change the parameters. Click (View Mode) after editing to reflect the changes in [Method View].
4	Displays the calibration curve for the compound selected on the [Compound] tab in [Method View] or the spectra specified in [Chromatogram View].
5	Displays the [Chromatogram] and [Sample Info] for the selected data file. Clicking or to double or halve the intensity axis (Y-axis), respectively.
6	Click this icon to expand the view to the full screen size.

NOTE

- The [Quant Browser] views that are separated by dividers. Drag the dividers with the mouse to resize the views.
- Use the [Quant Browser] to check the quantitative calculation results of up to 1024 data files.
- Click [Save Browsing File As] on the [Layout] menu to save the name of the method and data file, file sort order, layout information, and other details as a browsing file (file extension *.lcm).
- Files are [Read Only] if they are currently being edited in other windows and cannot be edited. Close the file in the other window, and open the file again to edit these files.

9.2 Check Quantitative Results in the Quant Browser

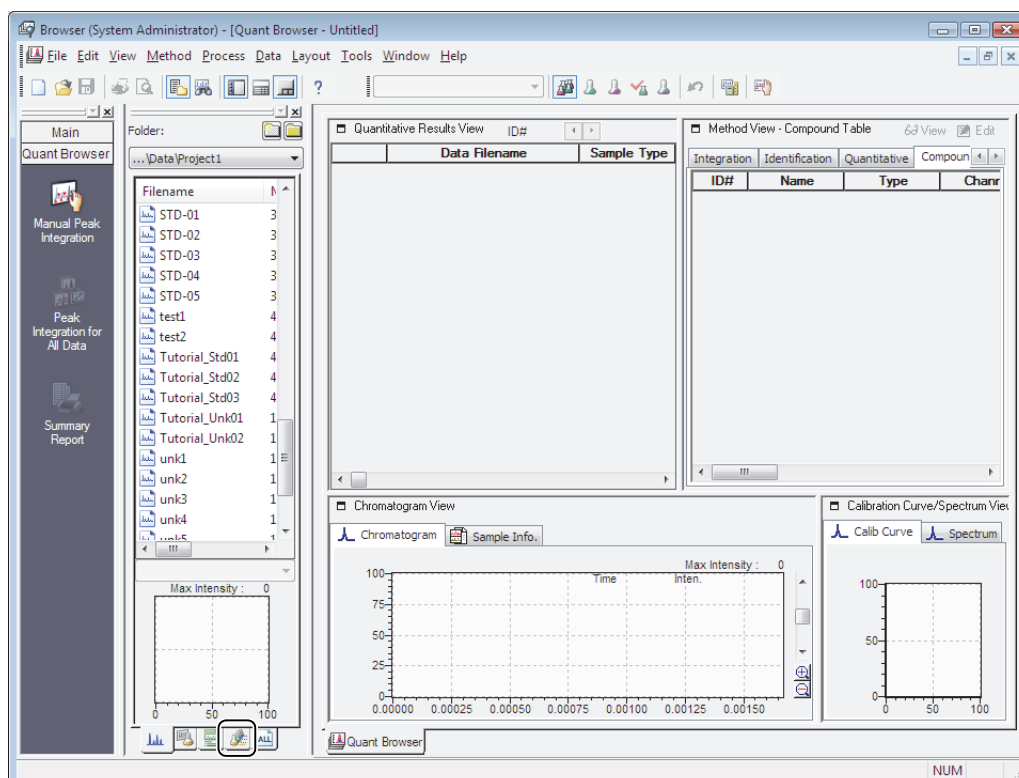
Multiple data can be displayed in a simple form in the [Quant Browser] window.

This section describes how to display data in each of the [Quant Browser] views.

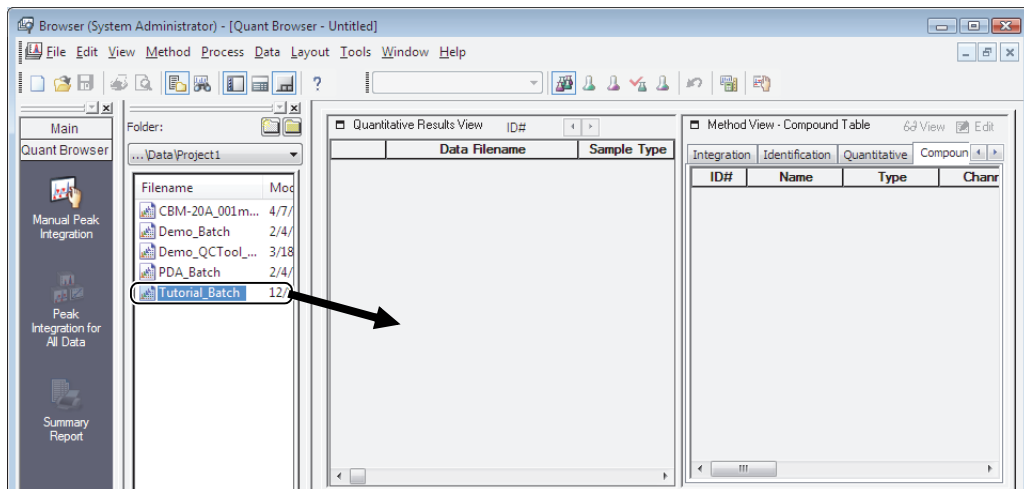
9.2.1 Open Batch Files

This section describes how to open batch files to display the contents of the method file and data files.

- 1 Click the  (Batch) tab at the bottom of the [Data Explorer] sub-window.



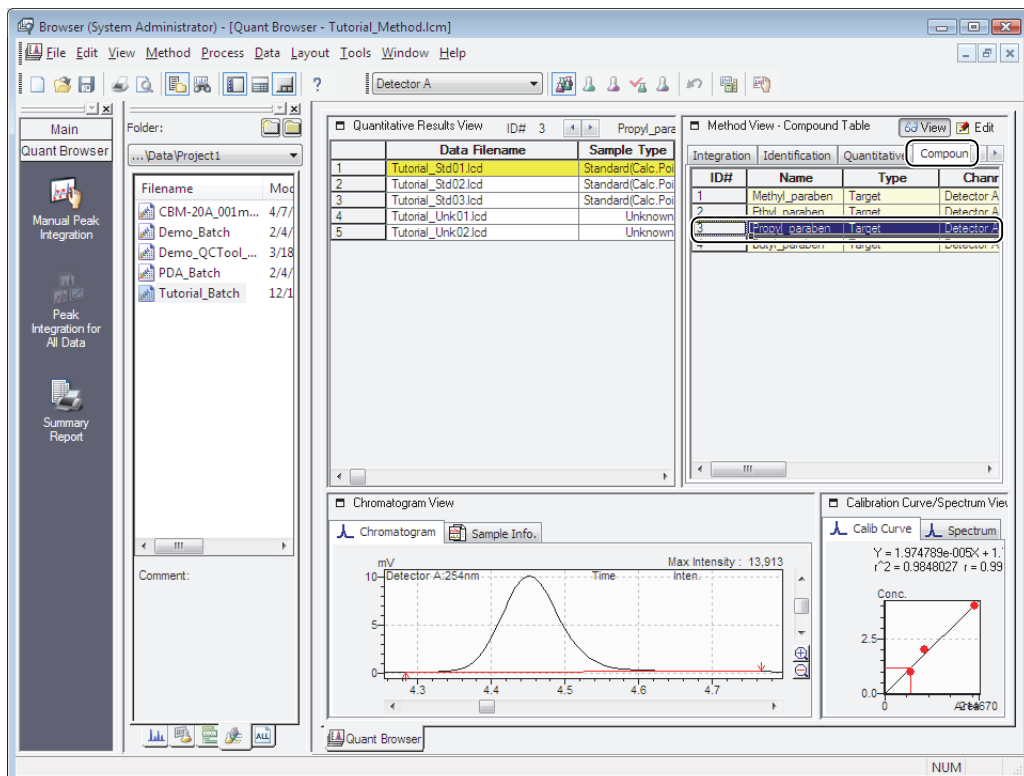
2 Drag-and-drop the batch file onto the [Quant Browser] window from the [Data Explorer] sub-window.



The contents of the method file and data files are displayed in the [Quant Browser] window.

3 Click the [Compound] tab in [Method View], and select the desired compound.

The quantitative results of the selected compound are displayed in [Quantitative Results View], and the calibration curve is displayed in the [Calibration Curve/Spectrum View].



4

Select the data file from [Quantitative Results View], and click the data file.

The chromatogram of the selected data file is displayed in the [Chromatogram View].

The screenshot displays the Quant Browser software interface. The main window is titled "Browser (System Administrator) - [Quant Browser - Tutorial_Method.lcm]". The interface is divided into several panes:

- Quantitative Results View:** A table with columns "Data Filename" and "Sample Type". The selected row is "Tutorial_Std02.lcm" with "Standard(Calc. Poi)".
- Method View - Compound Table:** A table with columns "ID#", "Name", "Type", and "Chan#". The selected row is "3" with "Ethyl_paraben", "Target", and "Detector A".
- Chromatogram View:** A plot showing a single peak at approximately 4.4 minutes. The y-axis is labeled "mV" and the x-axis is "Time". The peak is labeled "Detector A.254nm" and "Max Intensity : 48,956".
- Calibration Curve/Spectrum View:** A plot showing a linear relationship between concentration and intensity. The equation is $Y = 1.974789e-005X + 1$ and the correlation coefficient is $r^2 = 0.9848027$ with $r = 0.99$.

NOTE

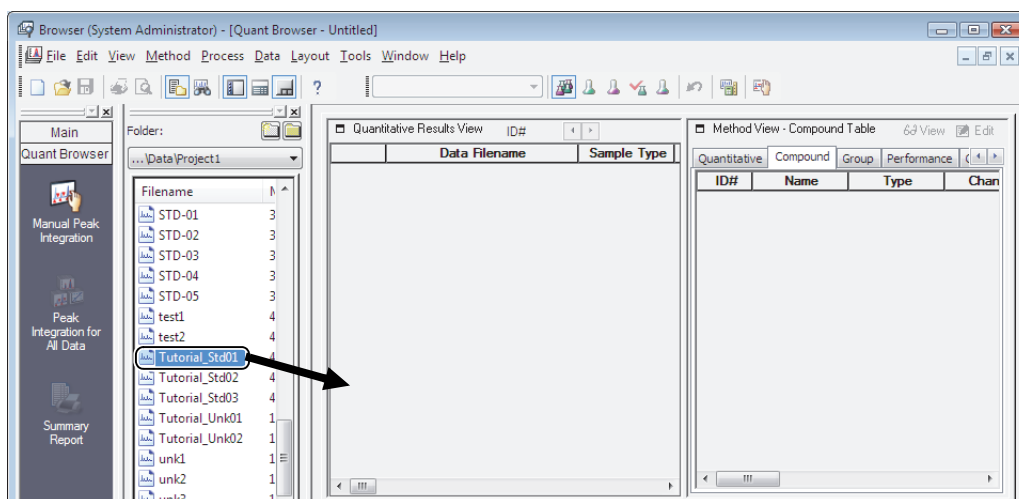
- The method file in the top row of the Batch Table is displayed in [Method View] when a batch file is selected in the [Data Explorer] sub-window. If the method file contains calibration curve information, the standard sample data file used for making the calibration curve is loaded.
- The data file and method file must be saved to the same folder as the batch file to display the content of the method file and data file using a batch file.
- Edit the method file and data file in the [Quant Browser] window. The batch file is not changed when data is displayed.

9.2.2 Open Data Files

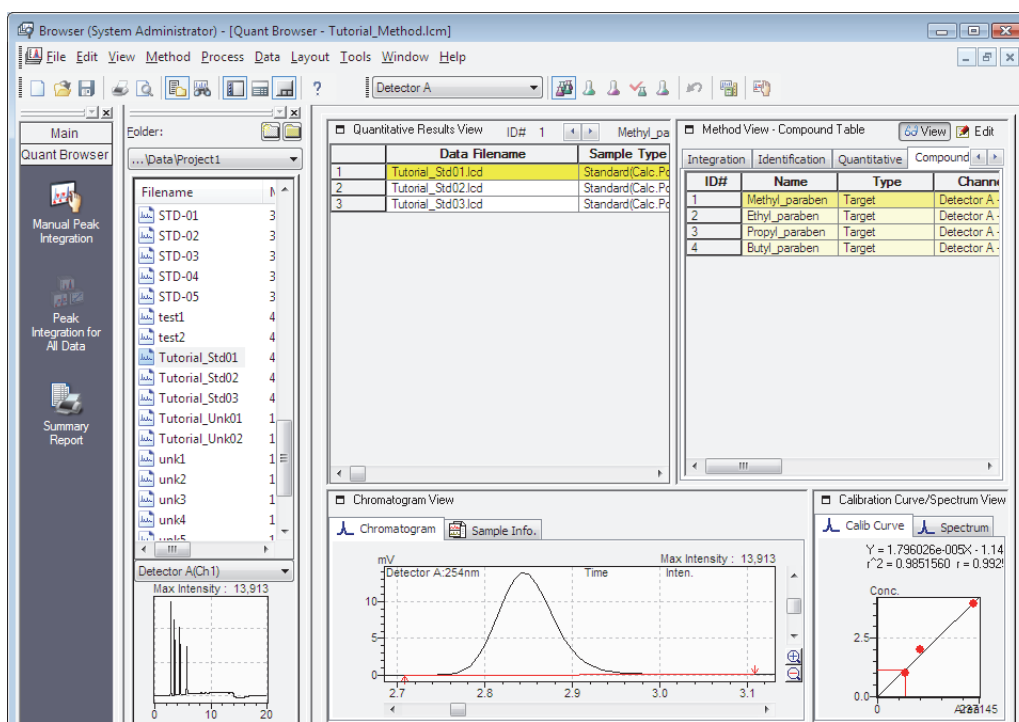
Open data files to display the contents of data files in each view.

This section describes how to open the data file of an unknown sample.

- 1 Drag-and-drop the data file onto the [Quant Browser] window from the [Data Explorer] sub-window.



The contents of the data file and method file are displayed in the [Quant Browser] window.



NOTE

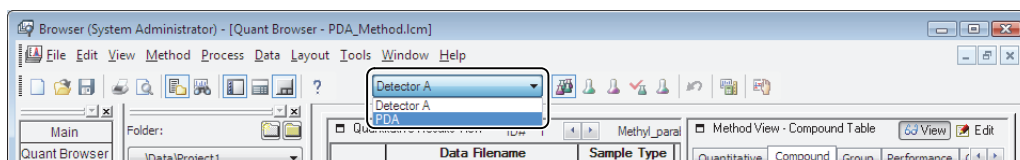
Multiple files are selected when the data file is dragged-and-dropped onto the [Quant Browser] window from the [Data Explorer] sub-window. The method file in the top data file is displayed in [Method View]. If the loaded method file contains calibration curve information, the content of the standard sample data file used to make the calibration curve is also displayed.

9.2.3 Change the Detector

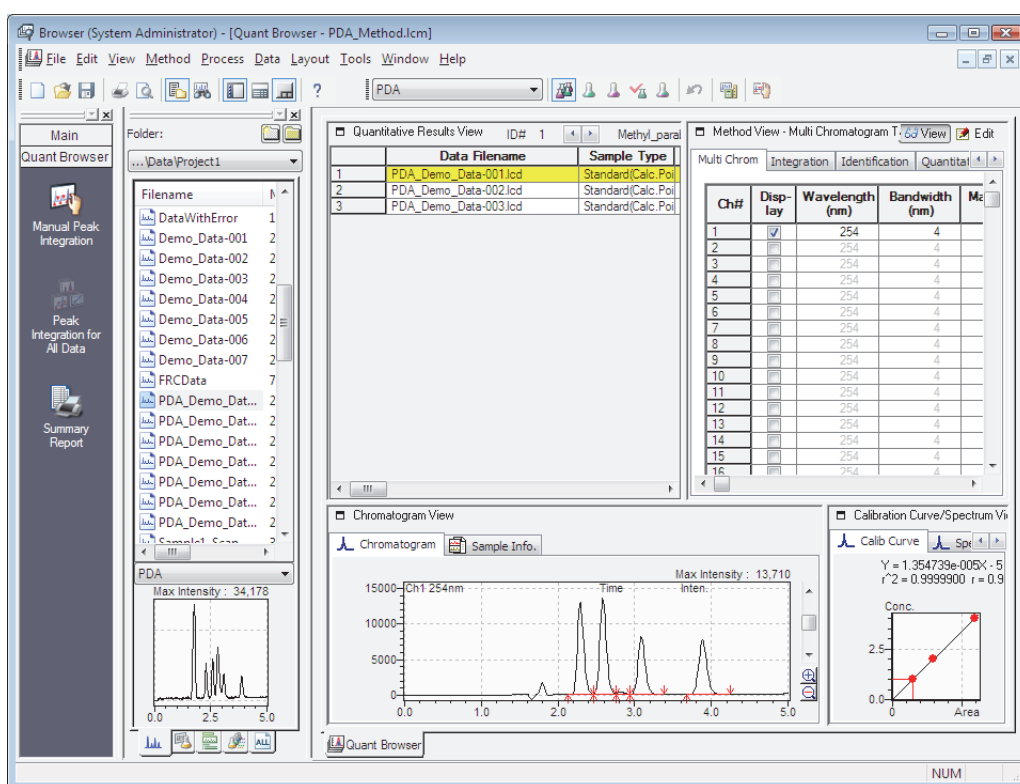
The method for the targeted detector can be changed if the method files contains methods for multiple detectors.

This section describes how to change [Select Detector] from [Detector A] to [PDA].

- 1 Select and click [PDA] from the [Select Detector] list.



The [Quant Browser] window changes to display the PDA detector.

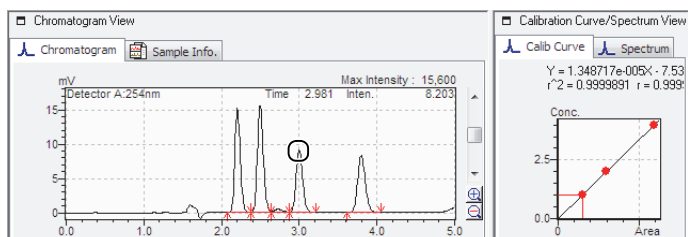


9.2.4 Check Spectra from [Chromatogram View]

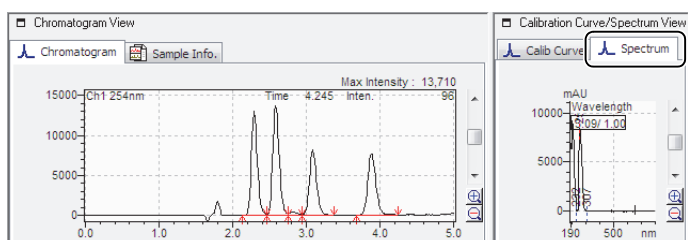
Double-click the PDA chromatogram displayed in [Chromatogram View] to display the spectrum at that retention time.

This section describes how to display a PDA spectrum.

- 1 Select the [Chromatogram] tab in [Chromatogram View], and double-click the PDA chromatogram.



[Calibration Curve/Spectrum View] changes to the [Spectrum] tab, and the PDA spectrum is displayed.



NOTE

To display chromatograms in all time ranges in [Chromatogram View], right-click on [Chromatogram View], and click [All Peaks] on the displayed menu.

9.3 Postrun Analysis of Multiple Data

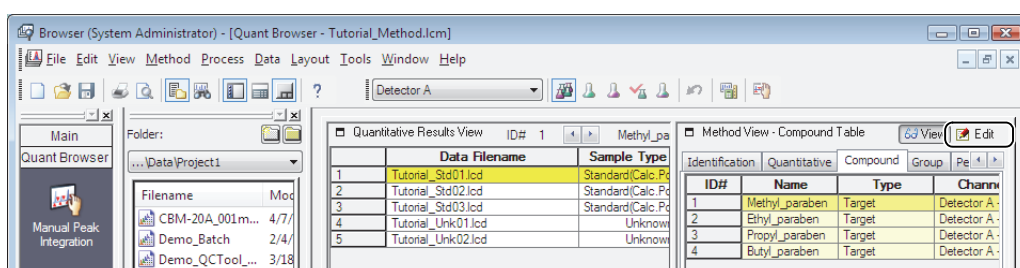
This section describes how to edit [Quantitative Results View] and [Method View] and perform collective postrun analysis on multiple data.

9.3.1 Edit the Compound Table

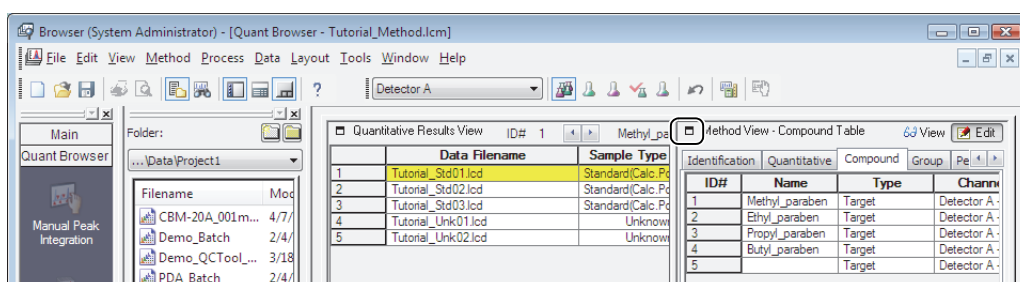
Compound Tables that were used for data acquisition can be edited in [Method View].

This section describes how to change [Conc. (1)] in the Compound Table.

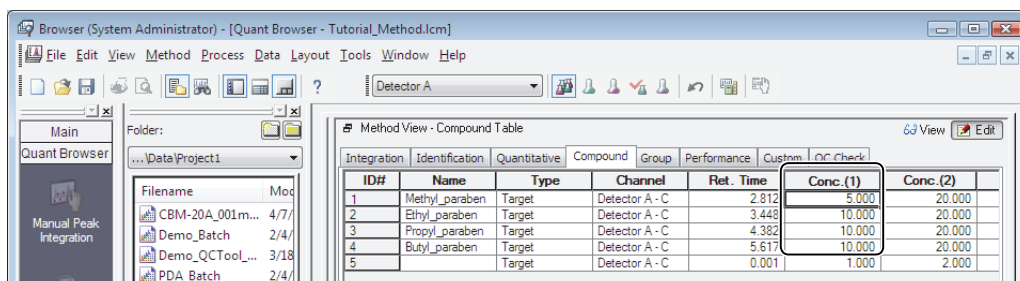
- 1 Click  **Edit (Edit Mode)** in [Method View].



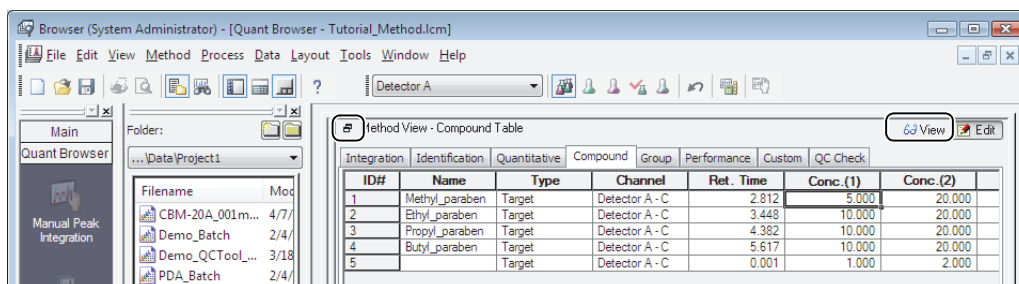
- 2 Click  **(Full Size)** in [Method View].



- 3 Click the [Compound] tab, select the desired compound, and change [Conc. (1)].
In this example, change the [Conc. (1)] setting from “10.000” to “5.000”.



4 Click (Normal Size) and (View Mode) in [Method View].



The calibration curve is recreated, the quantitative results are re-calculated, and [Quantitative Results View] is updated.

Quantitative Results View ID# 2 Ethyl_paraben						
	Data Filename	Ret. Time	Area	Conc. (mg/L)	Std. Conc.	
1	Tutorial_Std01.lcd	3.494	57.862	11.608	10.000	
2	Tutorial_Std02.lcd	3.473	89.605	17.940	20.000	
3	Tutorial_Std03.lcd	3.450	202.46	40.452	40.000	
4	Tutorial_Unk01.lcd	3.525	61.153	12.264	-----	
5	Tutorial_Unk02.lcd	3.495	143.48	28.687	-----	

Quantitative Results View ID# 1 Methyl_paraben						
	Data Filename	Ret. Time	Area	Conc. (mg/L)	Std. Conc.	
1	Tutorial_Std01.lcd	2.844	64.618	8.429	5.000	
2	Tutorial_Std02.lcd	2.831	100.03	15.602	20.000	
3	Tutorial_Std03.lcd	2.816	225.28	40.970	40.000	
4	Tutorial_Unk01.lcd	2.864	68.295	9.173	-----	
5	Tutorial_Unk02.lcd	2.848	159.50	27.647	-----	

NOTE

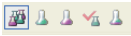
- Right-click on [Method View] and click [Cancel Edit] to cancel method editing.
- Select the columns that are displayed in the Compound Table in the [Table Style] sub-window. Right-click on the Compound Table and click [Table Style] to open the [Table Style] sub-window.

9.3.2 Edit [Quantitative Results View]

This section describes how to change the items displayed in the [Quantitative Results View].

Quantitative results are automatically re-calculated when each item is changed.

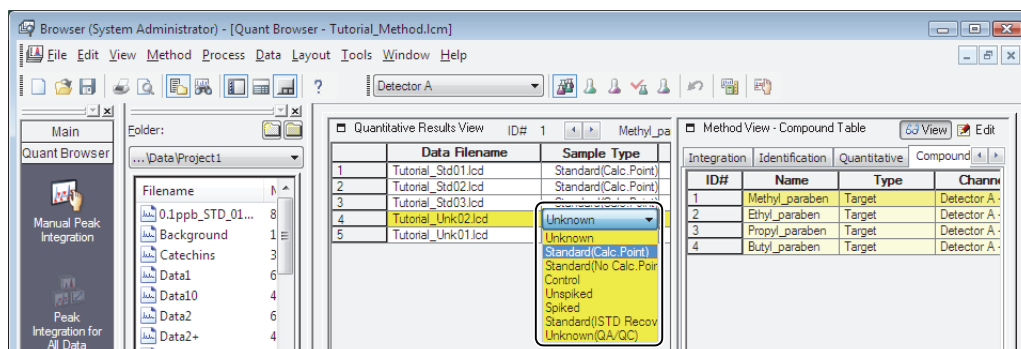
NOTE

- Right-click on [Quantitative Results View] and click [Remove] to delete a data file in [Quantitative Results View]. If deletion of a data file affects the calibration curve, all data files are re-calculated.
- Click the  icon on the toolbar to filter the data files displayed in [Quantitative Results View] by individual sample type.
- Right-click on [Quantitative Results View] and click [Full Path] to display the folder and file name at [Data Filename].
- Click the title of a column in the [Quantitative Results View] table to sort the data by [Data Filename], [Sample Name], [Sample ID], [Sample Type], [Level #], [Vial #], [Tray], and [Date Acquired].
 - Select the columns that are displayed in the [Quantitative Results View] table in the [Table Style] sub-window. Right-click on the [Quantitative Results View] table and click [Table Style] to open the [Table Style] sub-window.
- Click [Save Method File] on the [File] menu to save changes made to the data and method files in [Quantitative Results View].

Change the Sample Type

Sample types that were set at data acquisition can be changed.

- 1 Click the [Sample Type] cell of the sample to be changed, and select the sample type from the displayed list.



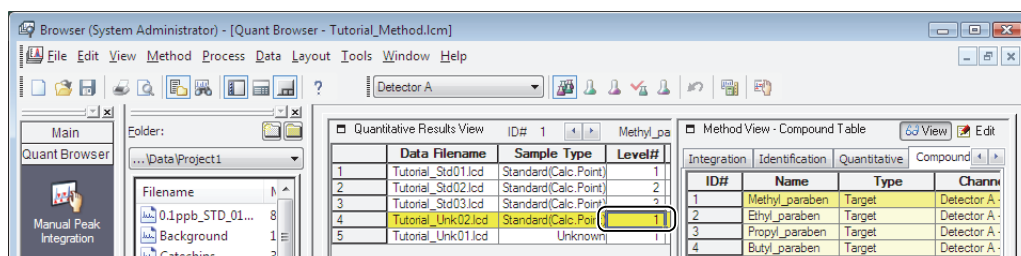
NOTE

If [Standard (Calc. Point)] is changed to another sample type, or another sample type is changed to [Standard (Calc. Point)], the calibration curve is re-created, and all data files are re-calculated.

Change the [Level#]

The level numbers that were set at data acquisition can be changed.

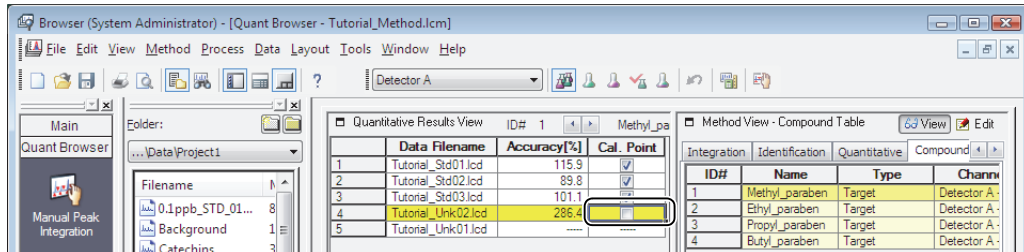
- 1 Change the [Level#] of the desired sample.



■ Disable Calibration Points

Calibration curve points can be disabled if the standard samples were not analyzed appropriately.

1 Deselect [Cal. Point].



If a [Cal. Point] is disabled, the calibration curve is re-created.



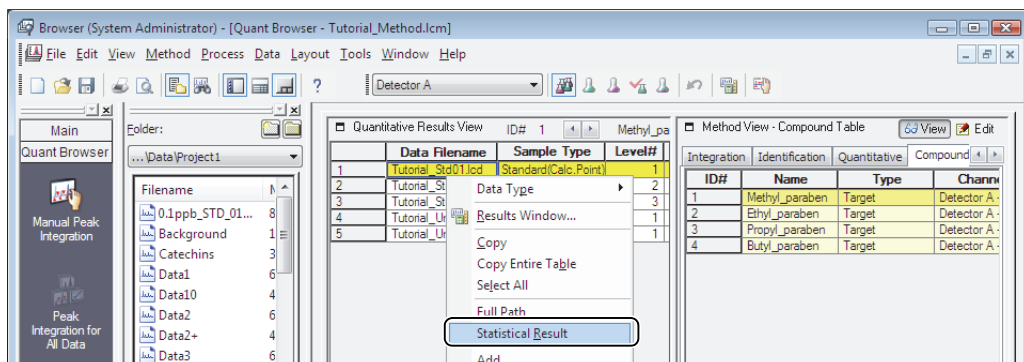
NOTE

Calibration points for individual compounds can be enabled or disabled on the [Compound] tab in [Method View].

■ Display Statistical Results

Statistical calculations can be applied to quantitative results and the results can be displayed in the [Quantitative Results View].

1 Right-click on [Quantitative Results View], and click [Statistical Result].



The statistical calculation results are added to the bottom of the table.

	Data Filename	Sample Type	Level#	Ret. Time	Area	Height	Conc. (mg/L)	Std. Conc.	Area%
1	Tutorial_Std01.lcd	Standard(Calc. Point)	1	2.844	64.619	13.853	1.159	1.000	28.474
2	Tutorial_Std02.lcd	Standard(Calc. Point)	2	2.831	100.034	21.685	1.795	2.000	28.416
3	Tutorial_Std03.lcd	Standard(Calc. Point)	3	2.816	225.287	48.881	4.045	4.000	28.303
4	Tutorial_Unk02.lcd	Unknown	0	2.848	159.506	34.674	2.864	---	28.389
5	Tutorial_Unk01.lcd	Unknown	1	2.864	68.295	14.595	1.225	---	28.320
Average				2.841	123.548	26.738	2.218		28.380
%RSD				0.637374	55.374827	55.860302	55.419995		0.247536
Maximum				2.864	225.287	48.881	4.045		28.474
Minimum				2.816	64.619	13.853	1.159		28.303
Std. Dev.				0.018108	59.414502116	14.926704056	1.228804		0.070262



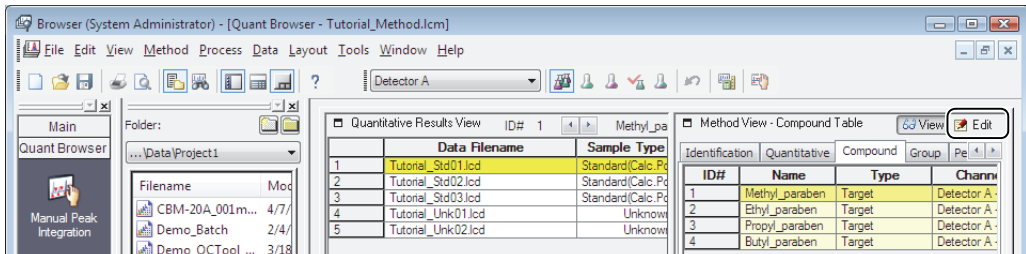
NOTE

Select the [Statistic] column in the [Quantitative Results View] table to target a data file for statistical calculation. [Statistic] is not displayed in [Quantitative Results View] by default. Right-click on the [Quantitative Results View] table and select [Table Style] to display the [Statistic] column.

9.3.3 Change Peak Integration Parameters

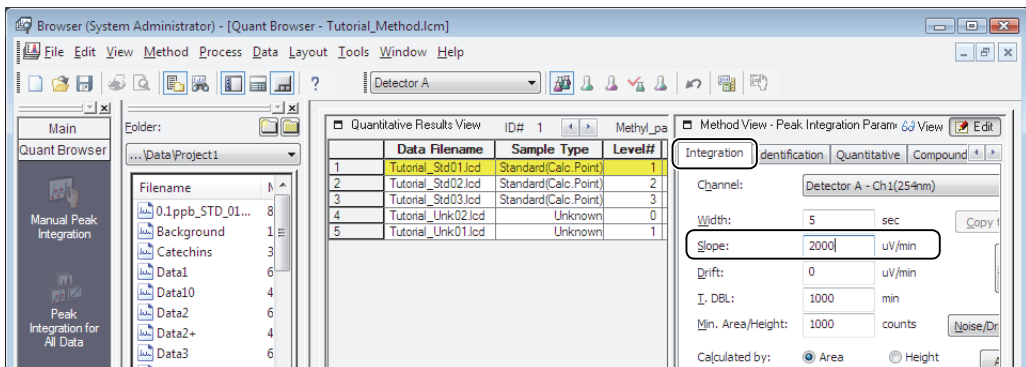
This section describes how to change the peak integration parameters and re-integrate the peak.

- 1 Click  **Edit (Edit Mode)** in **[Method View]**.



- 2 Click the **[Integration]** tab, and set each parameter as required.

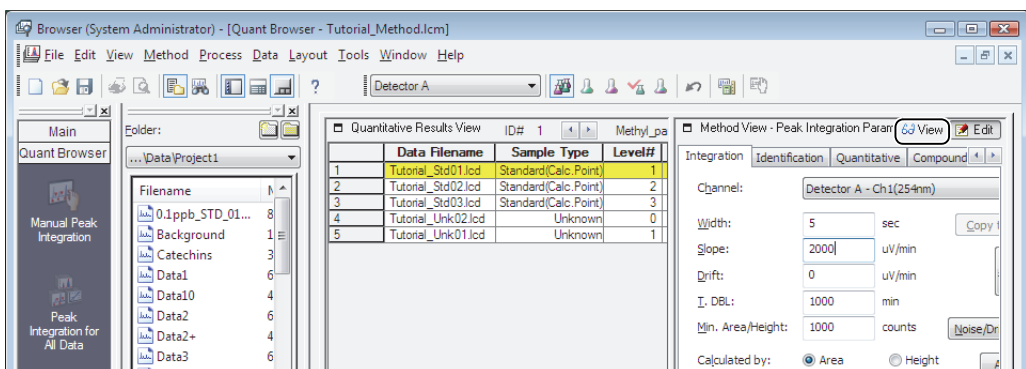
In this example, change the [Slope] to "2000".



Reference

Refer to the Data Acquisition & Processing Theory Guide for details on peak integration.

- 3 Click  **(View Mode)** in **[Method View]**.



The results of peak integration and quantitation are displayed in the **[Quantitative Results View]**.

ID#	Data Filename	Area	Height	Conc. (ppm)	Std. Co
1	Tutorial_Std01.lcd	-----	-----	-----	0.500
2	Tutorial_Std02.lcd	15,230,436	1,152,193	1,000	1,000
3	Tutorial_Std03.lcd	80,746,261	4,833,989	5,000	5,000
4	Tutorial_Unk01.lcd	11,077,384	835,152	0,746	-----
5	Tutorial_Unk02.lcd	10,886,185	846,829	0,735	-----

9.3.4 Calibration Curve Correction

During calibration curve creation, low-concentration samples may not be integrated properly. If the low-concentration calibration point is disabled, a 3-point calibration curve becomes a 2-point calibration curve.

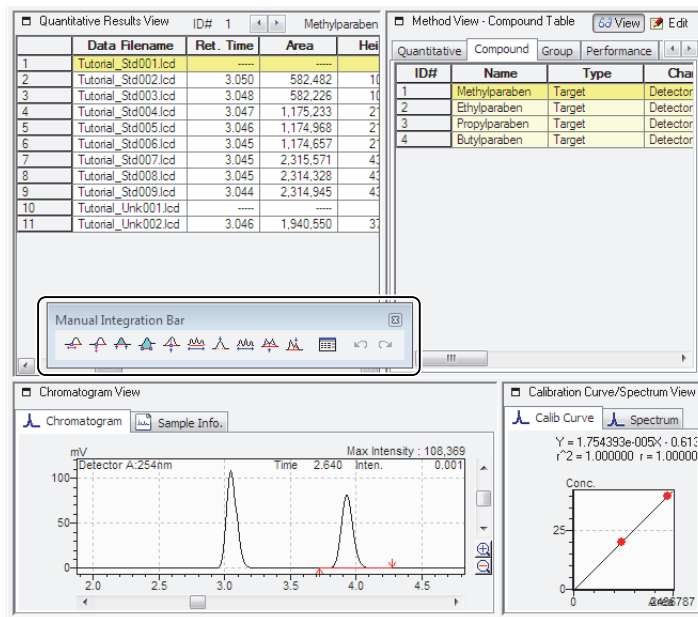
This section describes how to manually integrate the data of a standard sample that could not be automatically integrated, and correct the calibration curve.

This section describes an example where peak integration failed, resulting in 2-point calibration curve.

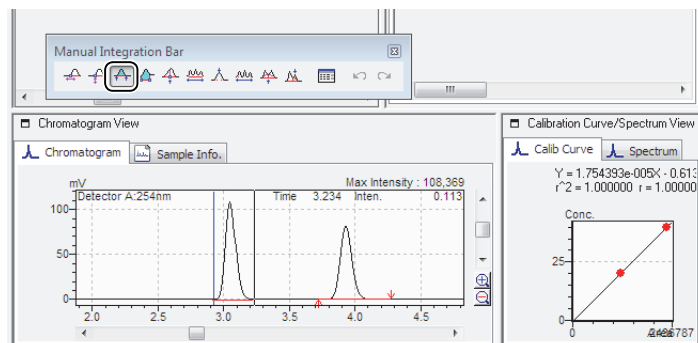
- 1 Click the  (Manual Peak Integration) icon on the [Main] assistant bar in the [Browser] program.



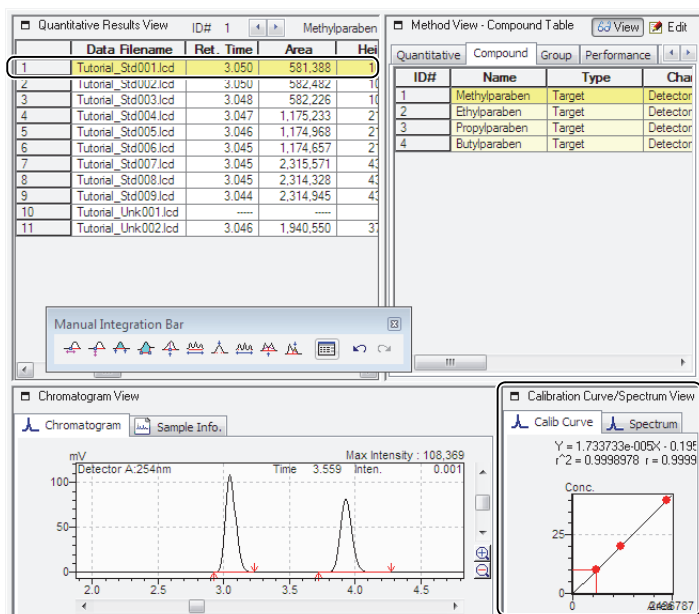
The [Manual Integration Bar] is displayed.



- 2 Click  (Insert Peak) on [Manual Integration Bar], and click the peak start point and then the peak end point.



The peak is detected, and the results are re-calculated.
 The 3-point calibration curve is re-created, and all data files are recalculated.

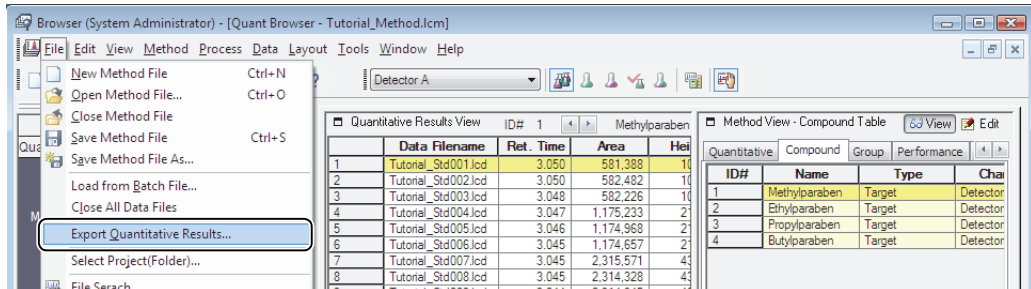
**NOTE**

To confirm the calibration curve information, right-click on the calibration curve on the [Calib Curve] tab in [Calibration Curve/Spectrum View], and click [Calibration Information] on the displayed menu.

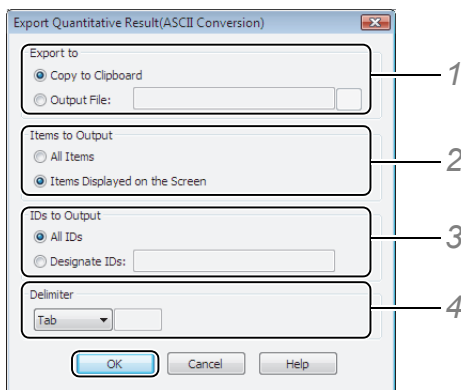
9.3.5 Export the Quantitative Results

The contents of the [Quantitative Results View] table can be converted to the ASCII text format and saved to a file or copied to the Clipboard.

- 1 Click [Export Quantitative Results] on the [File] menu.




- 2 Select the desired parameters, and click [OK].

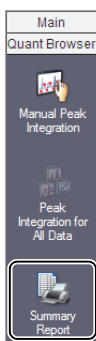


- 1 Select [Export to].
Enter the folder and file name to output files.
- 2 Set [Items to Output].
Select [Items Displayed on the Screen] to output the items displayed in the [Quantitative Results View].
- 3 Set [IDs to Output].
Select [All IDs] to display the results of all compound IDs.
Select [Designate IDs] and enter the ID numbers of the compounds to output.
 - Enter multiple ID numbers to output with a comma or space. (example: 1,3,8)
 - Enter a range of continuous ID numbers with a hyphen. (example: 2-8)
- 4 Select a [Delimiter].

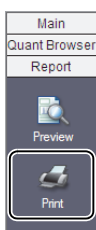
9.4 Print Quantitative Results

The [Quant Browser] window has a summary report function for collectively reporting multiple data.

- 1 Click the  (Summary Report) icon on the [Quant Browser] assistant bar.

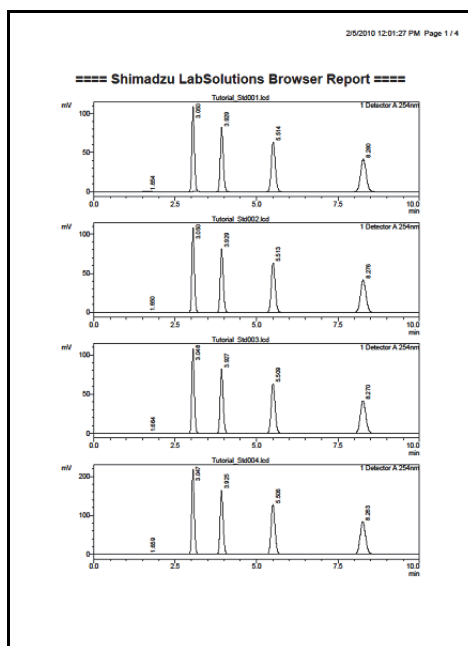


- 2 Click the  (Print) icon on the [Report] assistant bar.



An image of the table is printed for each compound.

Example of Quant Browser printout



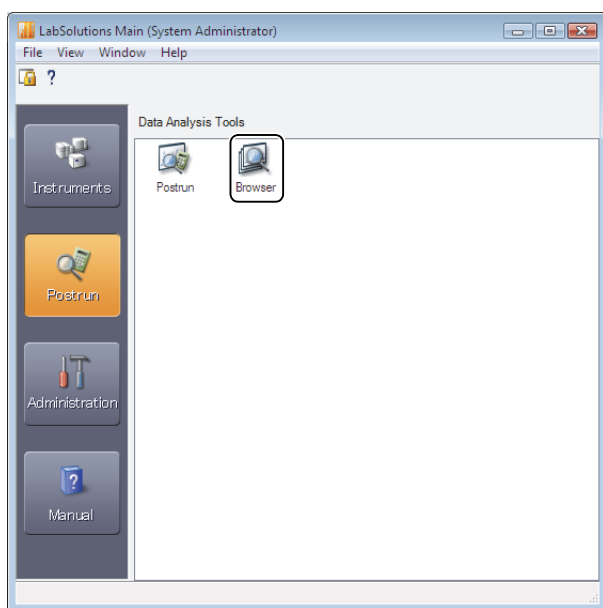
10 Data Browser

Use the [Data Browser] window to compare multiple data, compare the data of different detectors, set the layout of display data, perform peak integration of chromatograms, and print browser reports. This chapter describes how to collectively check multiple chromatograms and spectra.

10.1 Open the [Data Browser] Window

Up to 64 chromatogram data, sample information, etc. can be displayed as a list in the [Data Browser] Window.

- 1 Select the  icon on the [LabSolutions Main] icon bar, and double-click the  Browser icon.

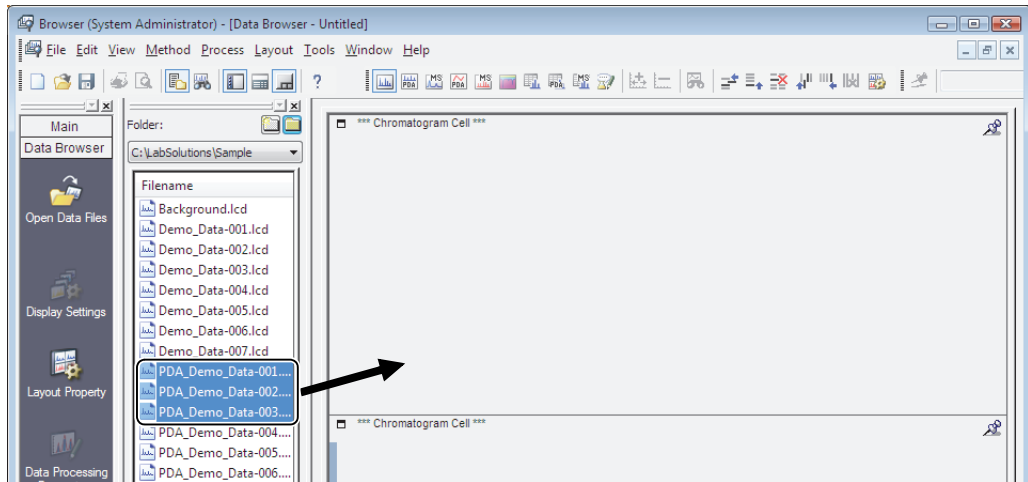


The [Browser] program opens.

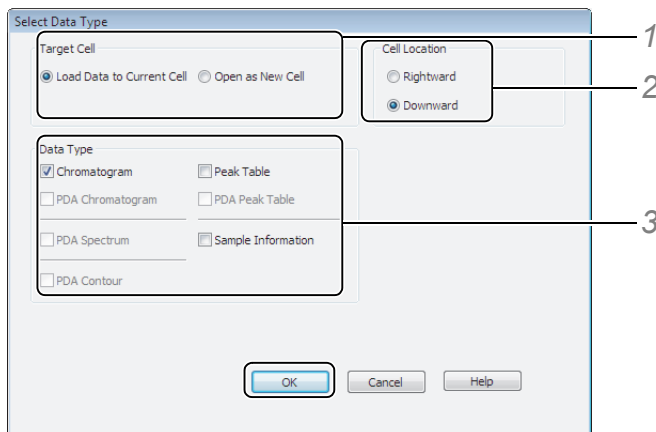
- 2 Click the  (Data Browser) icon on the [Main] assistant bar in the [Browser] program.



- 3** Drag-and-drop the data files onto the [Data Browser] window from the [Data Explorer] sub-window.



- 4** Select the Data Type parameters, and click [OK].



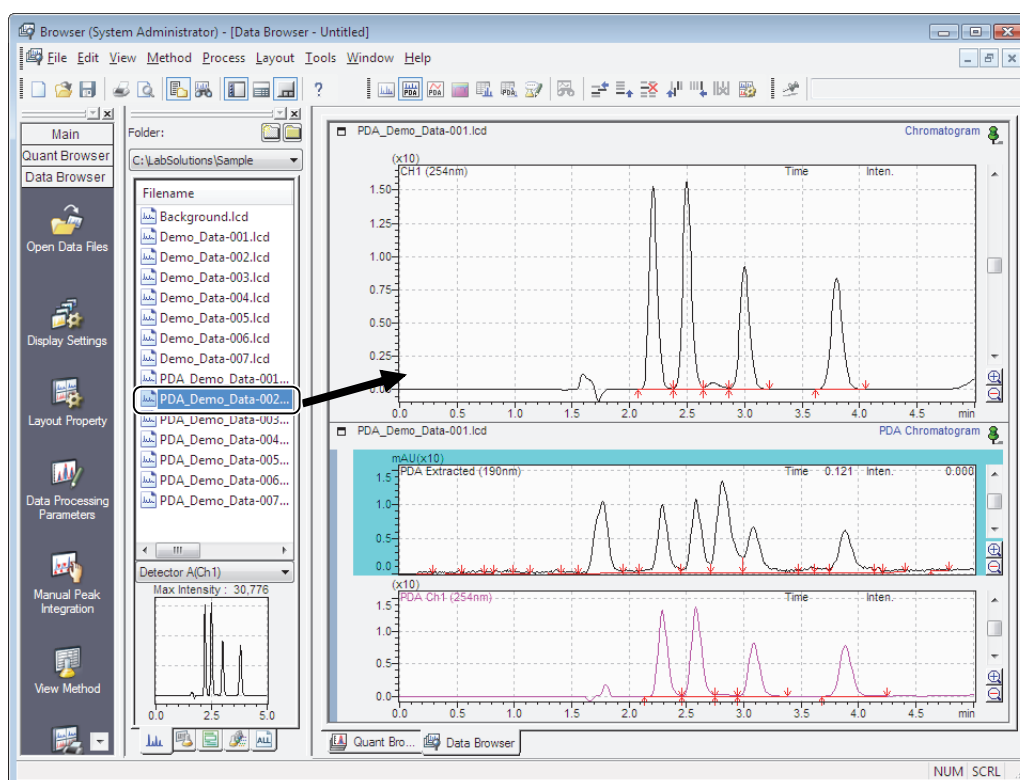
NOTE

If the cell fixed function is not enabled, the [Select Data Type] sub-window is displayed. Refer to ["10.3 Cell Fixed Function" P.288](#) for details on the cell fixed function.

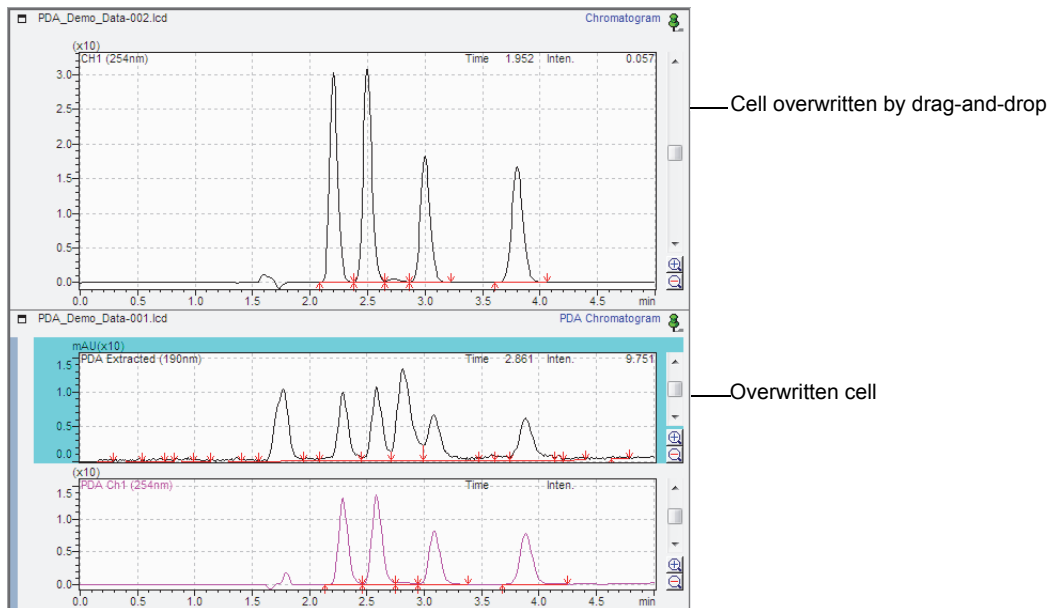
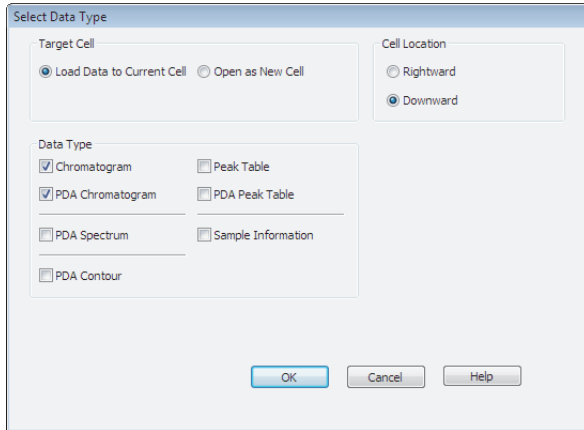
- 1 Select the [Target Cell].
Select [Load Data to Current Cell] to display the selected data files in the cell where the files were dragged-and-dropped into from the [Data Explorer] sub-window.
- 2 Set [Cell Location].
If [Open as New Cell] was selected at [Target Cell], set the direction that new cells will be added.
Select [Rightward] to create columns and select [Downward] to create rows.
- 3 Set [Data Type].
Select the multiple types of data to be displayed.
The contents of the data files are displayed in the [Data Browser] window.

■ [Target Cell]

Cells are created according to the [Target Cell] setting in the [Select Data Type] sub-window. The following example assumes that a data file is already loaded in a layout whose [Row] and [Col] settings are set to “3” and “1”, respectively.



- [Load Data to Current Cell] is selected at [Target Cell]
The [Chromatogram] cell contents are replaced by the data file that is dragged-and-dropped into that cell. In this example, the cell contents are overwritten with the [Chromatogram] and the [PDA Chromatogram] are opened in the direction specified at [Cell Location]. Here, the [PDA Chromatogram] cell is overwritten to cells below the cell that the data file was dragged-and-dropped into.

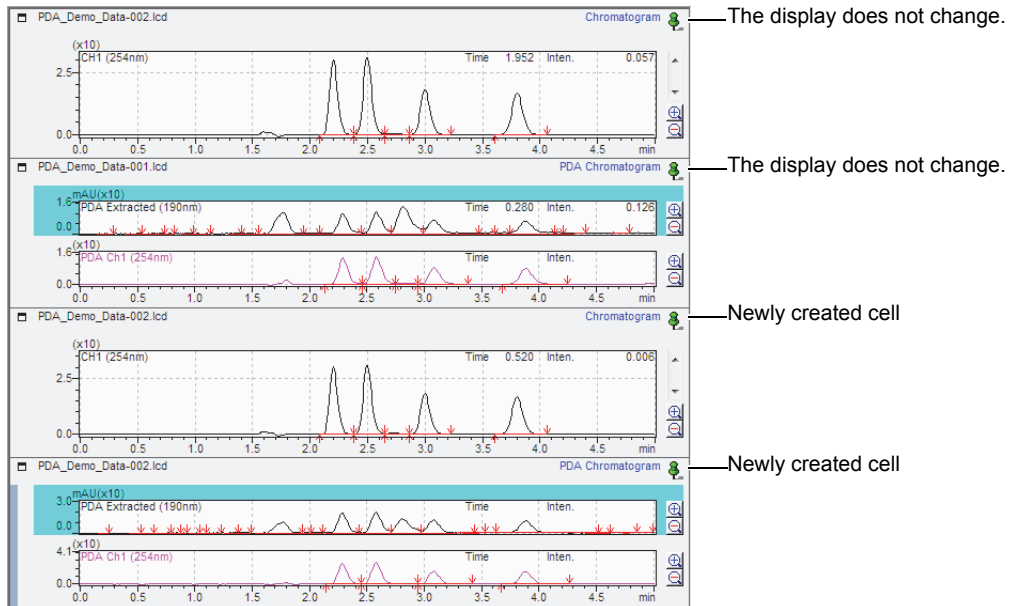
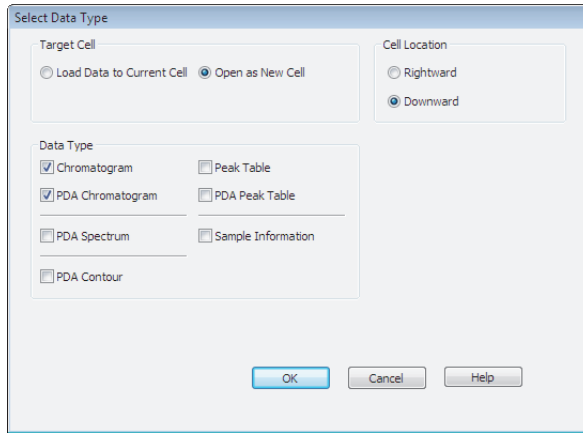


NOTE

The cell order becomes [Chromatogram] and [PDA Chromatogram].

If multiple data files are dragged-and-dropped, only the data file initially selected in the [Data Explorer] sub-window is processed.

- [Open as New Cell] is selected
New cells are created to individually display the [Chromatogram] and [PDA Chromatogram].

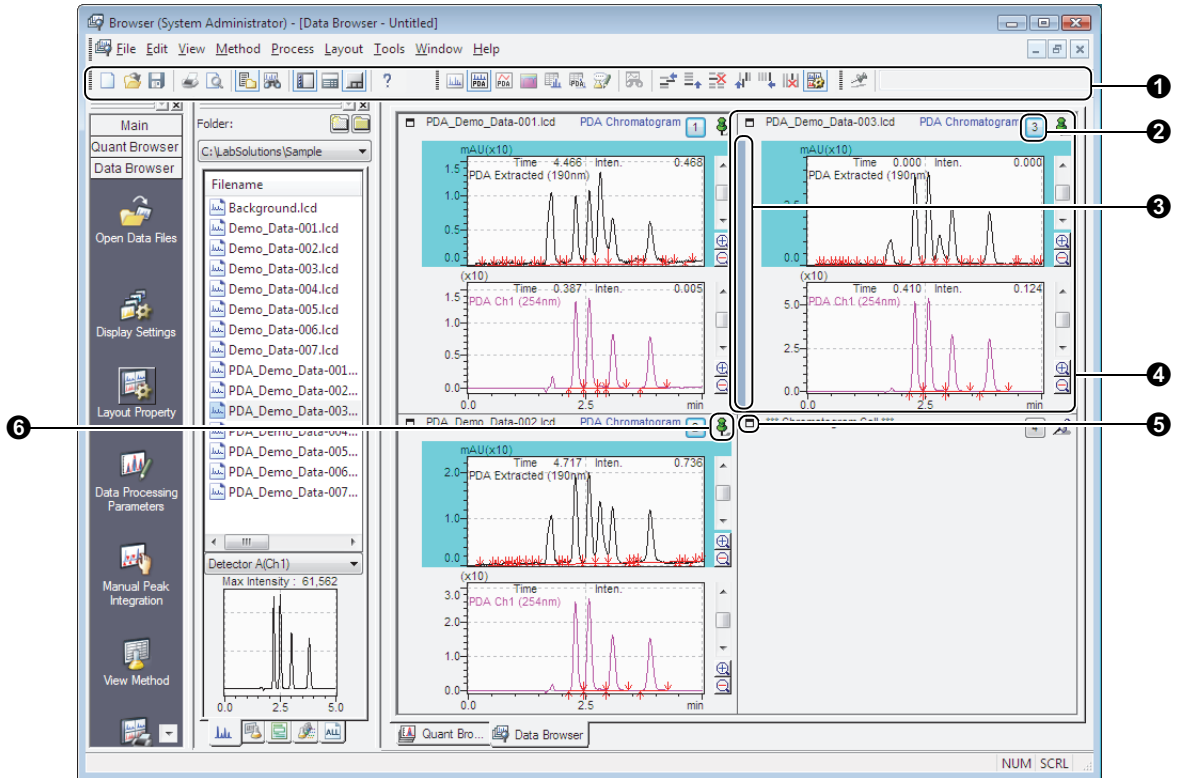



NOTE

If the [Row] or [Col] display reaches the maximum number of 8 each (8 rows, 8 columns), a new [Row] or [Col] is created to display the additional data files.

10.1.1 [Data Browser] Window Description

This section describes how to view and use the [Data Browser] window.



No.	Explanation
①	Displays the [Standard] and [Data Browser] toolbars.
②	Displays the preset cell number. The cell number can be changed by clicking <input type="text" value="1"/> . If the cell fixed function is enabled, <input type="text" value="1"/> is displayed. Refer to "10.3 Cell Fixed Function" P.288 for details on the cell fixed function.
③	The focus bar is displayed in the currently selected cell.
④	Displays the content of the data file in the cell. Place the mouse pointer over the data file name display area to display the sample information.
⑤	Clicking this button to expand the cell to the full screen view.
⑥	When the focus pin is upright and green () , it is linked to other cells. Refer to "10.4.2 Link Content Between Cells" P.292 for details on linking cells.

NOTE

- Files currently being edited in other windows are [Read Only] and cannot be edited. Close the file in the other window and open the file again to edit these files.
- The arrangement of cells in the vertical direction is referred to as [Row], and the arrangement of cells in the horizontal direction is referred to as [Col].
- The maximum number of [Row] and [Col] is 8 each, which means that up to 64 cells can be displayed.

10.2 Adjust Layouts

Adjust and re-arrange layouts so that the content of the currently displayed data can be easily compared.

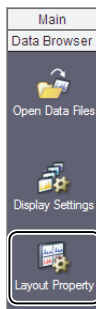
NOTE

- Drag the border of the [Data Browser] cell with the mouse to resize the cell. The size of [Data Browser] is automatically determined so that it is split into equal lengths according to the number of displayed cells.
- Use the cell connect function to partially create larger cells. Refer to "[10.2.3 Connect Cells](#)" P.287 for details on connecting cells.

10.2.1 Adjust Display Layouts

This section describes how to adjust the layout of display cells.

- 1 Click the  (Layout Property) icon on the [Data Browser] assistant bar.

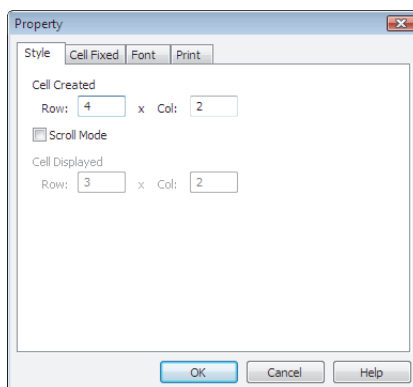


NOTE

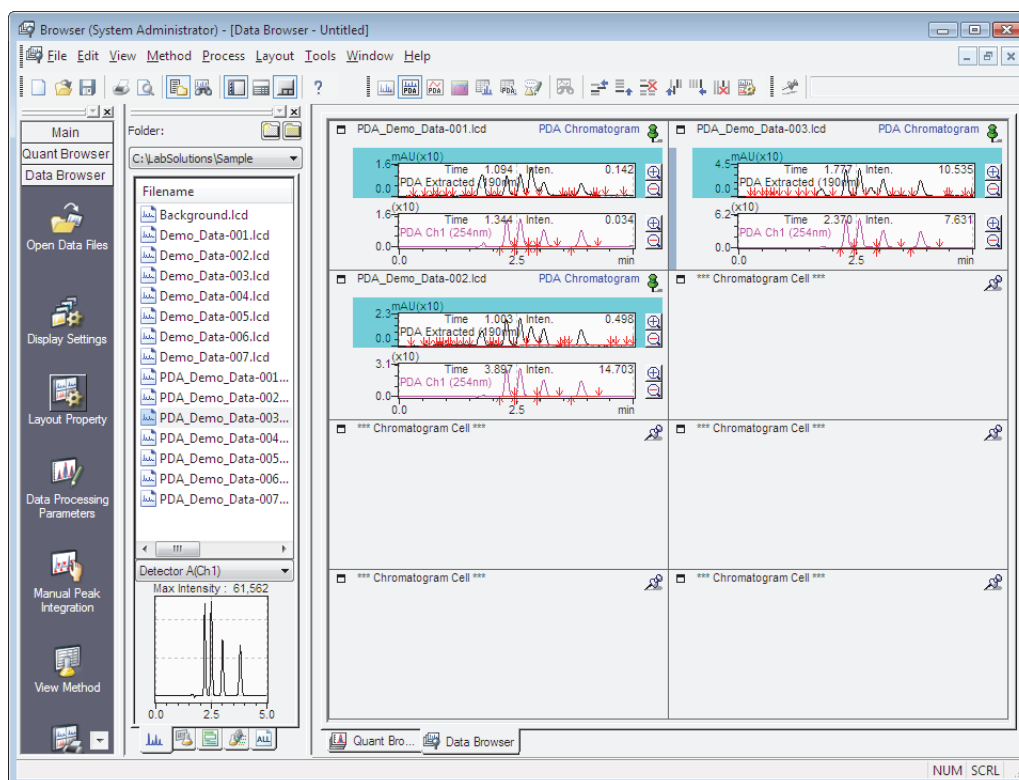
The [Property] sub-window can also be opened by clicking [Property] on the [Layout] menu of the [Data Browser] window.

- 2 Select the [Style] tab, set the number of rows and columns of the cell to display, and click [OK].



In this example, set [Row] and [Col] at [Cell Created] to "4" and "2", respectively.



A 4 × 2 grid of cells is displayed.



NOTE

- Select [Scroll Mode] in the [Style] tab to display additional cells using the scroll bars. For example, when [Row] and [Col] at [Cell Displayed] are set to “3” and “2”, respectively, a 3 × 2 grid of cells is displayed in the sub-window and the remaining cells are displayed by scrolling with the scroll bars.
- To delete rows or columns, either right-click a cell in the row or column to be deleted, select [Adjust Layout], and click [Delete Row] or [Delete Column], or click  (Delete Row) or  (Delete Column) on the toolbar. Select the cell and click [Delete Cell] from the [Edit] menu to delete a single cell.
- Select [Save Layout File As] on the [Layout] menu to save cell layouts or the display information of data loaded to each cell. This data can be saved as layout files (file extension *.lyt).

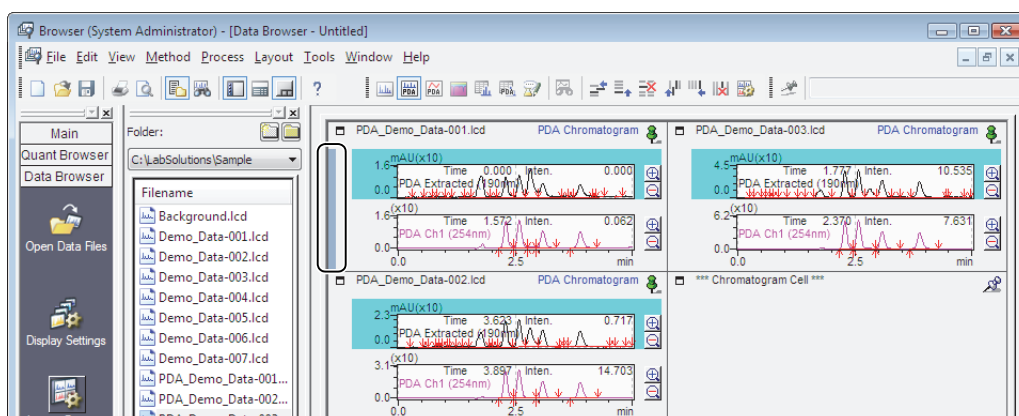
10.2.2 Change the Contents of Cells

The contents displayed in cells in the [Data Browser] window can be changed.

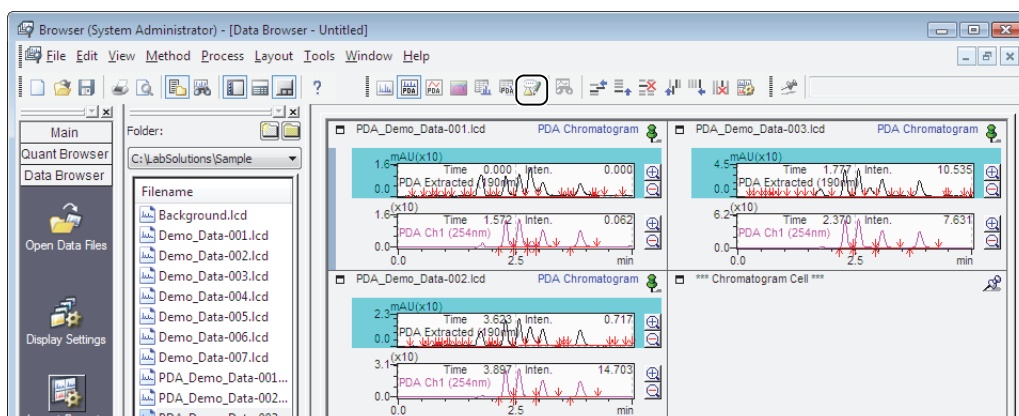
This section describes how to change the cell content from [LC Chromatogram] to [Sample Information].

1 Click the desired cell.

The focus bar is displayed.



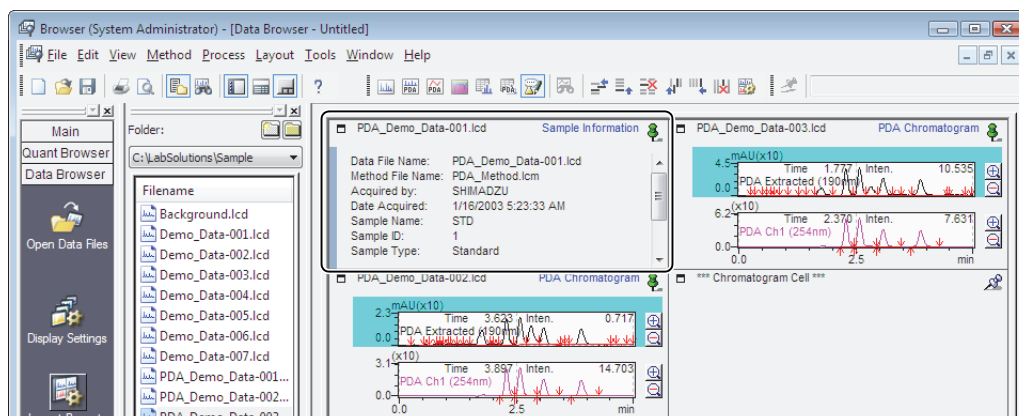
2 Click (Sample Information) on the toolbar.




NOTE

The display data can also be changed by right-clicking on the cell, selecting [Change Data Type], and clicking [Sample Information].

The display content of the cell is switched from a chromatogram to the sample information.



NOTE

- Click the  (Display Settings) icon on the [Data Browser] assistant bar to set the display mode and range of each cell.
- Right-click on the source cell and click [Copy Cell] then right-click on the destination cell and click [Paste Cell] to copy the contents to other cells. This function is handy for displaying the contents of the same data file in multiple cells.
- To swap the contents of the currently selected cell with the contents of another cell, drag the title (file name) of the selected cell and drop it on the target cell.
- Right-click on the desired cell and click [Release Data from Cell] to delete the display contents of a cell.

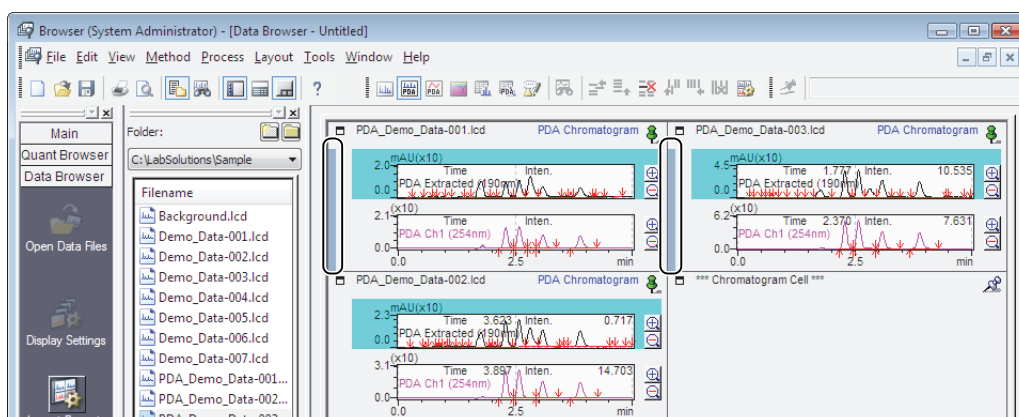
10.2.3 Connect Cells

Adjacent cells can be connected or disconnected.

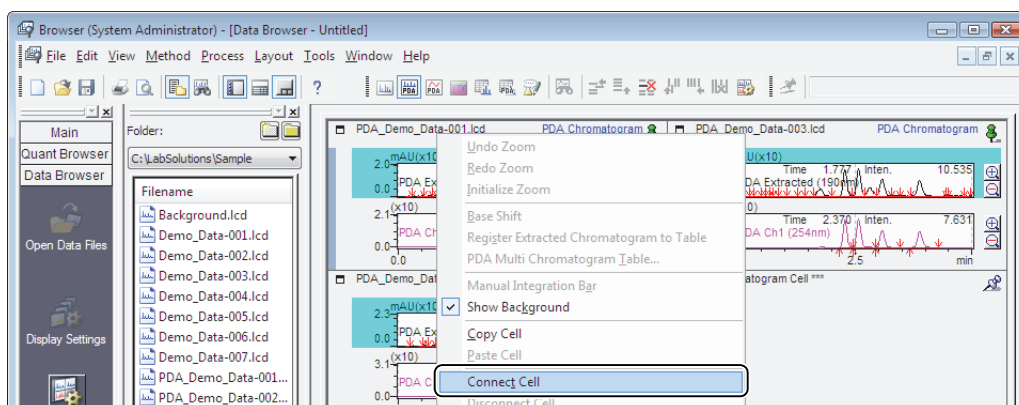
This section describes how to connect cells.

1 Select the cells to connect with the [Ctrl] key held down.

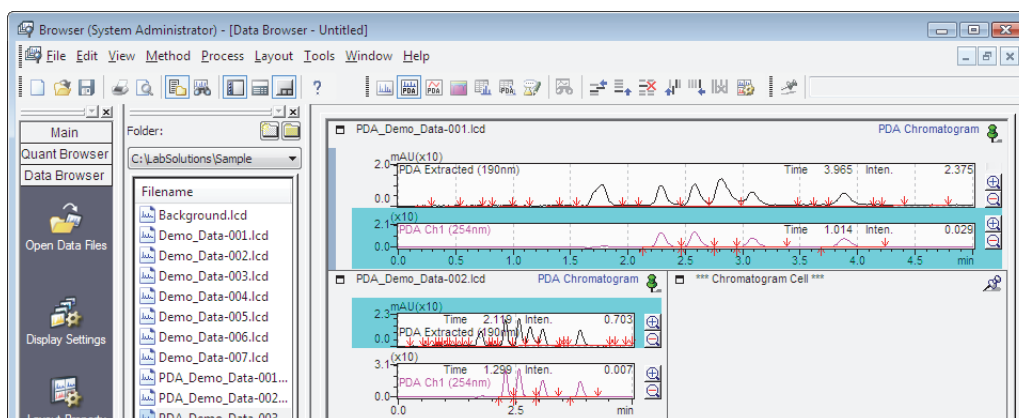
The focus bar is displayed on the multiple cells.



2 Right-click on one of the selected cells and click [Connect Cell].



The cells are connected.



NOTE

- When cells are connected, data which is open in secondary cells is closed.
- Right-click on the connected cell and click [Disconnect Cell] to disconnect cell connections.
- Select cells to be connected so that the shape of the resulting cell is a rectangle.

10.3 Cell Fixed Function

Use the cell fixed function to efficiently compare different data files. For example, compare the peaks of the control sample and target sample.

When the cell fixed function is used, the cell numbers are displayed in each cell. The contents of the same data file is displayed in cells of the same cell number.

Reference

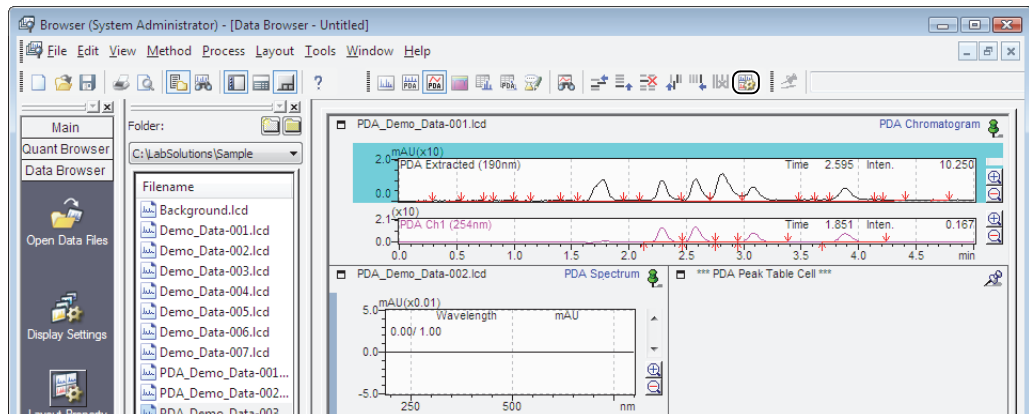
"10.4.1 Load a Data File in Multiple Cells" P.289


"10.4.3 Peak Integration on Chromatograms" P.294

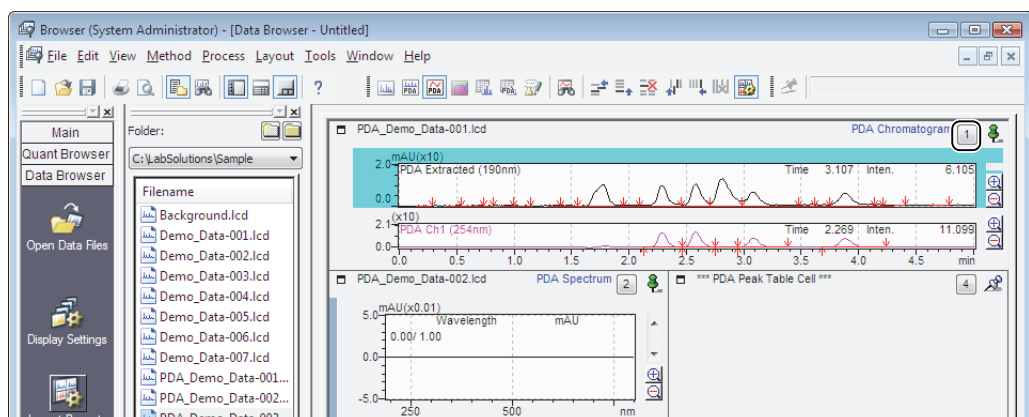
10.3.1 Use the Cell Fixed Function

This section describes how to turn the cell fixed function on.


- 1 Click the  (Cell Fixed) icon on the toolbar.



 (Cell Fixed) is selected, and cell number (1) is displayed in the cell.



NOTE

- Click the  (Cell Fixed) icon on the toolbar again, to turn the cell fixed function off.
- The cell fixed function can also be switched on and off by clicking [Cell Fixed] on the [Edit] menu in the [Data Browser] window.

10.4 Compare Data

10.4.1 Load a Data File in Multiple Cells

This section describes how to use the cell fixed function to display the chromatograms and PDA chromatograms of data files 1 and 2.

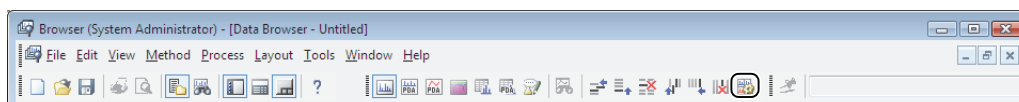
1 Determine the layout and cell type.


This example uses a 2 row × 2 column layout to display a chromatogram in the 1st row and a PDA chromatogram in the 2nd row.

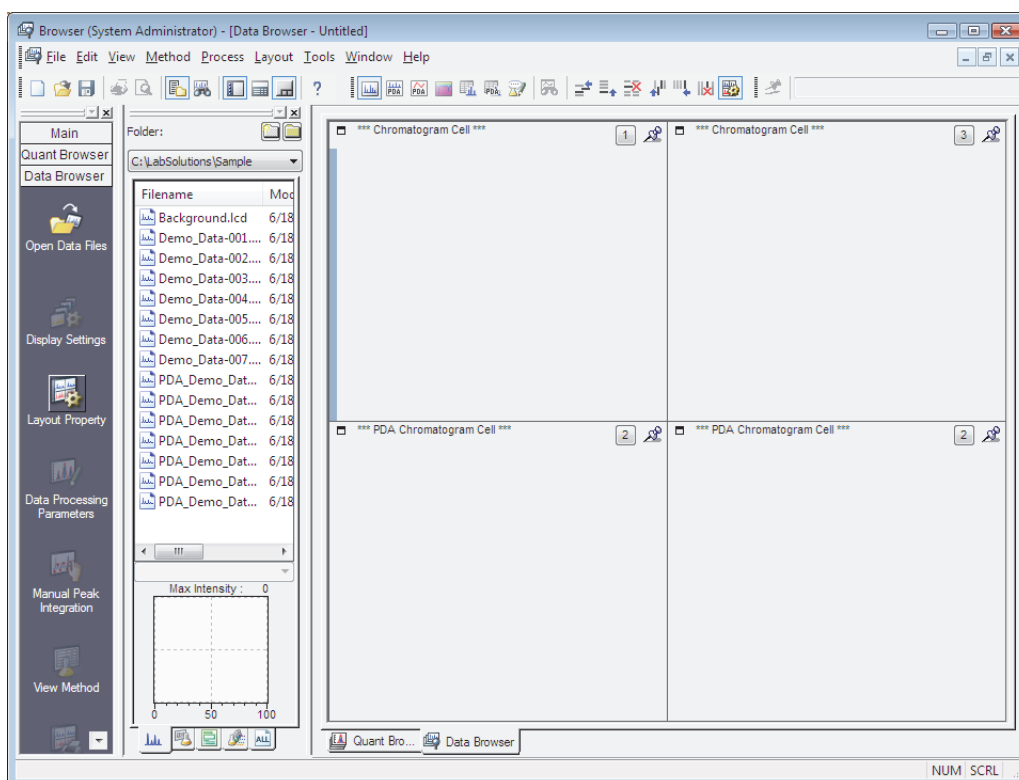
Reference

Refer to *"10.2.1 Adjust Display Layouts" P.283* for details on changing layouts, and *"10.2.2 Change the Contents of Cells" P.285* for changing cell type.

2 Click the (Cell Fixed) icon on the toolbar.



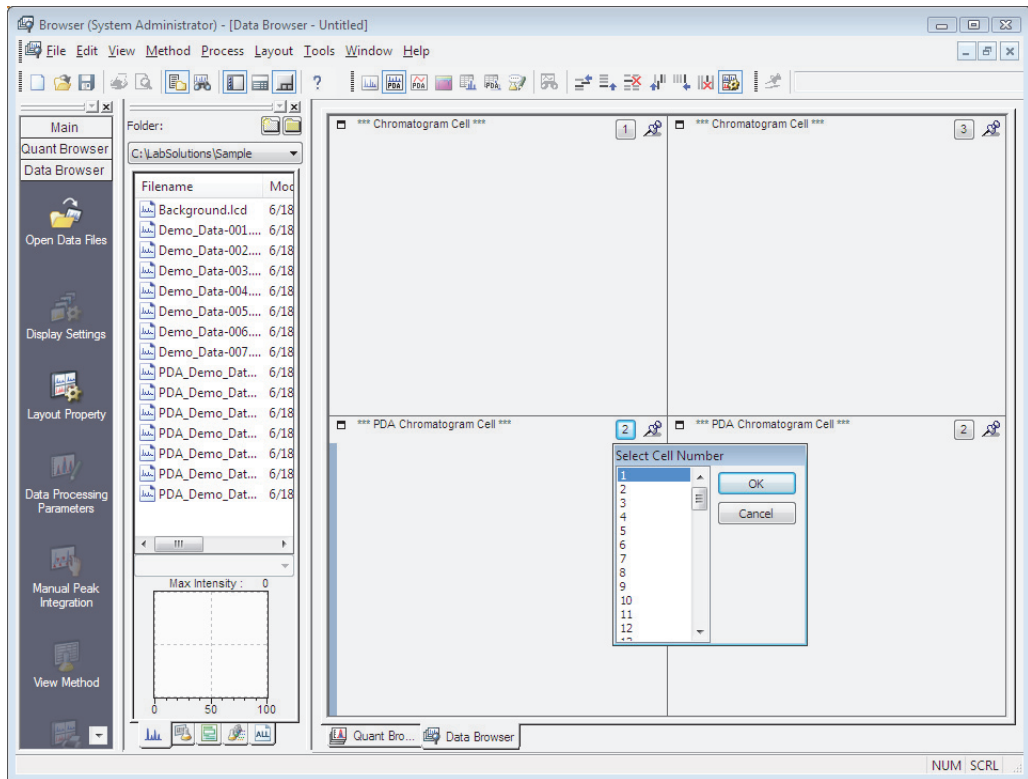
 (Cell Fixed) is selected and cell number (1) is displayed in the cell display area.



3

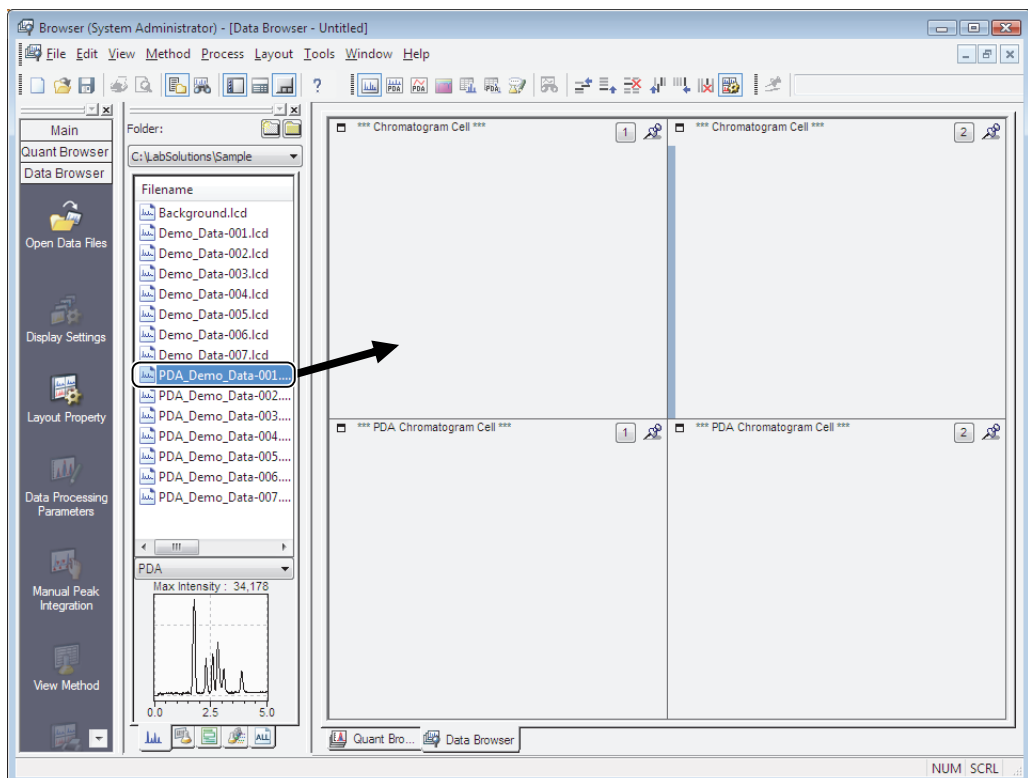
Click the cell number (1) that is to be changed, and set the cell number.

In this example, set the cells in the 1st column to “1” and the cells in the second column to “2”.

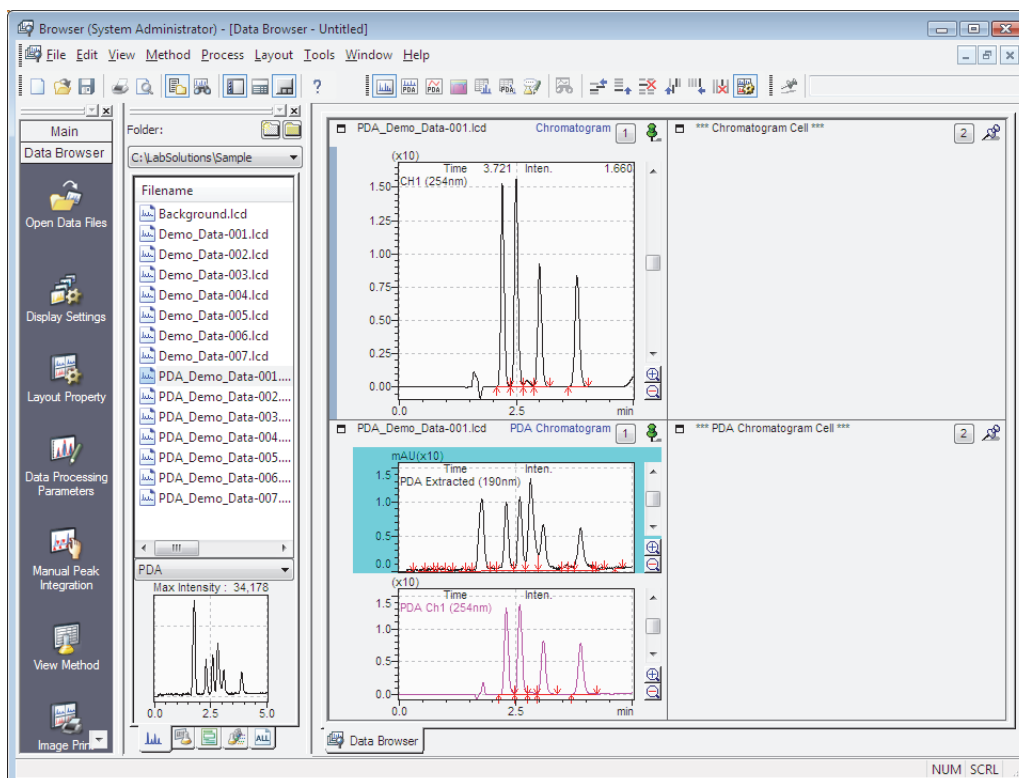


4

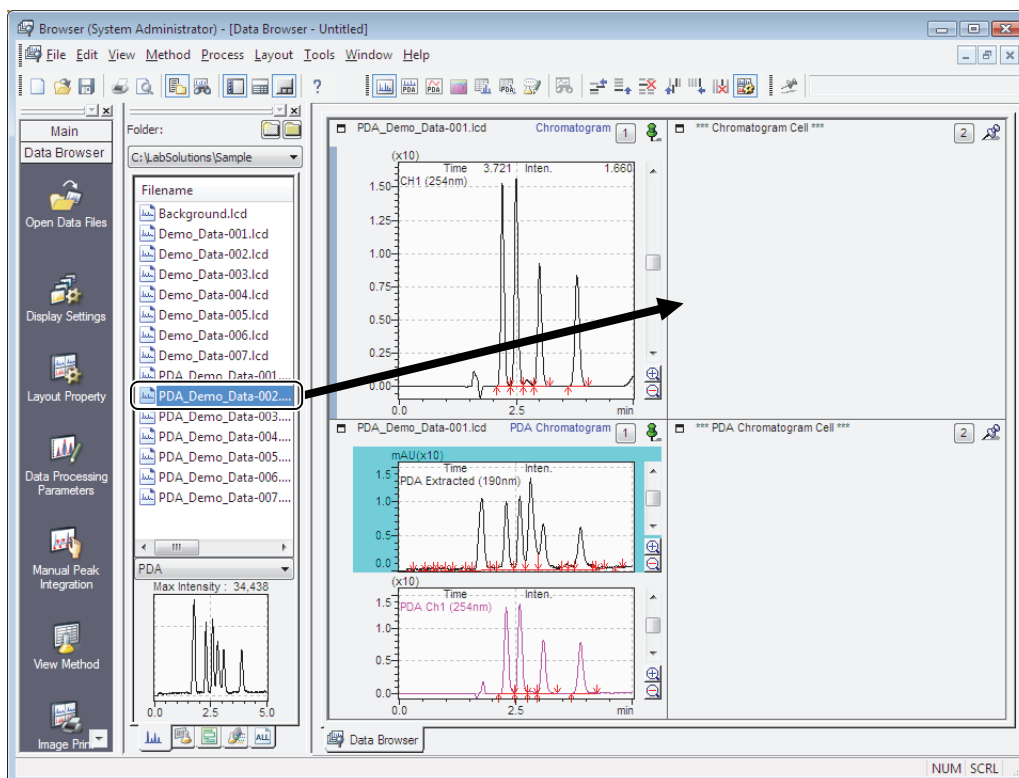
Drag-and-drop data file 1 onto the number 1 chromatogram cell from the [Data Explorer] sub-window.



The contents of the data file are displayed in the number 1 cells.

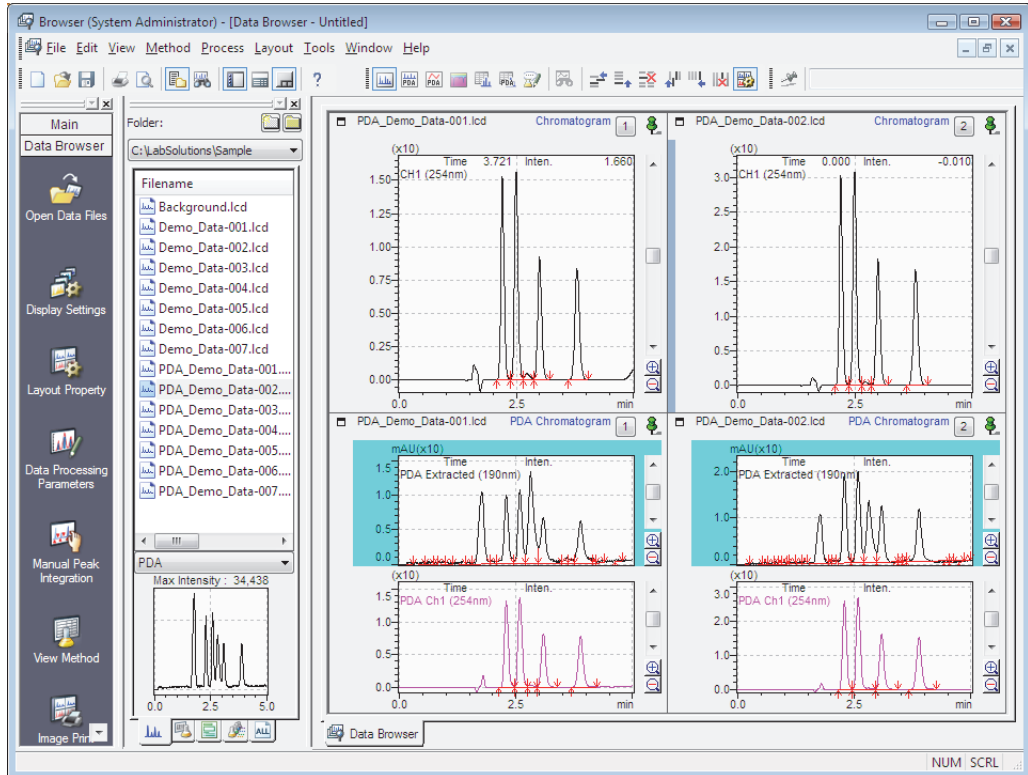


5 Drag-and-drop data file 2 onto the number 2 chromatogram cell from the [Data Explorer] sub-window.




10

The contents of the data file are displayed in the number 2 cells.



10.4.2 Link Content Between Cells

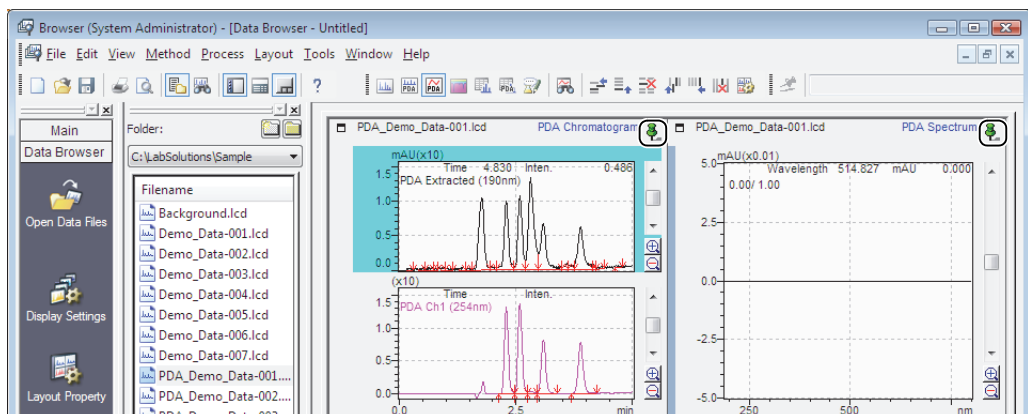
An upright focus pin () indicates that the cell is linked to other cells.

For example, if the [PDA Chromatogram] and [PDA Spectrum] cell are linked and the chromatogram is double-clicked, the displayed spectrum in the [PDA Spectrum] cell is updated.

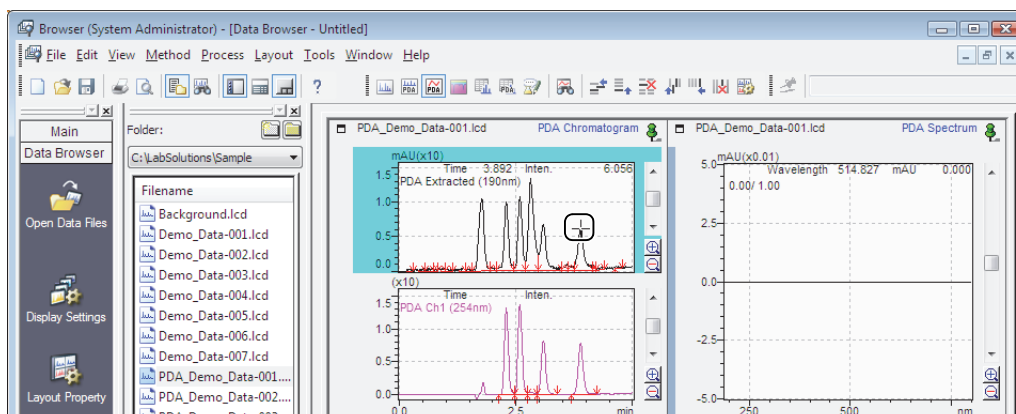
This section describes how to link the [PDA Spectrum] cell display with the [PDA Chromatogram] cell.

1 Ensure that the focus pin is upright () on the [PDA Chromatogram] and [PDA Spectrum] cells.

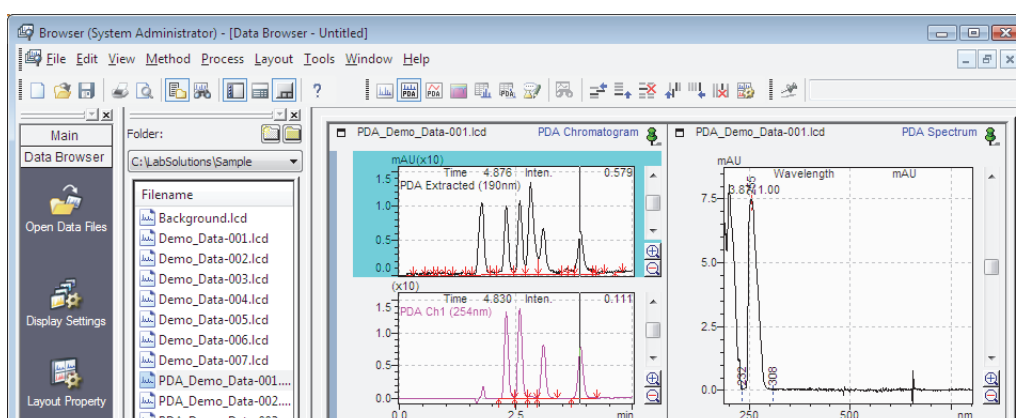
If the focus pin is down (), click  to change it to the upright state ().



2 Double-click the desired time position in the [PDA Chromatogram] cell.



The spectrum at that time is displayed in the [PDA Spectrum] cell.



NOTE

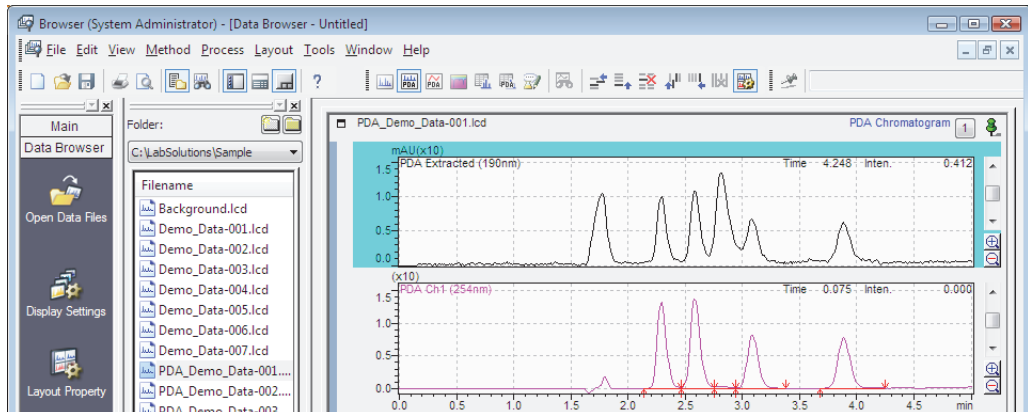
- Depending on the type of cell, the display may be altered to display other information.
- The default state of the focus pin in the cell is upright.
- Click an upright focus pin to disable cell links.

10.4.3 Peak Integration on Chromatograms

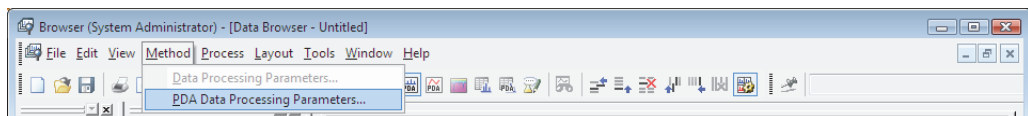
This section describes how to perform peak integration on [PDA Chromatogram] in the [Data Browser] window.

■ Perform Peak Integration

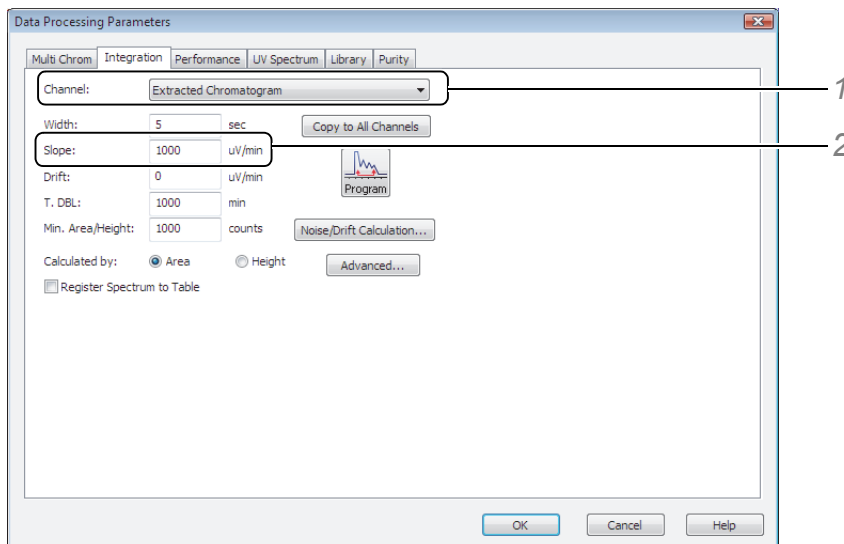
1 Open the [PDA Chromatogram] to be integrated.



2 Click [PDA Data Processing Parameters] on the [Method] menu.



3 Click the [Integration] tab, set each of the integration parameters, and click [OK].



- 1 Select the channel to be integrated. In this example, select [Extracted Chromatogram].
- 2 Change the [Slope] setting to "1000".

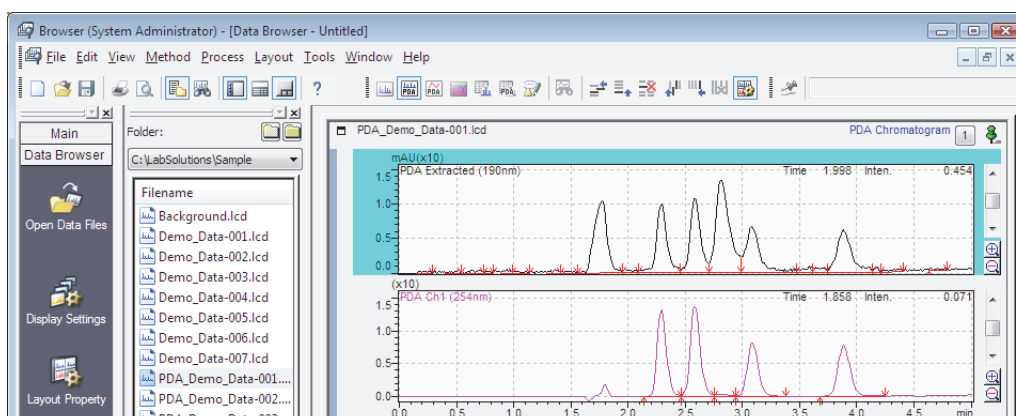
👉 Reference

Refer to the Data Acquisition & Processing Theory Guide for details on each of the parameters.

 **NOTE**

If automatic peak integration is not successful, try manual peak integration. Right-click on the PDA chromatogram and click [Manual Integration Bar] to display the [Manual Integration Bar]. The [Manual Integration Bar] cannot be displayed if an overlaid PDA chromatogram is displayed. Select [Stack] or [Single] to display the [Manual Integration Bar]. Refer to Help for details on the [Manual Integration Bar]

Peak integration is performed on the extracted chromatogram and the results are displayed. The baseline and peak top comment are displayed on the PDA chromatogram.



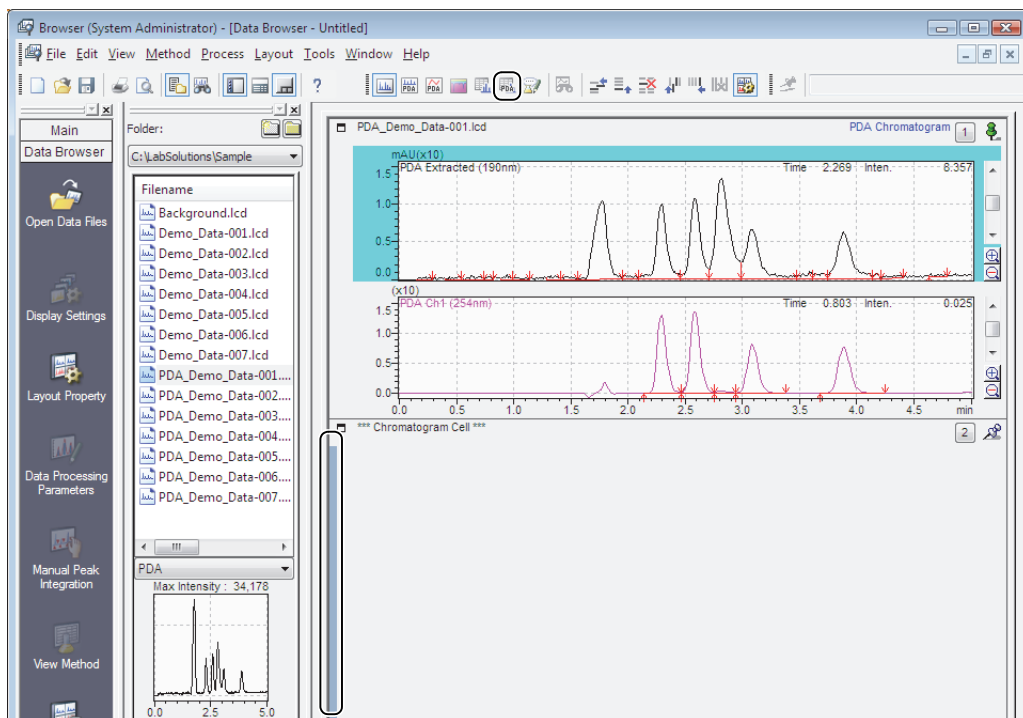
■ Examine the Peak Integration Results

The results of peak integration can be examined in the [PDA Peak Table] cell.

This section describes how to change the displayed cell to the [PDA Peak Table] cell to examine the peak integration results of the extracted PDA chromatogram.

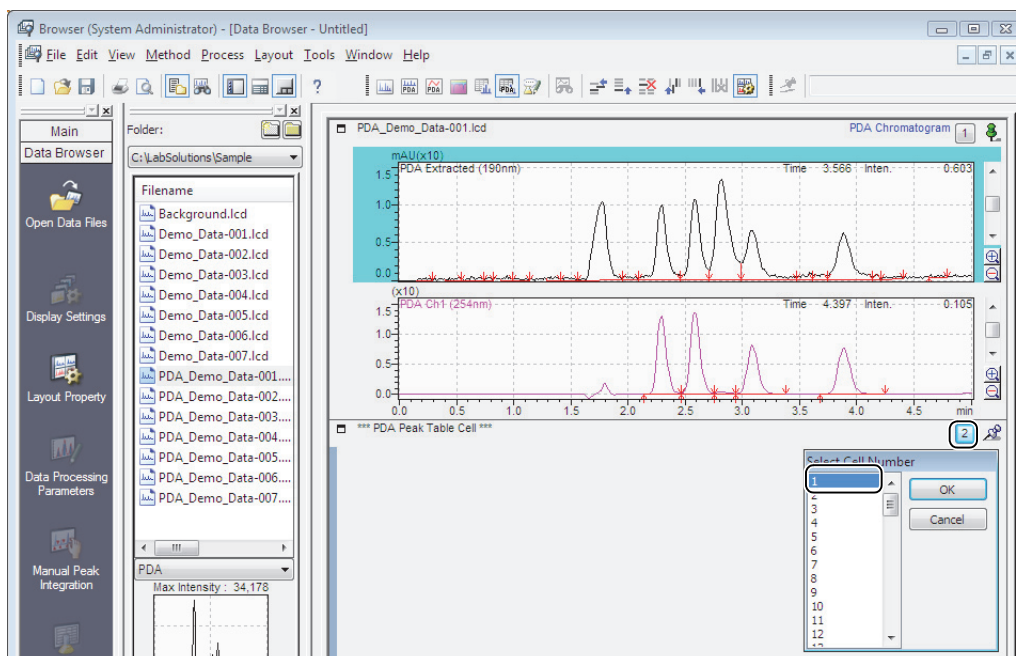
- 1** Select the cell to be changed to the [PDA Peak Table] and click  (PDA Peak Table) on the toolbar.

Click the cell to display the focus bar in that cell. Click  (PDA Peak Table) on the toolbar to change the cell to the [PDA Peak Table] cell.



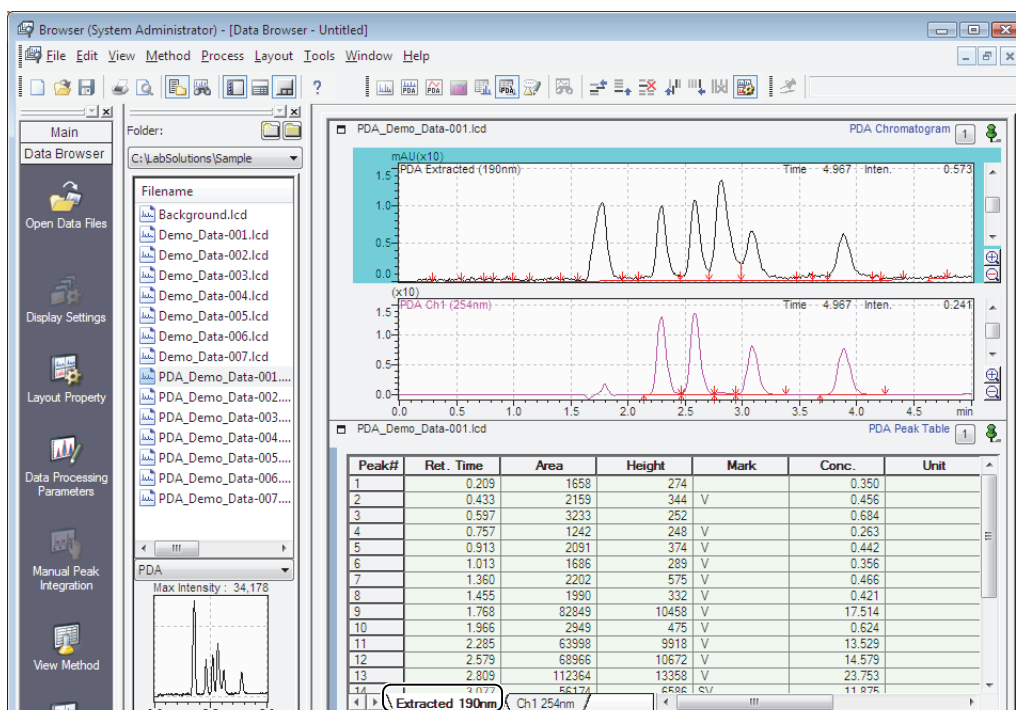
2 Click the cell number and select the cell number in the [Select Cell Number] sub-window.

If the cell number is not displayed, refer to "10.3.1 Use the Cell Fixed Function" P.288 to turn the cell fixed function off.



3 Click the [Extracted] tab.

The peak integration results of the extracted PDA chromatogram are displayed.



NOTE

The peak integration results of chromatograms are displayed in the [Peak Table] cell.

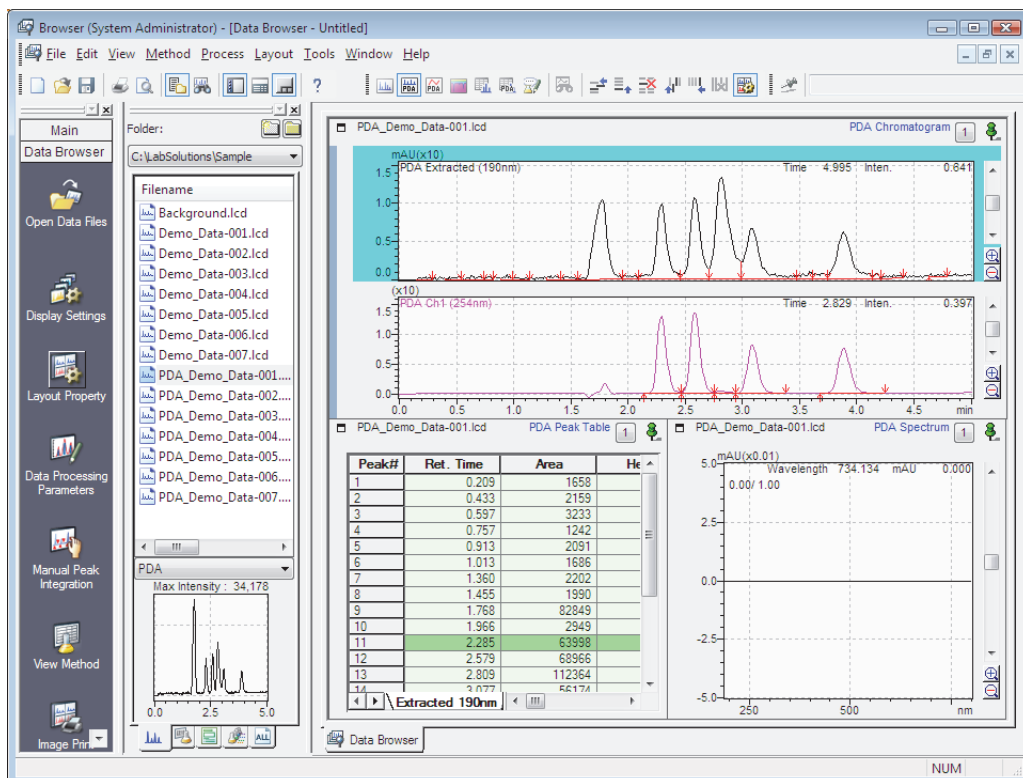
■ Link Cells to Check Peak Integration Results

This section describes how to link the [PDA Chromatogram], [PDA Peak Table] and [PDA Spectrum] cells to check peak integration results.

1 Position the [PDA Chromatogram], [PDA Peak Table] and [PDA Spectrum] cells as follows.

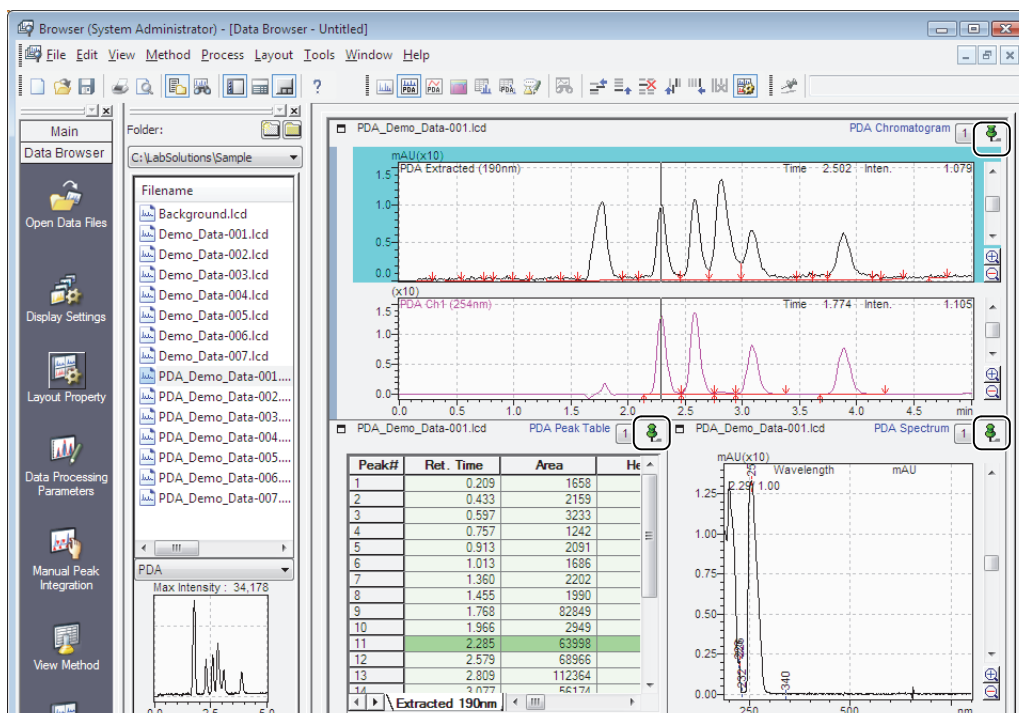
Reference

Refer to "10.2 Adjust Layouts" P.283 for details.



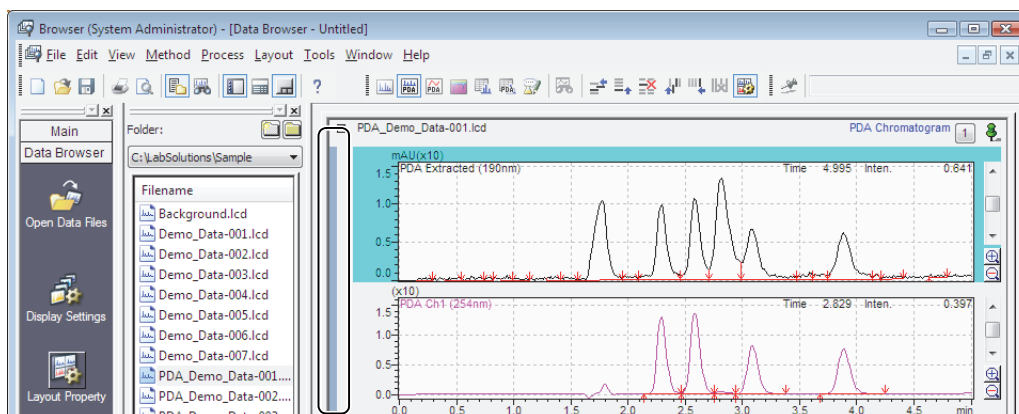
2 Ensure that the focus pins of the cells are in the upright (📌) position.

If the focus pin is down (📌), click 📌 to change it to the upright state (📌).



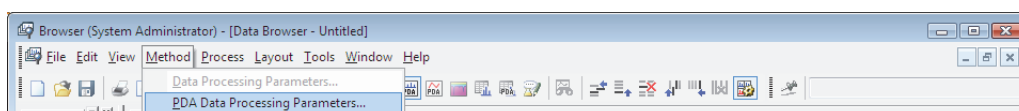
3 Click the [PDA Chromatogram] cell.

The focus bar is displayed on the [PDA Chromatogram] cell.

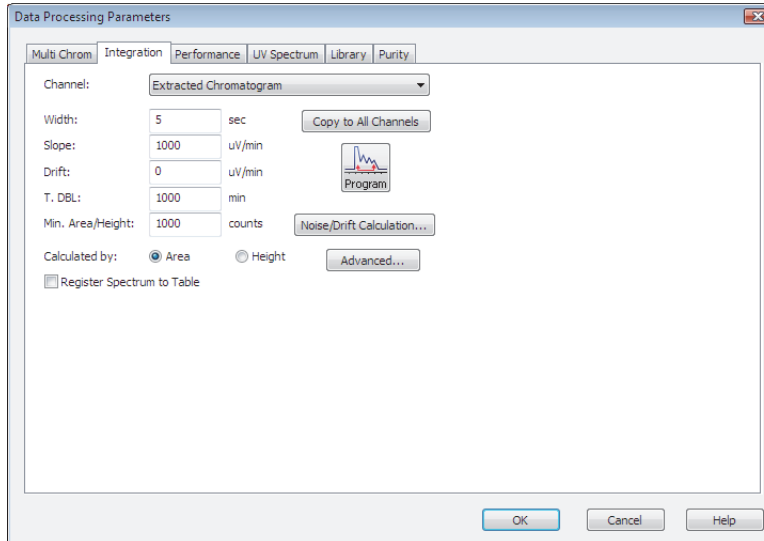


10

4 Click [PDA Data Processing Parameters] on the [Method] menu.



- 5** Enter the parameters in the [Data Processing Parameters] sub-window, and click [OK]. Peak integration is performed when [OK] is clicked, even if no changes were made in the [Data Processing Parameters] sub-window.



- 6** After peak integration, click a row on [PDA Peak Table]. The information for that peak is displayed in the [PDA Chromatogram] and [PDA Spectrum] cells.

Peak#	Ret. Time	Area	He
1	0.209	1658	
2	0.433	2159	
3	0.597	3233	
4	0.757	1242	
5	0.913	2091	
6	1.013	1686	
7	1.360	2202	
8	1.455	1990	
9	1.768	82849	
10	1.966	2949	
11	2.285	63998	
12	2.579	68966	
13	2.809	112364	
14	3.077	86174	

10.5 Print a Browser Report

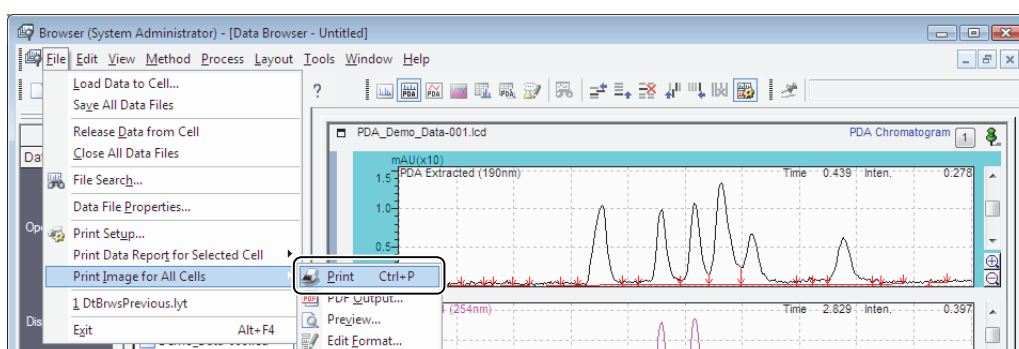
The [Data Browser] window has functions for printing all of the cells or only selected cells. Size, color and other information in the chromatogram and spectrum cells also are reflected in the printout.

10.5.1 Print All of the Cells

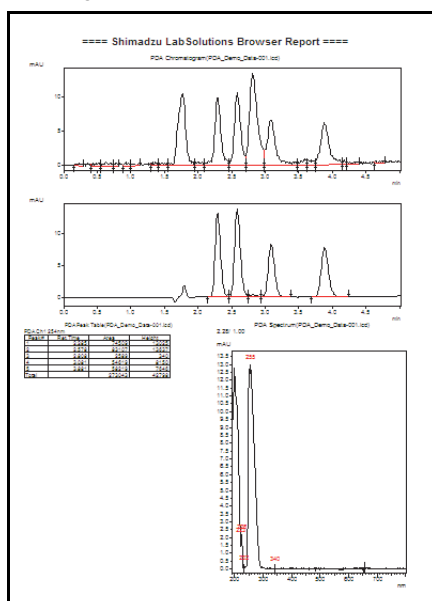
An image of all of the cells currently displayed in the [Data Browser] window can be printed.

This section describes how to print all of the cells.

- 1 Select [Print Image for All Cells] on the [File] menu, and click [Print].



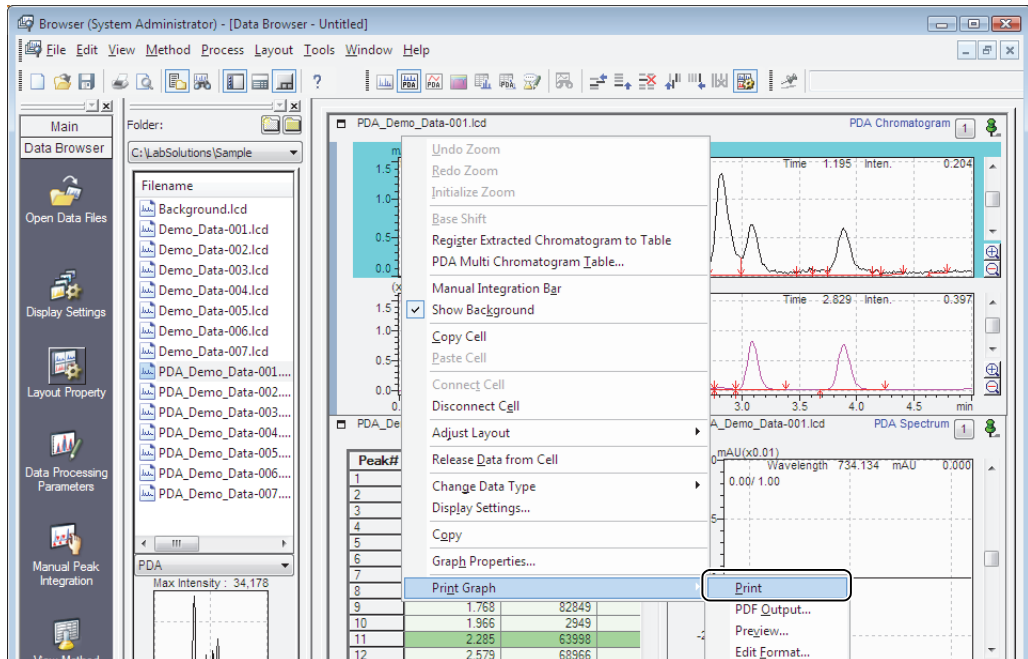
An image of all of the cells is printed in the preset report layout locations.



10.5.2 Print Selected Cells

An image of the cells currently selected in the [Data Browser] window can be printed. This section describes how to print the [PDA Chromatogram] cell.

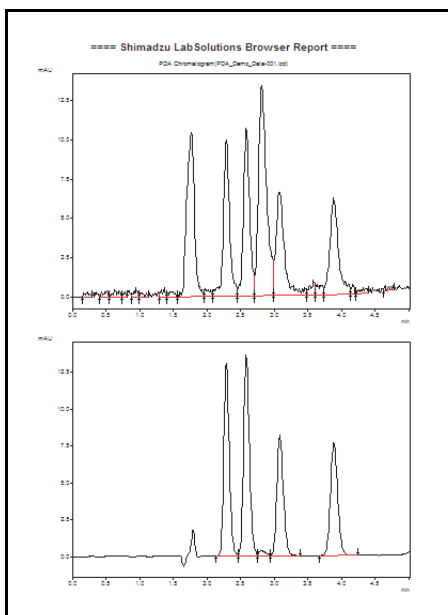
- 1 Right-click on the desired cell, select [Print Graph], and click [Print].



NOTE

The right-click menu changes to [Print Table] or [Print Sample Information] when the cell content is a table or sample information, respectively.

The image of the selected cell is printed.



11

Data Comparison

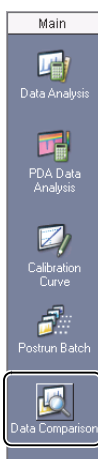
This chapter describes how to overlay multiple data overlaid and perform calculations in the [Data Comparison] window. Up to 16 chromatograms can be overlaid in the [Data Comparison] window for comparison.

Comparison calculations can be performed for the data of any currently specified chromatograms.

11.1 Open the [Data Comparison] Window

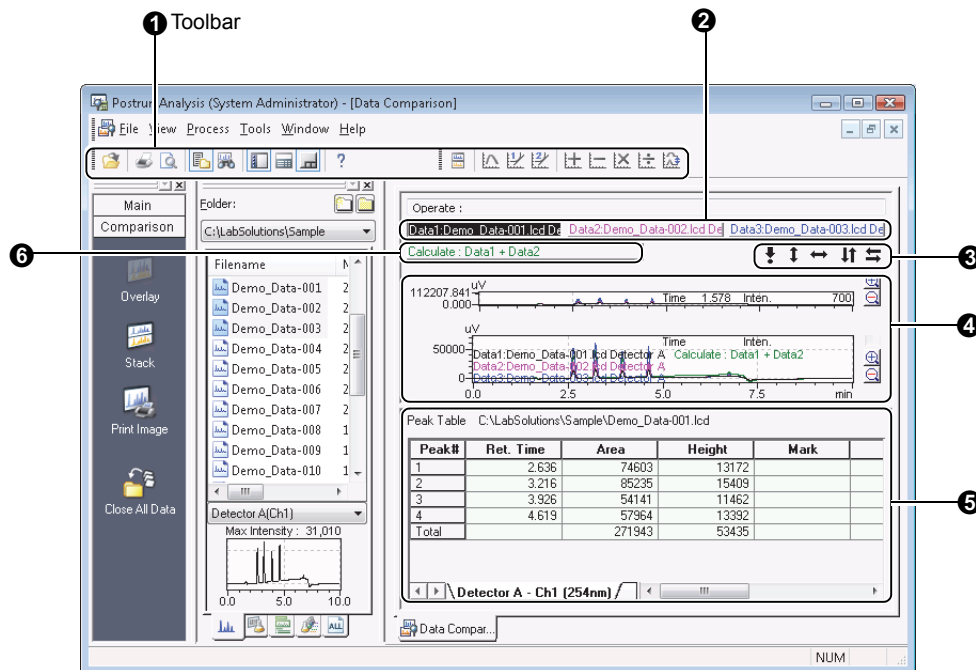
This section describes how to overlay the chromatograms of selected data in the [Data Comparison] window.

- 1 Click the  (Data Comparison) icon on the assistant bar in the [Postrun Analysis] program.



11.2 [Data Comparison] Window Description

This section describes how to view and use the [Data Comparison] window.



No.	Explanation
①	Displays the [Standard] and [Data Comparison] toolbars.
②	Displays the information for the displayed data file. Right-click on the data file information and click [Close] to close the data file.
③	Use these buttons to expand, reduce or moves a selected chromatogram to the top, bottom, left or right. <ul style="list-style-type: none"> To move a chromatogram up/down or left/right, click (Move Up/Down) or (Move Left/Right) and drag the chromatogram to the move destination position. Click (Base Point) to expand or reduce a chromatogram and the click the position of the base point on the chromatogram to determine that point. Next, click (Zoom Up/Down) or (Zoom Left/Right), and drag the chromatogram to the expand/reduce destination point. The chromatogram is expanded or reduced to that point.
④	Displays the chromatogram of the open data file as [Full Chromatogram] or [Zoomed Chromatogram]. Three view methods are available, [Overlay], [Stack] and [Base Shift].
⑤	Displays the Peak Table of the selected chromatogram.
⑥	Displays calculation formulas for operations performed between the data of selected chromatograms.

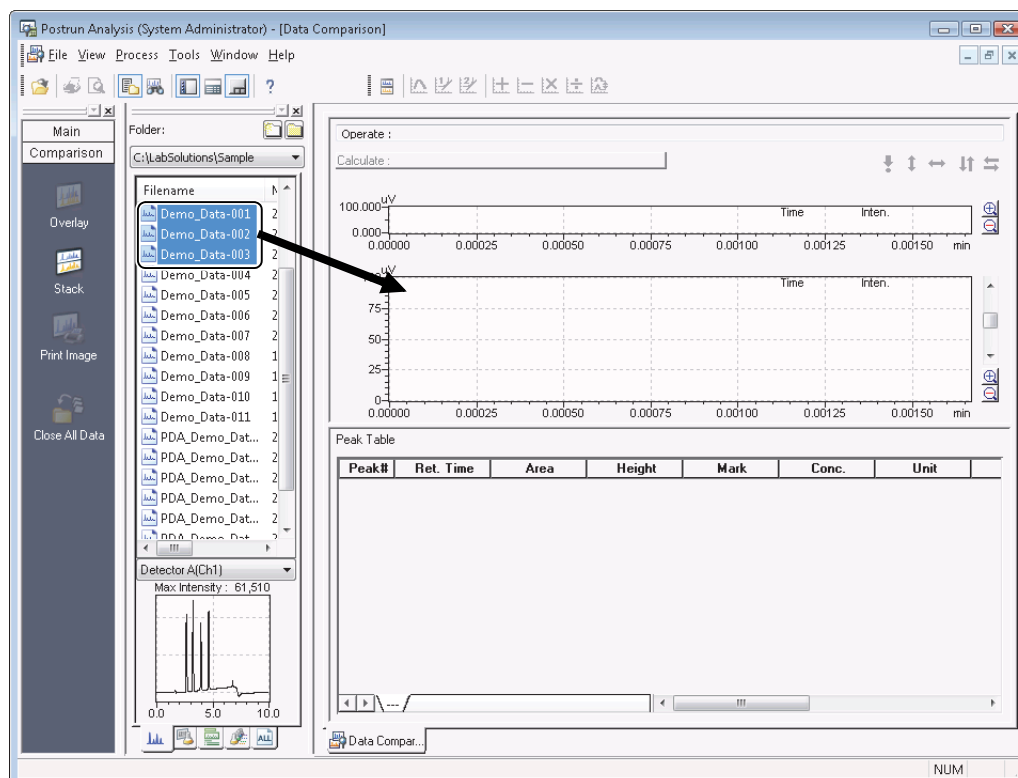
NOTE

- Right-click on the chromatogram and select [Base Shift] to shift the displayed chromatograms by an equal interval.
- Right-click on the chromatogram and select [Copy] to paste the chromatograms into other applications as image files.
- Select [Close] on the [File] menu, then select [All Data] to close all of the open data.

11.3 Overlay Multiple Data


This section describes how to display the chromatograms of selected data overlaid in the [Data Comparison] window.

- 1 Select the data file to overlay in the [Data Explorer] sub-window, and drag-and-drop that file onto the [Data Comparison] window.



The chromatogram and Peak Table of the data files are displayed in the [Data Comparison] window.

NOTE

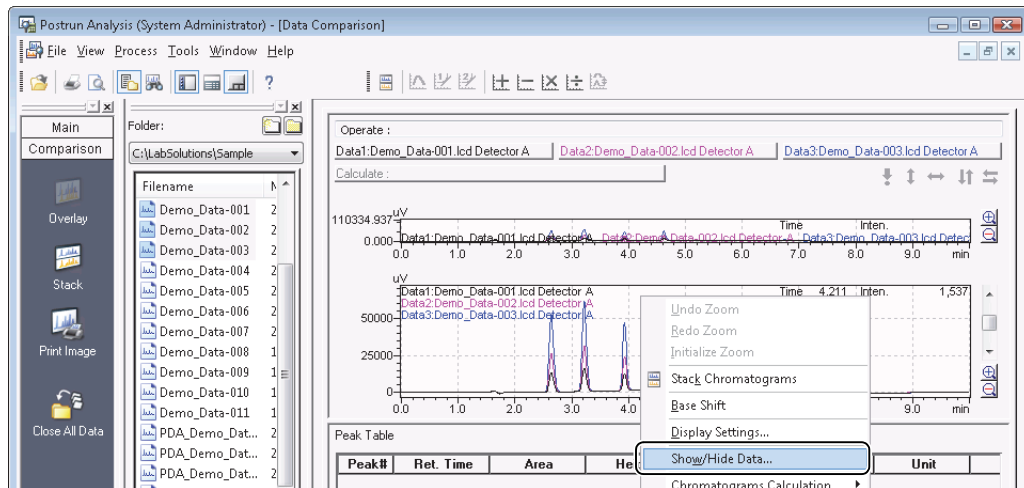
- A sub-window opens for channel selection when displaying a data file obtained by data acquisition on multiple channels. Select the checkbox of the channel to display.
- Data files obtained by a PDA detector cannot be displayed overlaid in the [Data Comparison] window.
To display in the [Data Comparison] window, select [Export Data] on the [File] menu in the [PDA Data Analysis] window, click [Export Chromatogram to Data File] and extract the multi chromatogram.
- Click the  (Stack) icon on the [Comparison] assistant bar to display chromatograms in a stacked format.

11.4 Perform Calculations on Chromatograms

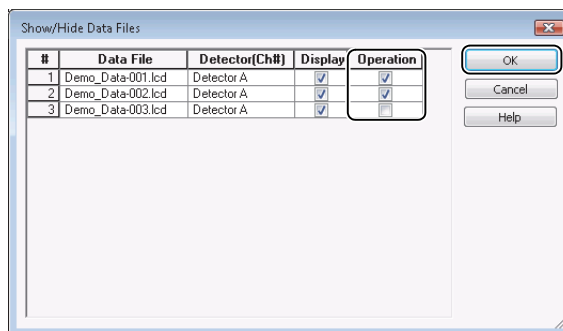
Specify any displayed chromatograms to perform arithmetic calculations (addition/subtraction/multiplication/division) on the data.

This section describes how to perform arithmetic operations on 2 chromatograms.

1 Right-click on [Chromatogram View], and click [Show/Hide Data].



2 Select [Operation] to perform the arithmetic operation on the data, and click [OK].



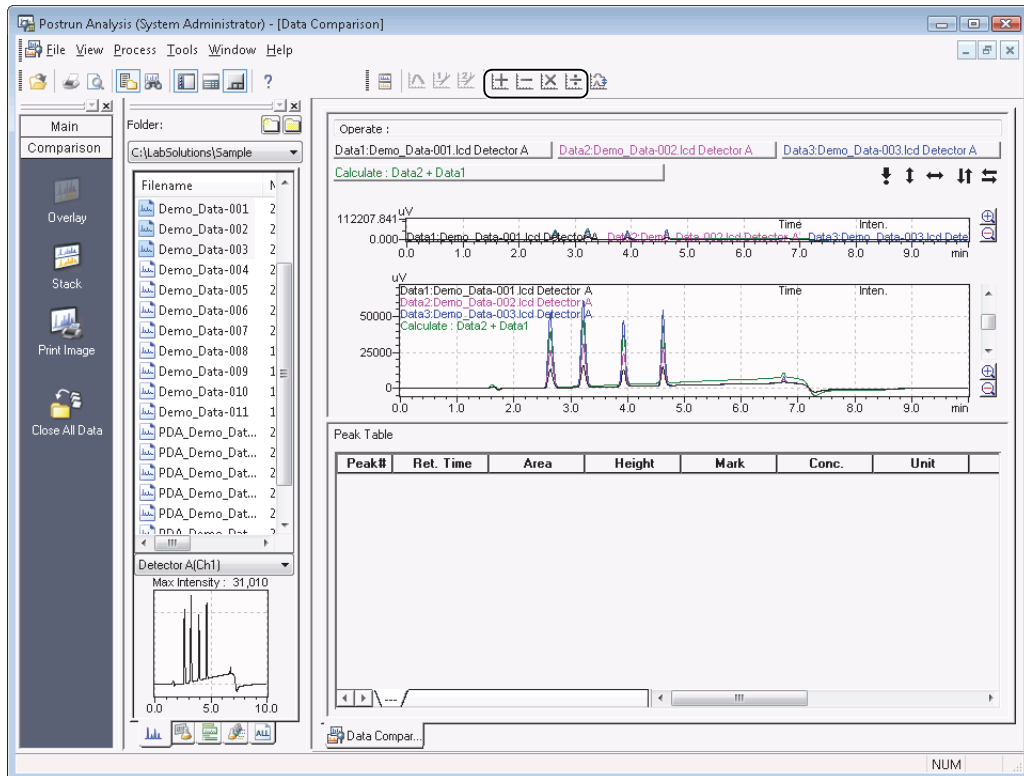
NOTE

Arithmetic operation can only be executed between 2 chromatograms.
An error occurs if 3 or more chromatograms are selected.


3 Click the desired arithmetic operation () on the toolbar.

The arithmetic operation is performed on the data of the selected chromatograms, and an additional green chromatogram is displayed.

The calculation formula can be checked by [Calculate : Data2 + Data1](#).



NOTE

- Click  (Reverse Data Order) on the toolbar to change [Calculate : Data2 + Data1](#) to [Calculate : Data1 + Data2](#) so that the calculation data is reversed.
- Right-click on [Chromatogram View], and select [Save Processed Data] to save the calculation result.

12

AART

12.1 AART (Automatic Adjustment of Retention Time)

If the column is cut to change the length or if a column from a different lot is used, the retention times in the measurement data may change. In this case, the times set in the instrument parameters and compound table must be modified so that the target compounds can be measured and identified reliably.

AART(Automatic Adjustment of Retention Time) allows you to modify all retention times based on retention indexes of target compounds.

Using the AART incorporated in this software makes it easier to modify the set times and helps reduce time-consuming work, even when analyzing various types of compounds in a batch.

This operation manual explains how to use the AART, which is based on the retention index.

<Retention Index>

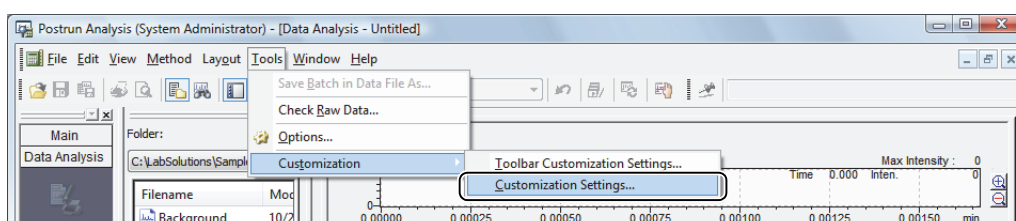
The retention index is calculated using the relationship between the n-alkanes retention time and the target compounds retention time. Usually, the elution position of a compound in a chromatogram is expressed in terms of the retention time. The retention time is, however, greatly affected by the type of column, the temperature, and the flow rate of the carrier gas. Expressing the retention time of compounds in terms of a value (the retention index) that correlates with the retention times of n-alkanes with different carbon numbers makes it possible to express the elution position as a value that remains constant even if the column length and internal diameter change. AART corrects the retention time using this retention index.

12.2 Before Using AART

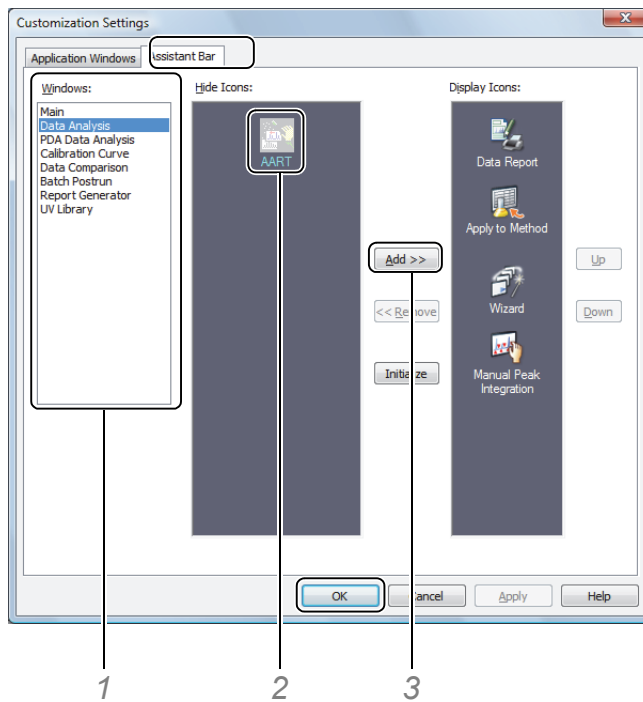
12.2.1 Add the [AART] icon on the [Data Analysis] assistant bar

To use AART, it is handy to add the [AART] icon on the [Data Analysis] assistant bar. This section describes how to add the [AART] icon on the [Data Analysis] assistant bar.

- 1 Select [Customization] on the [Tools] menu in the [Data Analysis] window, and click [Customization Settings].



- 2** Click the [Assistant Bar] tab, add the [AART] icon to the [Display Icons] list, and click [OK].



- 1 Select [Data Analysis] in the [Windows] list.
 - 2 Select the [AART] icon in the [Hide Icons] list.
 - 3 Click [Add].
- The [AART] icon is added to the [Display Icons] list.

The [AART] icon is added to the [Data Analysis] assistant bar.

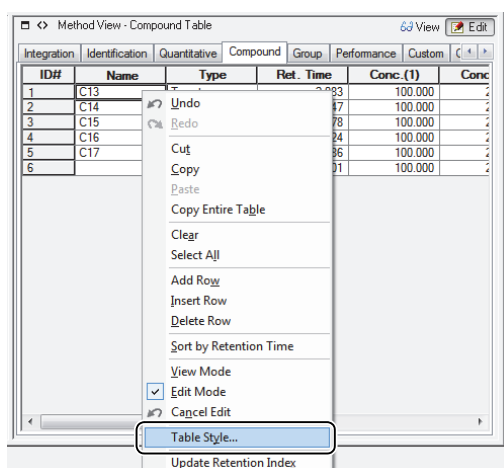
NOTE

To change the display order of icons on the assistant bar, select the icon to move at [Display Icons], and click [Up] or [Down].

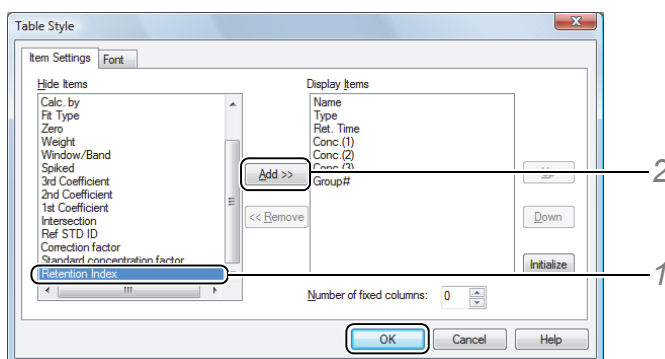
12.2.2 Display the [Retention Index] column in the Compound Table

When retention index is set in a data file or a method file, load the file in [Data Analysis] or [Calibration Curve] window and set [Table Style] so that the [Compound Table] can display the [Retention Index] column.

- 1 Click the [Compound] tab.
- 2 Right-click on the compound table, and click [Table Style].



- 3 Add the [Retention Index] column to the compound table in the [Table Style] sub-window, and click [OK].



- 1 Select [Retention Index] in the [Hide Items] list.
 - 2 Click [Add].
- The [Retention Index] item is added to [Display Items] list.

ID#	Name	Type	Ret. Time	Conc. (1)	Retention Index
1	C13	Target	2.083	100.000	0
2	C14	Target	2.747	100.000	0
3	C15	Target	3.678	100.000	0
4	C16	Target	4.824	100.000	0
5	C17	Target	6.086	100.000	0
6		Target	0.001	100.000	0



NOTE

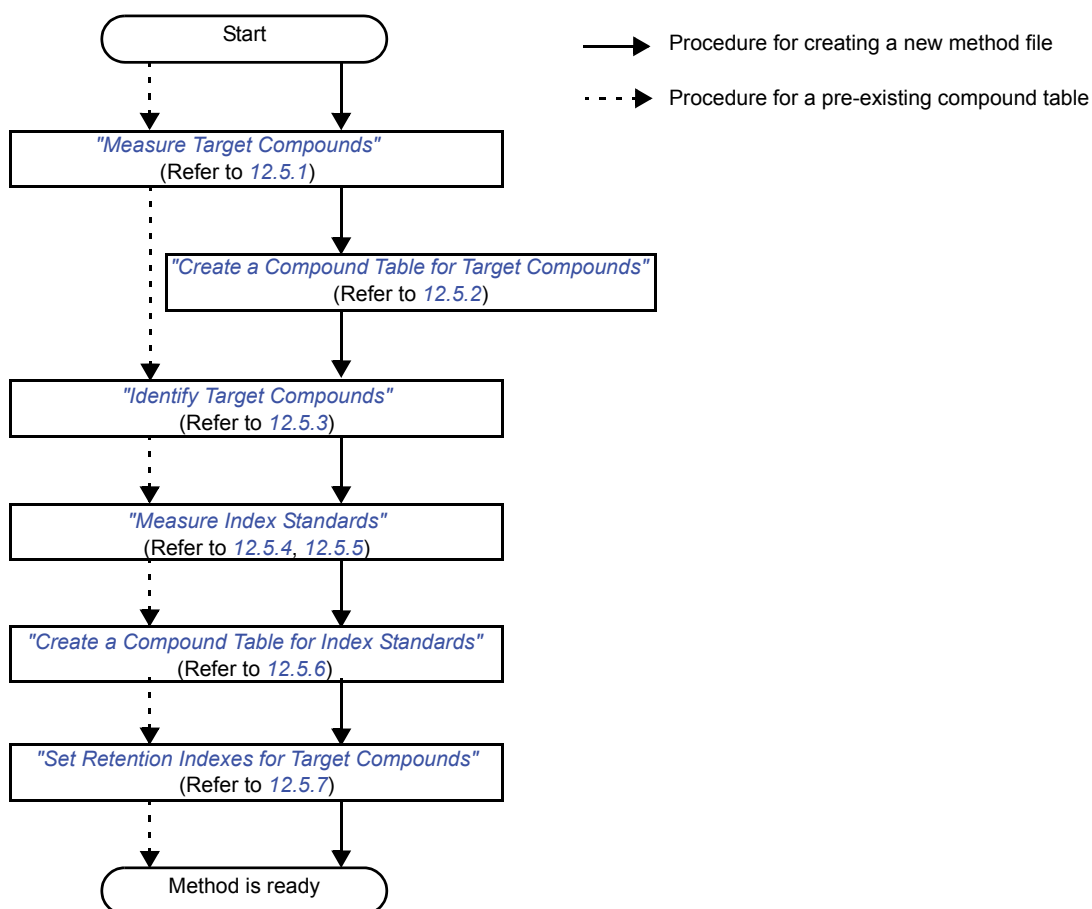
Change the display order of items in the compound table, by selecting the item in the [Display Items] list and then clicking [Up] or [Down].

12.3 How to run AART

The procedure for modifying retention times using retention indexes consists of the following steps. (Refer to the appropriate chapter for details.)

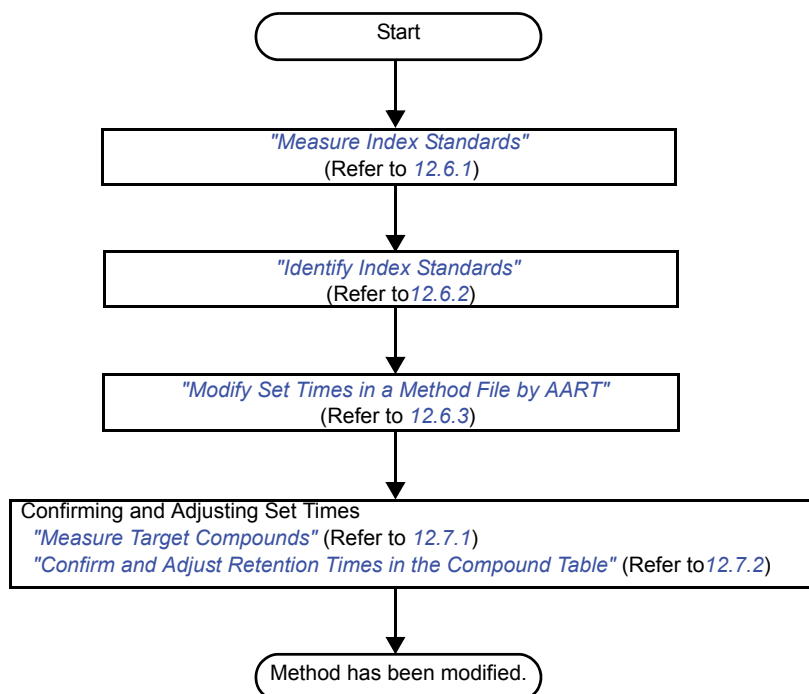
■ Setting up a method file applicable to AART

To perform AART, it is necessary to set retention index of each compound in a method file. Register the retention indexes in the method file's compound table beforehand.



■ Modifying Times by AART

If the instrument environment changes (e.g., because of changes in the column information), change the set times in the method file.



12.4 Index Standards

Measurement of index standards is required to perform AART.

n-alkanes are among the easiest-to-use compounds. Prepare a mixed solution of n-alkanes with the appropriate range of carbon numbers depending on the measurement parameters (especially the oven heating parameter) of the target compound.

Restek Corporation

n-Alkane

Cat.No.560295, Custom Retention Time Index Standard (Hexane solutions), 100ug/mL, 1mL, C7-C33 (n-alkane), Concentration C15, C30-C33 in 200ug/mL, Others in 100ug/mL

12

12.5 Set up a Method File Applicable to AART

To perform AART, it is necessary to set retention index of each compound in a method file. Register the retention indexes in the method file's compound table beforehand.

Files used here are the method file (AART_30m.gcm) and data file (AART_30m.gcd) for the target compounds, and the method file (alkane_30m.gcm) and data file (alkane_30m.gcd) for the index standards. This section describes an example using a 30 m column.

12.5.1 Measure Target Compounds

Prepare standard sample of target compounds and perform measurement with GC.

(Example: Method file AART_30m.gcm, Data file AART_30m.gcd)

NOTE

- It is recommended that "Linear Velocity" is used as the GC control mode to perform AART.
- The actual column length must be entered in order to more accurately estimate the retention time. In particular, enter the value obtained for column length if the offset between the adjusted results and the actual retention time is significant, and if using a column that has been cut in the past. The column length can be calculated by subtracting the cut length from 30 m, or by counting the number of column coils and multiplying 3.14 x (column coil diameter) x (number of column coils).

Reference

Refer to "3.4.1 Execute Single Run" P.52 for details on single run.

12.5.2 Create a Compound Table for Target Compounds

Create a Compound Table for target compounds using chromatograms (AART_30m.gcd) measured in "12.5.1 Measure Target Compounds". Retention Indexes are set in "12.5.7 Set Retention Indexes for Target Compounds".

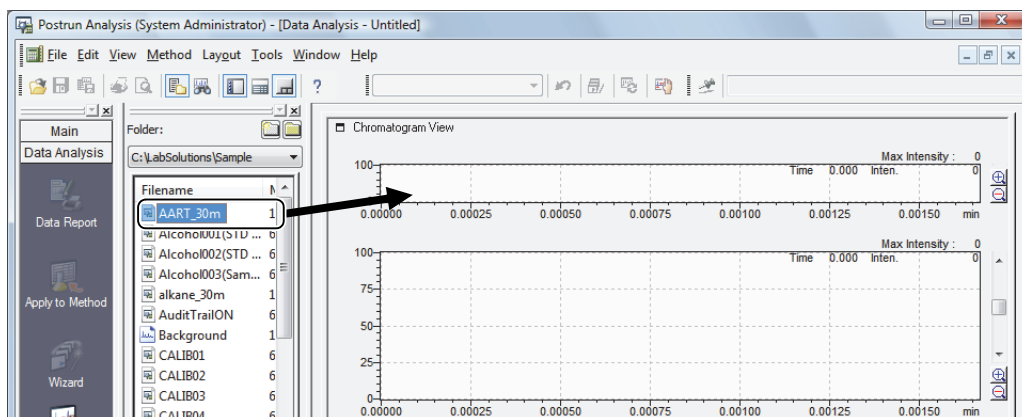
Reference

Refer to "6.5 Compound Table" P.160 for details on creating the compound table.

12.5.3 Identify Target Compounds

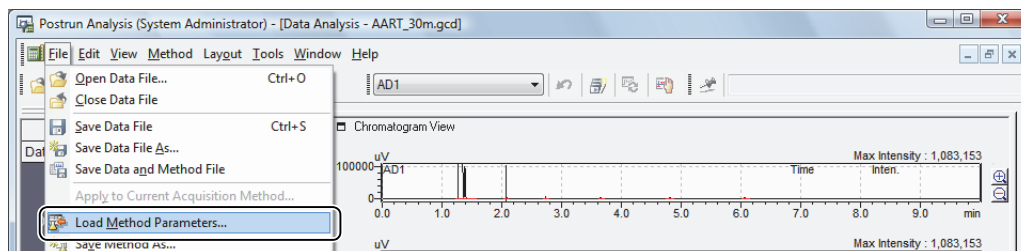
Load the data file (AART_30m.gcd) in the [Data Analysis] window, perform data processing with the method file (AART_30m.gcm), and verify that the peak has been correctly identified.

- 1 Drag-and-drop the the data file (AART_30m.gcd) in measured "12.5.1 Measure Target Compounds" onto the [Data Analysis] window from the [Data Explorer] sub-window.

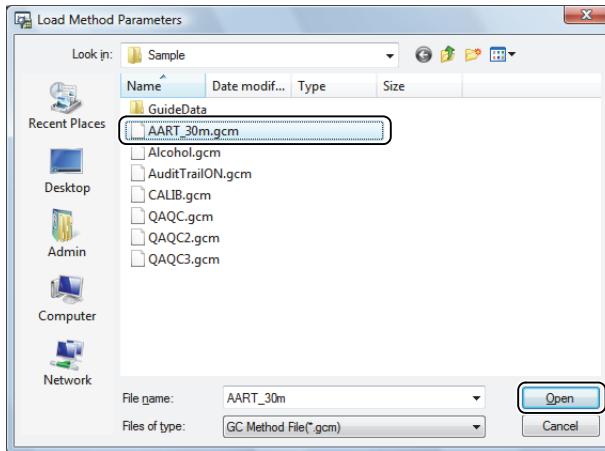


The data file (AART_30m.gcd) for the target compounds is opened.

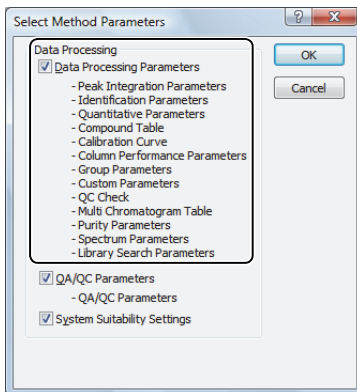
- 2 Click [Load Method Parameters] on the [File] menu.



- 3** Select the method file (AART_30m.gcm) saved in "12.5.2 Create a Compound Table for Target Compounds", and click [Open].



- 4** Select [Data Processing Parameters], click [OK].



The compound table saved in "12.5.2 Create a Compound Table for Target Compounds" is loaded.

5 Check whether or not the target compounds registered in the compound table have been identified correctly.

If they have not, change the retention time on the [Compound] tab in [Method View] to identify them.


The screenshot displays the Postrun Analysis software interface. The main window is titled "Postrun Analysis (System Administrator) - [Data Analysis - AART_30m.gcd]". The interface includes a menu bar (File, Edit, View, Method, Layout, Tools, Window, Help), a toolbar, and a sidebar with various icons. The central area is divided into several panels:

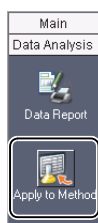
- Chromatogram View:** Shows two chromatograms. The top one is labeled "AD1" and has a peak at 3.642 min with a maximum intensity of 1,083,153. The bottom one is also labeled "AD1" and has a peak at 4.374 min with a maximum intensity of 1,083,153.
- Results View - Compound Table:** A table with columns: ID#, Name, Ret. Time, Conc. The data is as follows:

ID#	Name	Ret. Time	Conc.
1	C13	2.072	100.0
2	C14	2.732	100.0
3	C15	3.659	100.0
4	C16	4.803	100.0
5	C17	6.065	100.0
- Method View - Compound Table:** A table with columns: ID#, Name, Type, Ret. Time. The data is as follows:

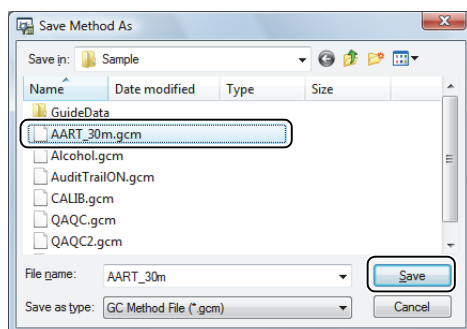
ID#	Name	Type	Ret. Time
1	C13	Target	2.083
2	C14	Target	2.747
3	C15	Target	3.678
4	C16	Target	4.824
5	C17	Target	6.086

6 If the compound table have been changed in step 5, save the method file.

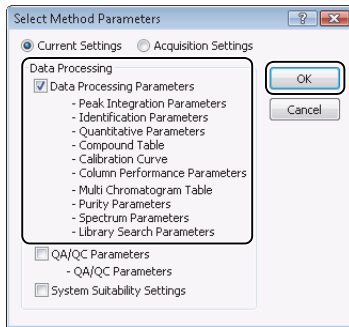
1 Click the  (Apply to Method) icon on the [Data Analysis] assistant bar.



2 Select the method file (AART_30m.gcm), and click [Save].



- 3 Select [Data Processing Parameters], and click [OK].

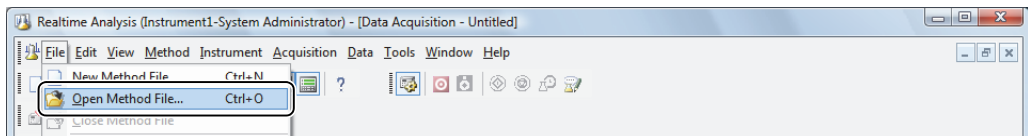


The compound table are saved to the method file (AART_30m.gcm).

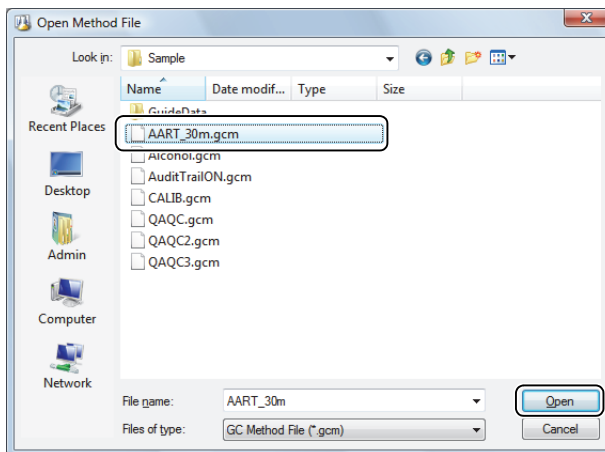
12.5.4 Create a Method File for Index Standards

Creating a method file for measuring index standards (e.g. n-alkanes), which are used to calculate retention indexes.

- 1 Select [Open Method File] on the [File] menu in the [Data Acquisition] window.

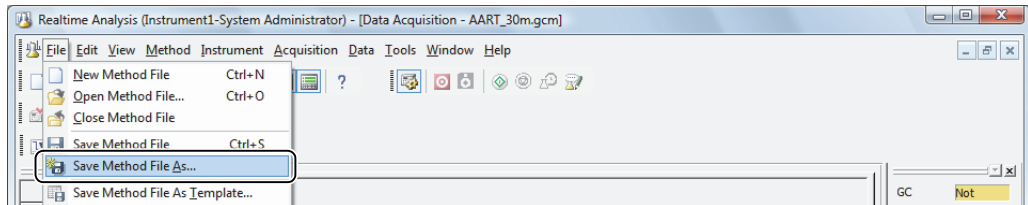


- 2 Select the method file (AART_30m.gcm) for measuring index standards, and click [Open].

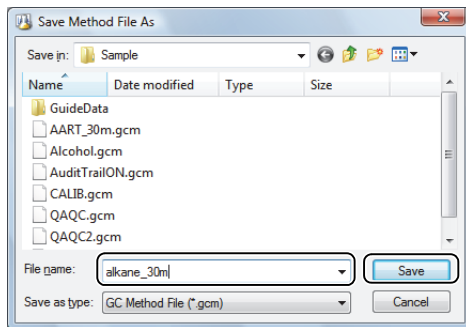


The method file (AART_30m.gcm) for measuring index standards is opened.

3 Click [Save Method File As] on the [File] menu.



4 Enter the file name, and click [Save].

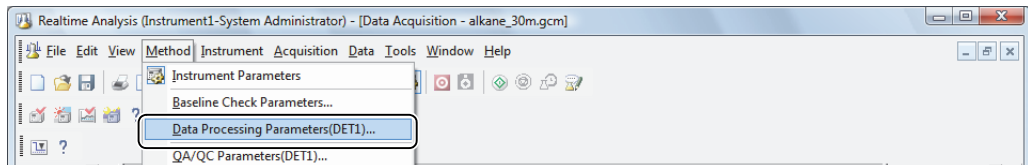


The file is saved as the method file (alkane_30m.gcm) for measuring index standards.

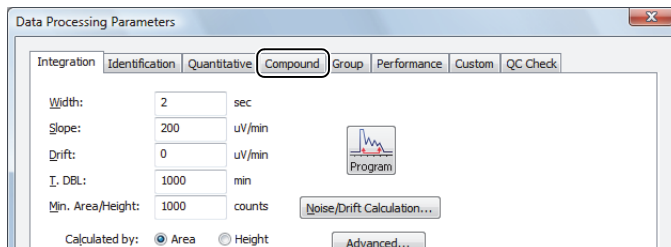
NOTE

Use the same parameters for measuring target compounds as they are to perform GC measurements.

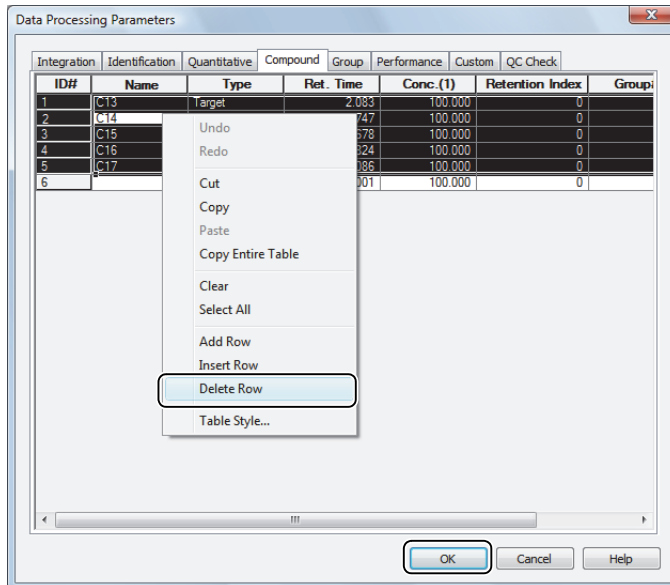
5 Click [Data Processing Parameters] on the [Method] menu.



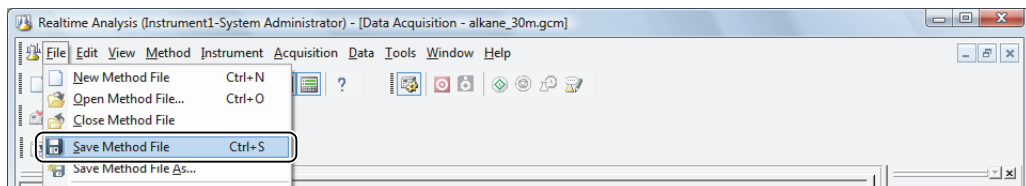
6 Click the [Compound] tab in the [Data Processing Parameters] sub-window.



7 Delete the settings of the compound table, click [OK].



8 Click [Save Method File] on the [Method] menu.



The method file (alkane_30m.gcm) for measuring index standards is saved.

12.5.5 Measure Index Standards

Prepare the index standards (e.g., n-alkane samples) used to calculate the retention indexes, and perform single run using method files (alkane_30m.gcm) that were created in ["12.5.4 Create a Method File for Index Standards"](#).

(Example: Data file alkane_30m.gcd)

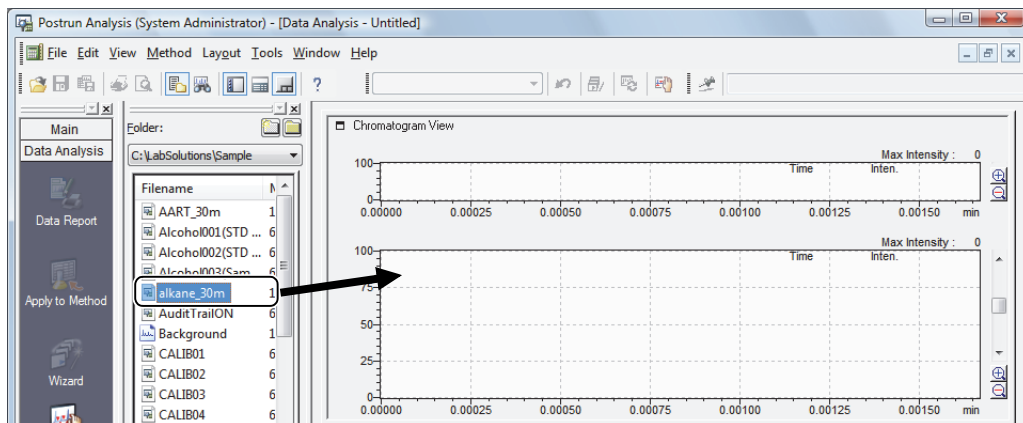
Reference

Refer to ["3.4.1 Execute Single Run" P.52](#) for details on single run.

12.5.6 Create a Compound Table for Index Standards

In the [Data Analysis] window, create a compound table for index standards and save it in a method file (alkane_30m.gcm).

- 1 Drag-and-drop the data file (alkane_30m.gcd) measured in "*12.5.5 Measure Index Standards*" onto the [Data Analysis] window from the [Data Explorer] sub-window.



The data file (alkane_30m.gcd) for the index standards is opened.

- 2 Click  **Edit** (Edit Mode) in [Method View].

Peak#	Ret. Time	Area	Height
1	1.302	3007156	10831
2	1.383	119332	1023
3	2.072	8309	78
4	2.732	8492	71
5	3.659	8462	63
6	4.803	9087	61
7	6.065	8560	52
Total		3169397	12182

The mode changes to the edit mode.

3 Referring to "6.5 Compound Table", create the Compound Table for the index standards.

4 Click [Compound] tab, and enter the Retention Index for the index standards.

Peak#	Ret. Time	Area	Height
1	1.302	3007156	10831
2	1.383	119332	1023
3	2.072	8309	78
4	2.732	8492	71
5	3.659	8462	63
6	4.803	9087	61
7	6.065	8560	52
Total		3169397	12182

ID#	Ret. Time	Retention Index	Conc.(1)
1	2.083	1300	100.
2	2.747	1400	100.
3	3.678	1500	100.
4	4.824	1600	100.
5	6.086	1700	100.
6	0.001	0	100.

Reference

Refer to "12.2.2 Display the [Retention Index] column in the Compound Table" P.311 if [Retention Index] column is not displayed in the compound table.

NOTE

The retention index of n-alkane is defined as follows.

Retention Index = carbon number x 100

Example:


Retention Index of Hexa (C16H34) = 16 x 100 = 1600

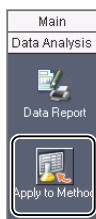
5 Click  (View Mode) in [Method View].

Peak#	Ret. Time	Area	Height
1	1.302	3007156	10831
2	1.383	119332	1023
3	2.072	8309	78
4	2.732	8492	71
5	3.659	8462	63
6	4.803	9087	61
7	6.065	8560	52
Total		3169397	12182

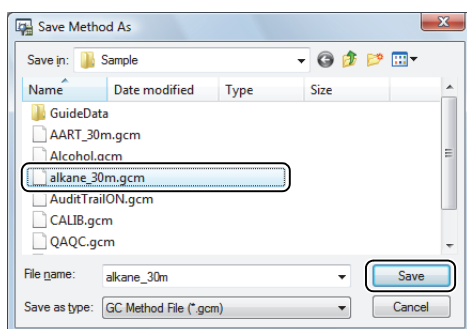
ID#	Ret. Time	Retention Index	Conc.(1)
1	2.083	1300	100.
2	2.747	1400	100.
3	3.678	1500	100.
4	4.824	1600	100.
5	6.086	1700	100.
6	0.001	0	100.

Postrun analysis is performed on the data.

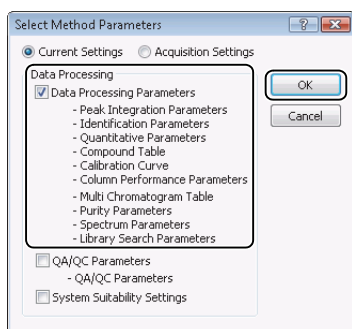
6 Click the  (Apply to Method) icon on the [Data Analysis] assistant bar.



- 7** Select the method file (alkane_30m.gcm) created in *"12.5.6 Create a Compound Table for Index Standards"*, and click [Save].



- 8** Select [Data Processing Parameters], and click [OK].



The compound table are saved to the method file (alkane_30m.gcm).

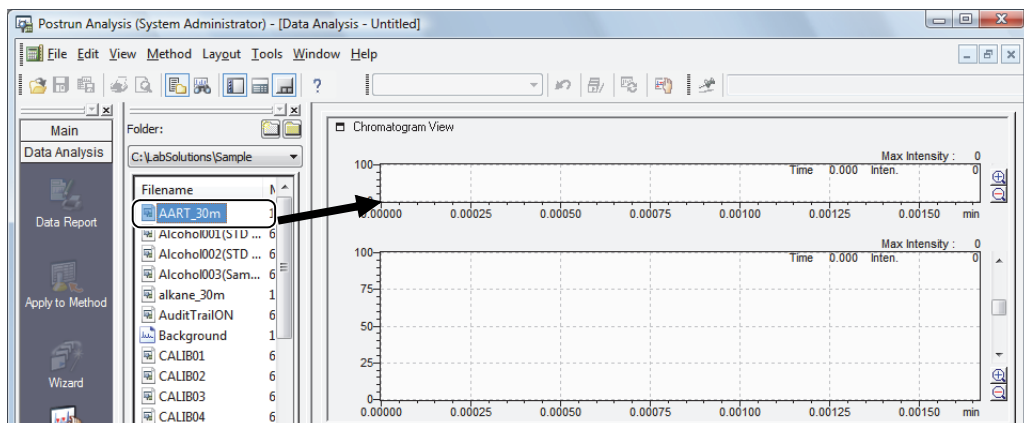
12.5.7 Set Retention Indexes for Target Compounds

The retention indexes in the compound table can be entered automatically using the data file for index standards.

This section describes two methods: how to set the retention index for an already created Compound Table and how to set the retention index during the creation of a Compound Table.

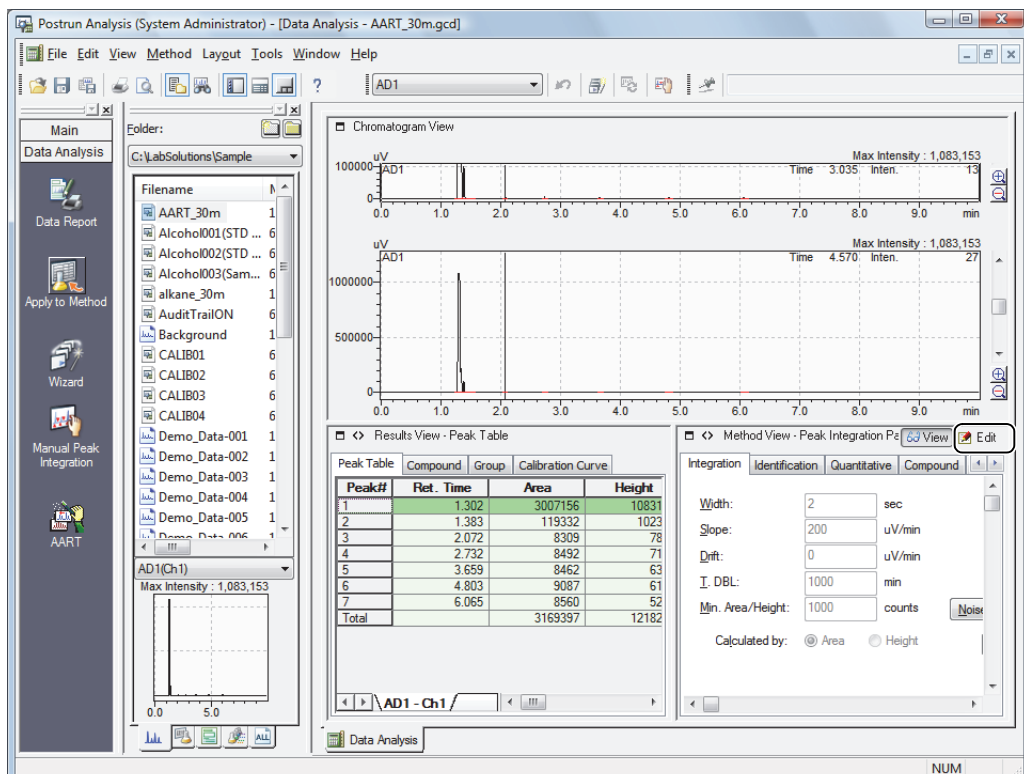
■ Set Retention Indexes for a Pre-existing Compound Table as One Batch

- 1 Drag-and-drop the data file (AART_30m.gcd) saved in "[12.5.3 Identify Target Compounds](#)" onto the [Data Analysis] window from the [Data Explorer] sub-window.





The data file (AART_30m.gcd) for the target compounds is opened.

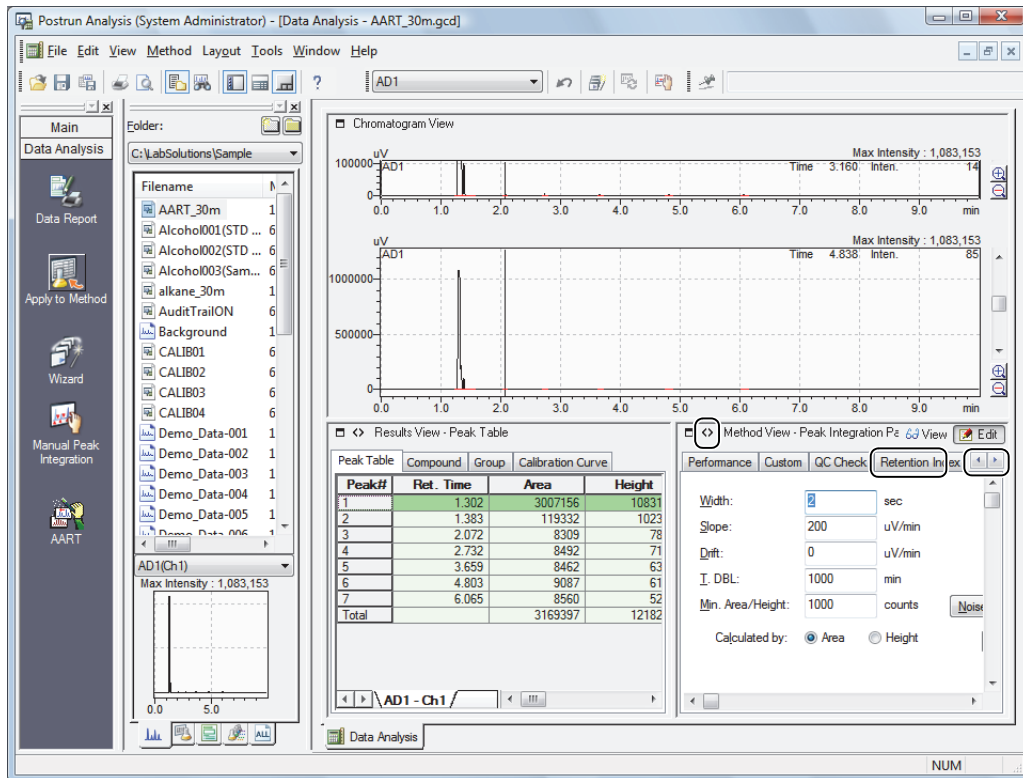
- 2 Click  **Edit** (Edit Mode) in [Method View].



The mode changes to the edit mode.

3 Click the [Retention Index] tab in [Method View].

Use  , if [Retention Index] tab is not displayed.

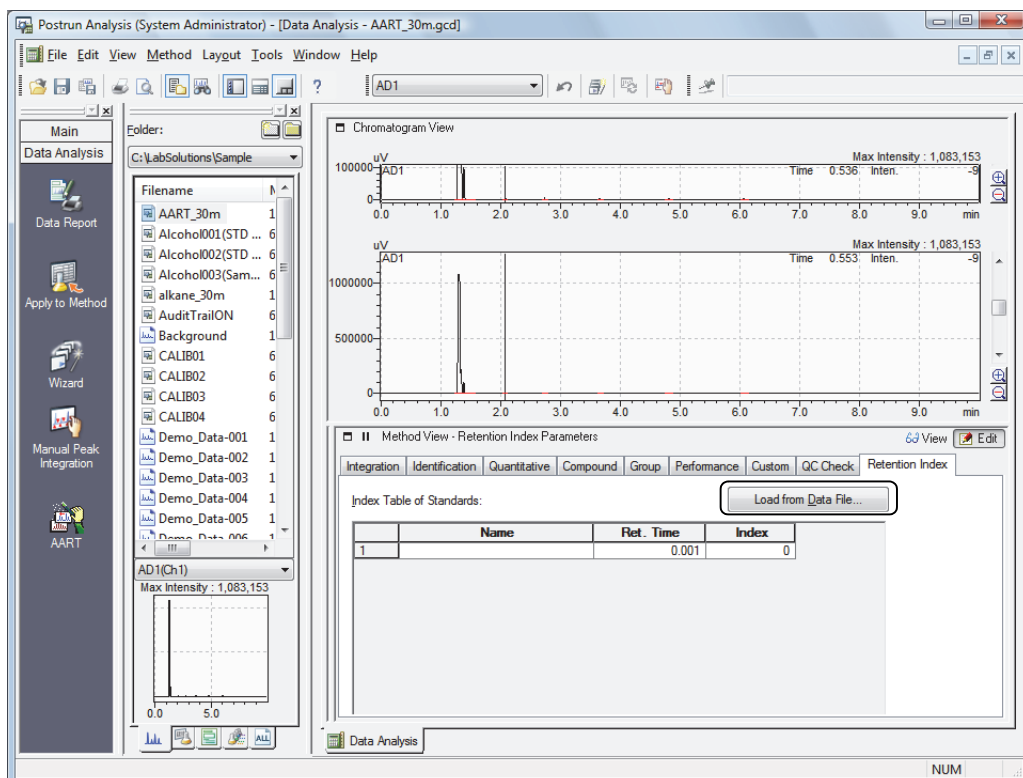


The screenshot shows the Postrun Analysis software interface. The main window displays a chromatogram view with two plots. The top plot shows a peak at 1.302 minutes with a maximum intensity of 1,083,153. The bottom plot shows a peak at 4.838 minutes with a maximum intensity of 1,083,153. The Peak Table is displayed below the chromatograms, showing the following data:

Peak#	Ret. Time	Area	Height
1	1.302	3007156	10831
2	1.383	119332	1023
3	2.072	8309	78
4	2.732	8492	71
5	3.659	8462	63
6	4.803	9087	61
7	6.065	8560	52
Total		3169397	12182

The Method View - Peak Integration Parameters dialog box is open, showing the Retention Index tab. The dialog box includes fields for Width (2 sec), Slope (200 uV/min), Drift (0 uV/min), I. DBL (1000 min), and Min. Area/Height (1000 counts). The Calculated by option is set to Area.

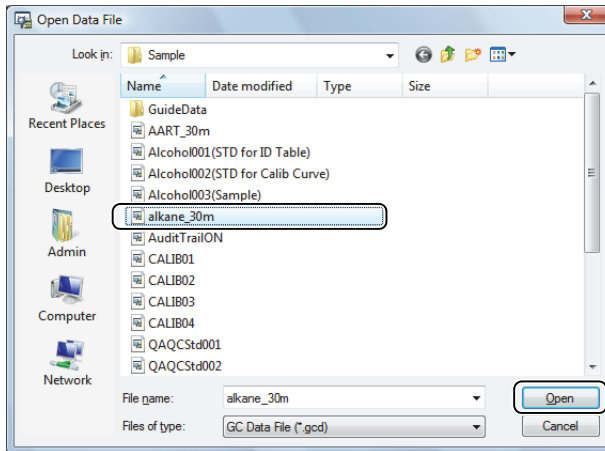
4 Click [Load from Data File].



The screenshot shows the Postrun Analysis software interface. The main window displays a chromatogram view with two plots. The top plot shows a peak at 0.536 minutes with a maximum intensity of 1,083,153. The bottom plot shows a peak at 0.553 minutes with a maximum intensity of 1,083,153. The Method View - Retention Index Parameters dialog box is open, showing the Retention Index tab. The dialog box includes a table for the Index Table of Standards and a button labeled "Load from Data File...".

Name	Ret. Time	Index
1	0.001	0

5 Select the data file (alkane_30m.gcd) saved in "12.5.6 Create a Compound Table for Index Standards", and click [Open].



The compound names, retention times and indexes are set in the [Index Table of Standards] table.

NOTE

The compound names set in the compound table for the index standards' measurement data are set in the [Name] column and the identified retention times in the compound result table are set in the [Ret. Time] column. The compounds not identified in the compound result table are not displayed in the [Index Table of Standards].

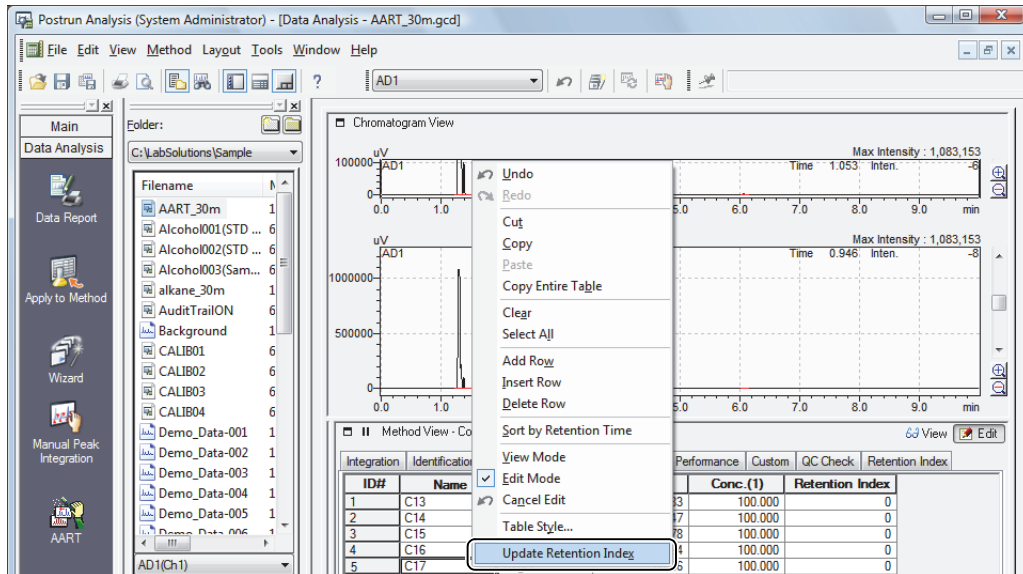
6 Edit [Index Table of Standard] as required.

All compounds needs retention indexes.

7 Click the [Compound] tab.

	Name	Ret. Time	Index
1	C13	2.072	0
2	C14	2.732	0
3	C15	3.659	0
4	C16	4.803	0
5	C17	6.065	0
6		0.001	0

8 Right-click on the compound table, and click [Update Retention Index].



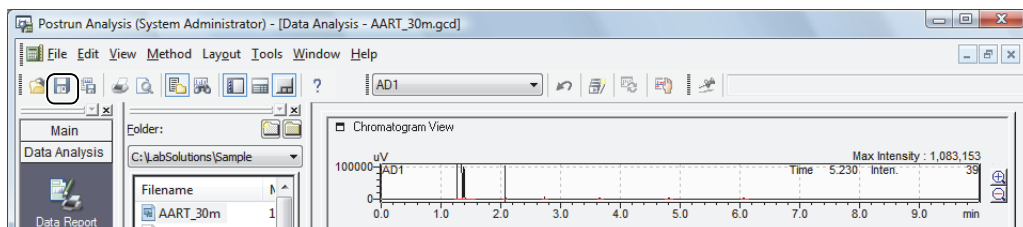
Retention indexes for each compound is calculated and displayed in the [Retention Index] column.

Reference

Refer to "12.2.2 Display the [Retention Index] column in the Compound Table" P.311 if [Retention Index] column is not displayed in the compound table.

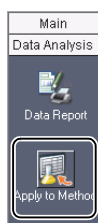
9 Click (View Mode) in [Method View].

10 Click the (Save) button on the toolbar.



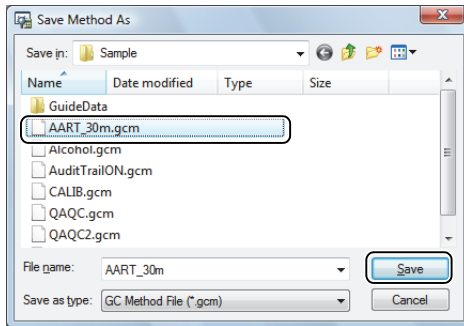
The compound table are saved to the data file (AART_30m.gcd).

11 Click the (Apply to Method) icon on the [Data Analysis] assistant bar.



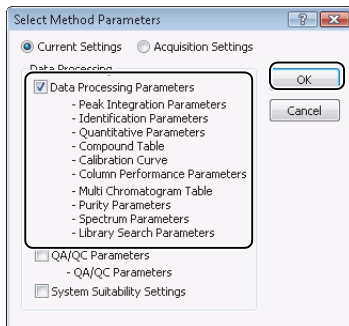
12

Select the method file (AART_30m.gcm), and click [Save].



13

Select [Data Processing Parameters], and click [OK].

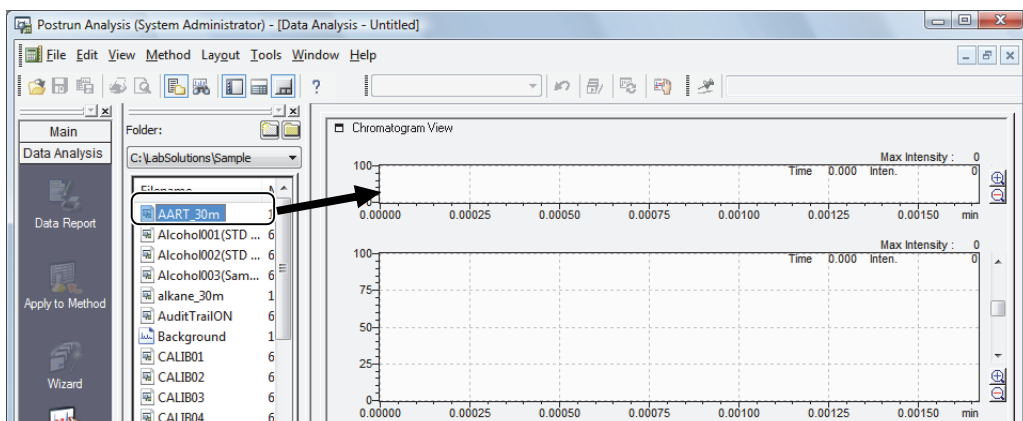


The compound table are saved to the method file (AART_30m.gcm).

■ Create a New Compound Table

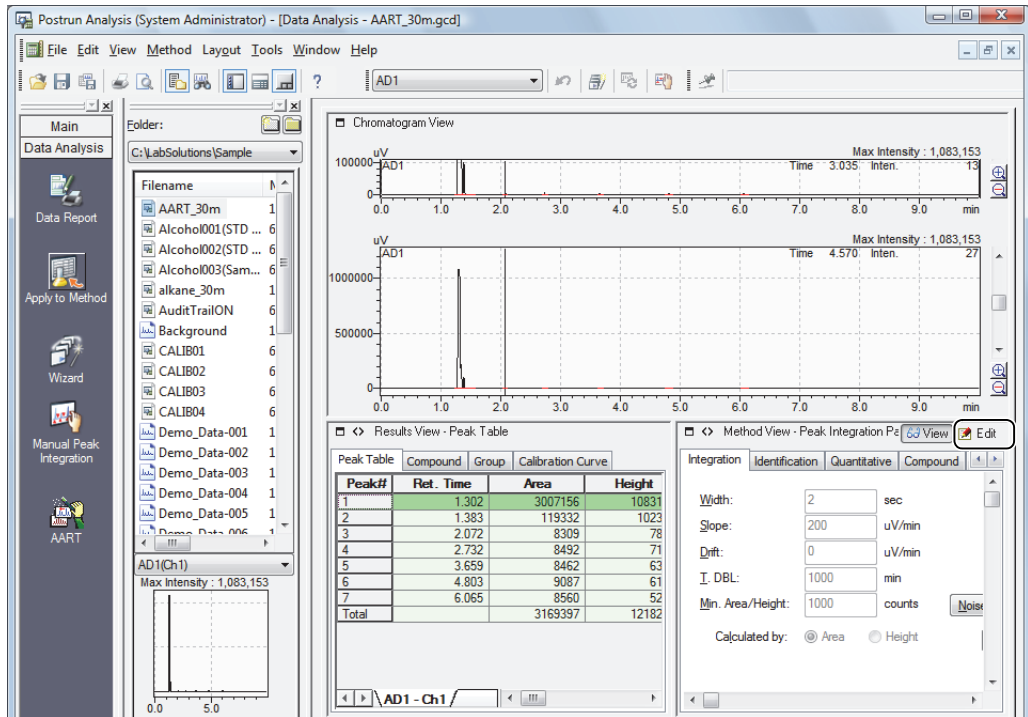
1

Drag-and-drop the data file (AART_30m.gcd) measured in *"12.5.1 Measure Target Compounds"* onto the [Data Analysis] window from the [Data Explorer] sub-window.



The data file (AART_30m.gcd) for target compounds is opened.

2 Click Edit (Edit Mode) in [Method View].





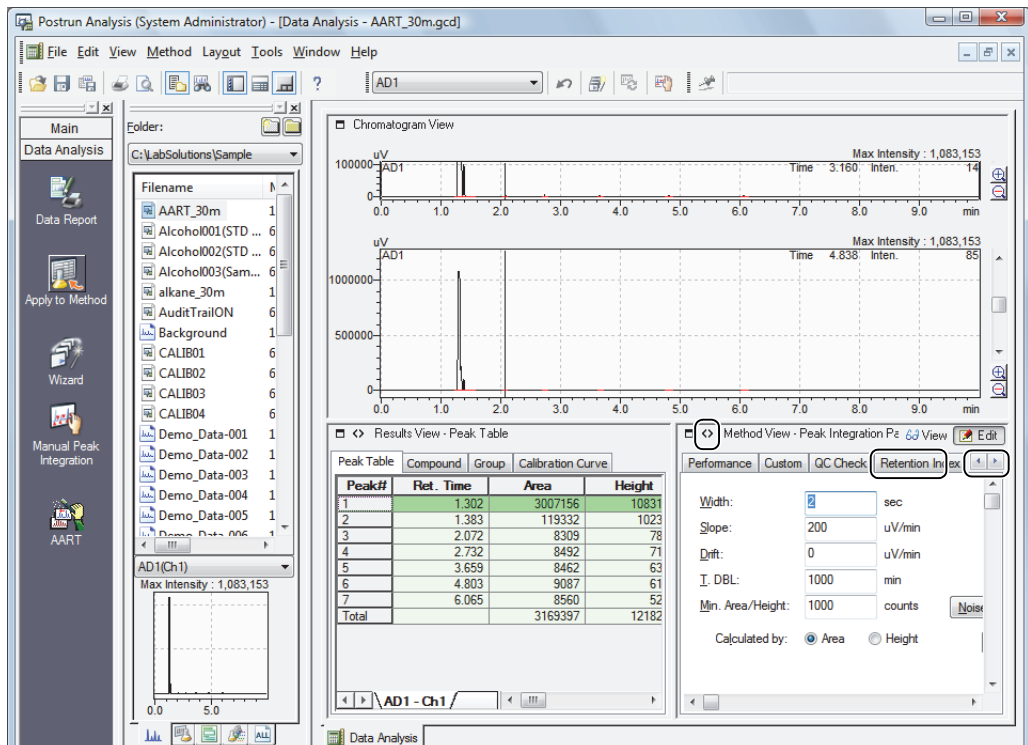
The screenshot shows the Postrun Analysis software interface. The 'Method View - Peak Integration Parameters' panel is open, and the 'Edit' button is highlighted. The peak table below shows the following data:

Peak#	Ret. Time	Area	Height
1	1.302	3007156	10831
2	1.383	119332	1023
3	2.072	8309	78
4	2.732	8492	71
5	3.659	8462	63
6	4.803	9087	61
7	6.065	8560	52
Total		3169397	12182

The mode changes to the edit mode.

3 Click the [Retention Index] tab in [Method View].

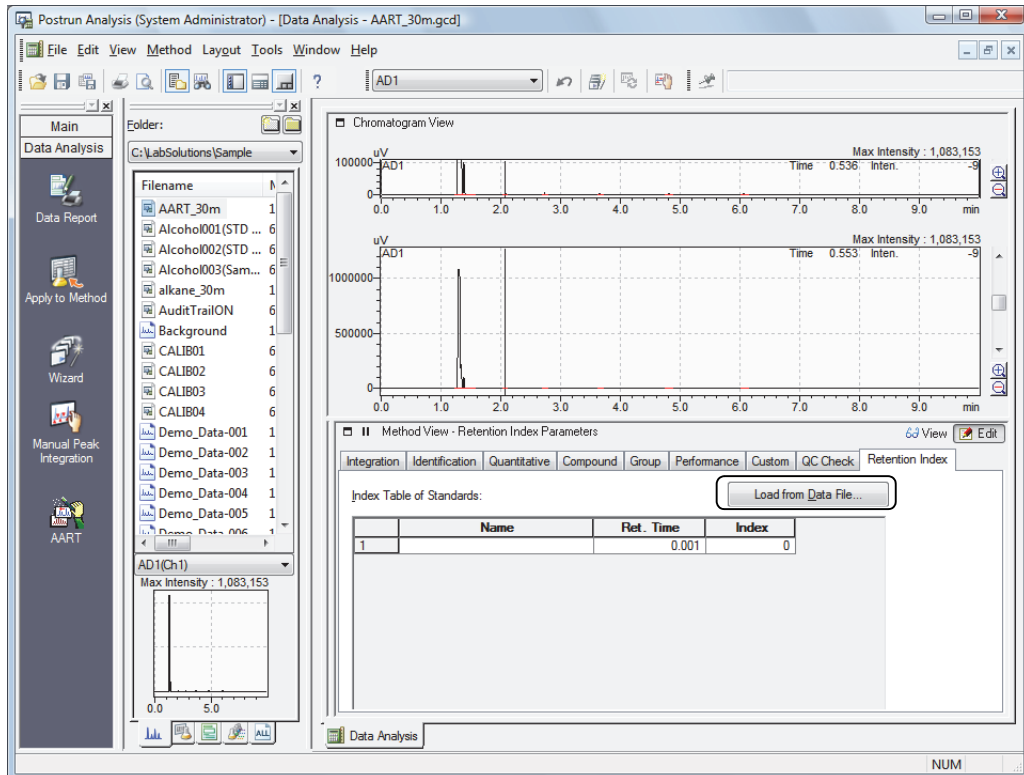
Use  , if [Retention Index] tab is not displayed.



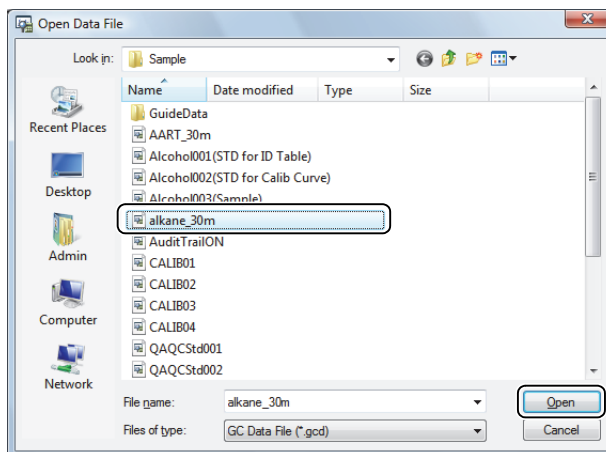
The screenshot shows the Postrun Analysis software interface. The 'Method View - Peak Integration Parameters' panel is open, and the 'Retention Index' tab is selected. The peak table below shows the following data:

Peak#	Ret. Time	Area	Height
1	1.302	3007156	10831
2	1.383	119332	1023
3	2.072	8309	78
4	2.732	8492	71
5	3.659	8462	63
6	4.803	9087	61
7	6.065	8560	52
Total		3169397	12182

4 Click [Load from Data File].



5 Select the data file (alkane_30m.gcd) saved in "12.5.6 Create a Compound Table for Index Standards", and click [Open].



The compound names, retention times and indexes are set in the [Index Table of Standards] table.

NOTE

The compound names set in the compound table for the index standards' measurement data are set in the [Name] column and the identified retention times in the compound result table are set in the [Ret. Time] column. The compounds not identified in the compound result table are not displayed in the [Index Table of Standards].

6 Edit [Index Table of Standard] as required.

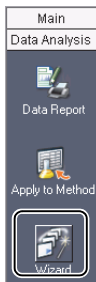
All compounds needs retention indexes.

7 Click the [Compound] tab.

The screenshot shows the Postrun Analysis software interface. The main window displays a chromatogram view with two plots. The top plot shows a peak at 5.230 minutes with a maximum intensity of 1,083,153. The bottom plot shows a peak at 4.623 minutes with a maximum intensity of 1,083,153. The 'Method View - Retention Index Parameters' window is open, showing the 'Compound' tab. The 'Index Table of Standards' table is displayed below the tabs.

	Name	Ret. Time	Index
1	C13	2.072	0
2	C14	2.732	0
3	C15	3.659	0
4	C16	4.803	0
5	C17	6.065	0
6		0.001	0

8 Click the (Wizard) icon on the [Data Analysis] assistant bar.



9 Referring to "6.5.1 Compound Table Wizard", create the Compound Table for the target compounds.

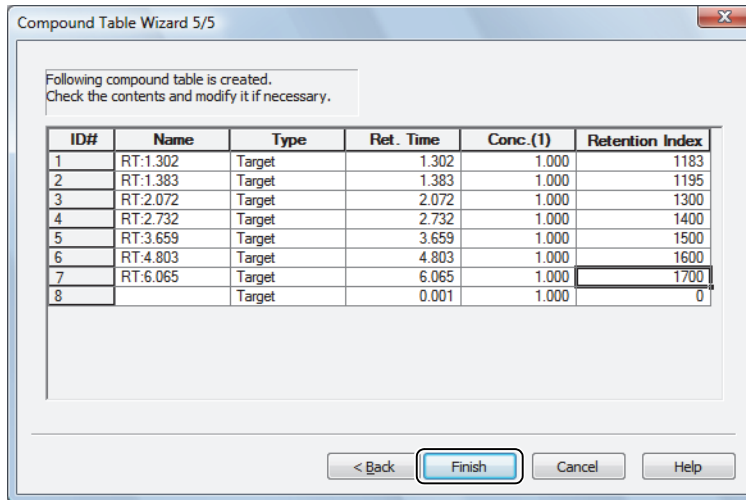
[Retention Index] displayed in [Compound Table Wizard 5/5] sub-window are calculated using the retention index parameters and the retention times in the compound table.

NOTE

Refer to [Data Acquisition & Processing Theory Guide] regarding the method for calculating the retention indexes from the retention index parameters and retention times.

10

Proceed to [Compound Table Wizard 5/5] sub-window and click [Finish].

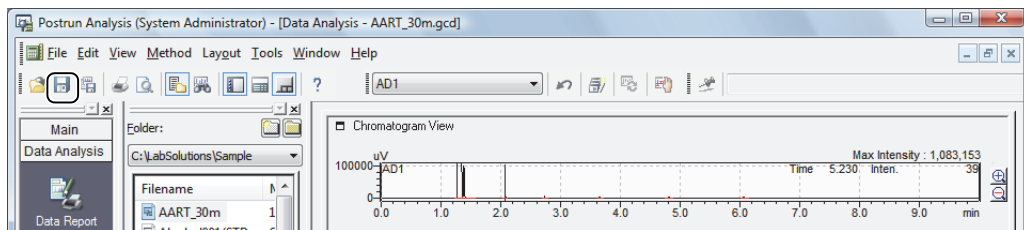


The compound table is created.


11

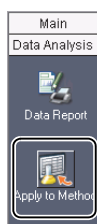
Click the  (Save) button on the toolbar.

The compound table are saved to the data file (AART_30m.gcd).



12

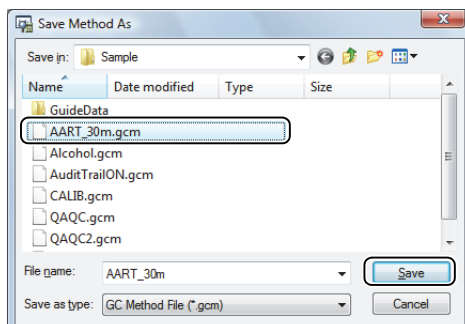
Click the  (Apply to Method) icon on the [Data Analysis] assistant bar.



12

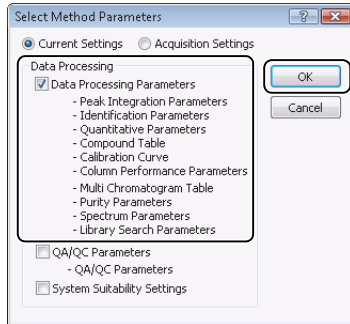
13

Select the method file (AART_30m.gcm), and click [Save].



14

Select [Data Processing Parameters], and click [OK].



The compound table are saved to the method file (AART_30m.gcm).

12.6 Modify Times by AART

If the instrument environment changes (e.g., because of changes in the column information), the change of the elution time makes it difficult to identify compounds. The AART corrects the retention times in a compound table for the target compound's method file, which uses the retention times for index standards.

12.6.1 Measure Index Standards

Prepare the index standards used to calculate the retention indexes, and perform single run using method files (alkane_30m.gcm) that were created in "[12.5.4 Create a Method File for Index Standards](#)".

(Example: Data file alkane_24m.gcd)

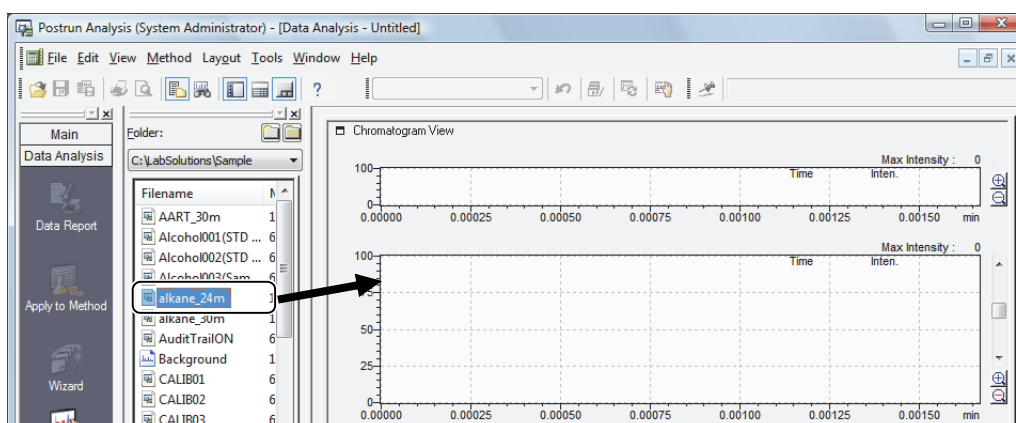
Reference

Refer to "[3.4.1 Execute Single Run](#)" P.52 for details on single run.

12.6.2 Identify Index Standards

In the [Data Analysis] window, perform identification processing for the index standards using the compound table. Identified information is used for AART in "12.6.3 Modify Set Times in a Method File by AART".

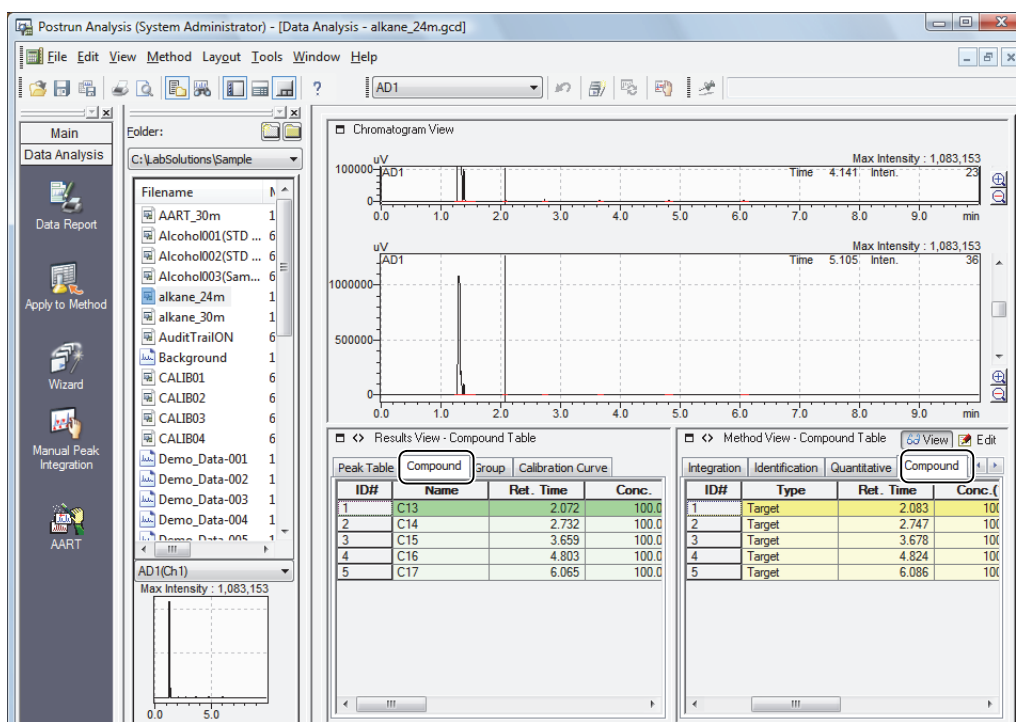
- 1 Drag-and-drop the data file (alkane_24m.gcd) measured in "12.5.5 Measure Index Standards" onto the [Data Analysis] window from the [Data Explorer] sub-window.



The data file (alkane_24m.gcd) for the index standards is opened.

- 2 Check whether or not the index standards registered in the Compound Table have been identified correctly.

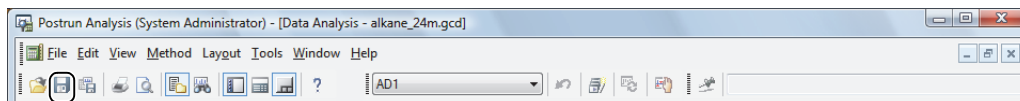
If they have not, change the retention time on the [Compound] tab in [Method View] to identify them.



NOTE

Due to differences in the column length, the retention time for index standards deviates from the settings in the Compound Table. Perform identification with care not to confuse the index standards for compounds with different carbon numbers.

- 3** Click the  (Save) button on the toolbar.



The data file (alkane_24m.gcd) is saved.

This data file is used as reference information when modifying the retention times as described in ["12.6.3 Modify Set Times in a Method File by AART"](#).

12.6.3 Modify Set Times in a Method File by AART

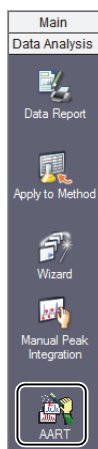
After conducting the steps in ["12.6.2 Identify Index Standards"](#), conduct the operations below after loading the index standards measurement data into the [Data Analysis] window.

- 1** With the data file for the index standards open, click the [AART] icon on the [Data Analysis] assistant bar.

Click [Automatic Adjustment of Retention Time [AART]] on the [Edit] menu if the [AART] icon is not displayed on the assistant bar.

Reference

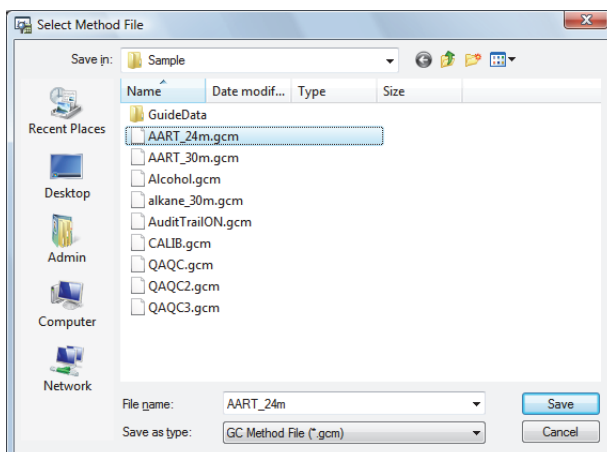
Refer to ["12.2.1 Add the \[AART\] icon on the \[Data Analysis\] assistant bar"](#) if the [AART] icon is not displayed on the assistant bar.



2 Select the method file to correct the preset time for, and click [Save].

NOTE

Times modified by AART are directly set in the method file selected here. To retain the original method file, copy the method file using Windows Explorer or by some other method. In this example, AART_30m.gcm is copied to create AART_24m.gcm.

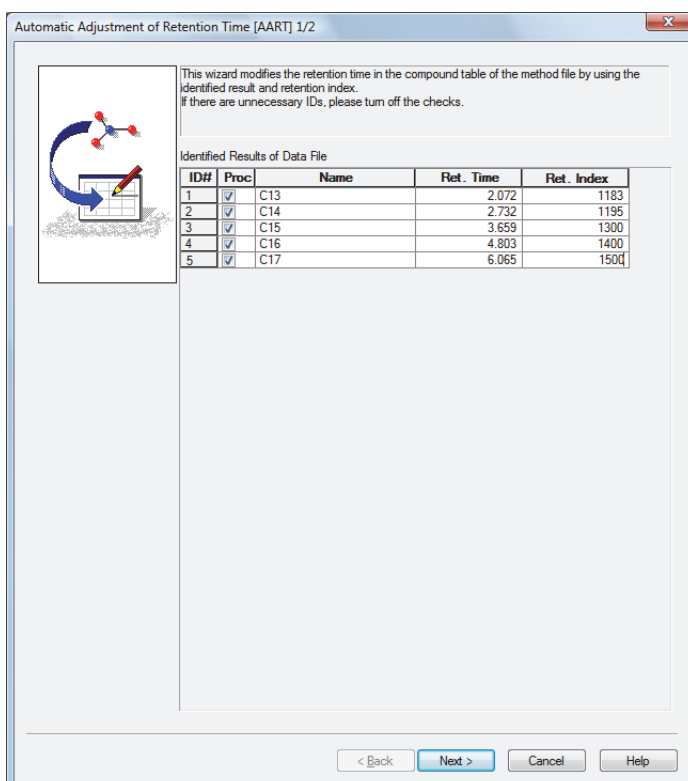


3 Check the settings, and click [Next].

NOTE

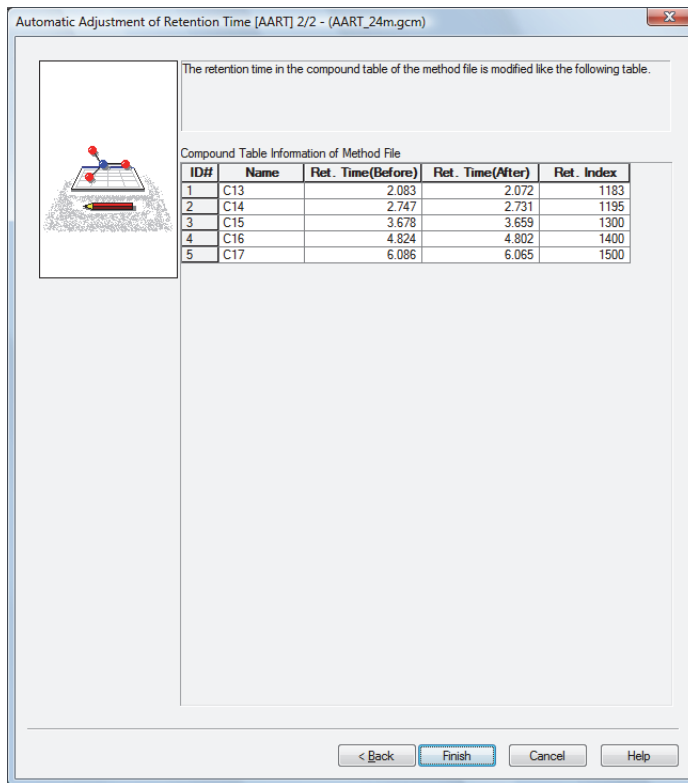
If there are compounds whose retention indexes are 0 or that are not required to perform AART for the method file, click to clear the [Proc.] columns for these compounds. Click [Next].

Identification results of index standards are displayed on the [Automatic Adjustment of Retention Time [AART] 1/2] sub-window.



The retention times modified using the retention indexes of compound table in the method file selected in step 2 and the identification results for the index standard data are displayed in the [Automatic Adjustment of Retention Time [AART] 2/2] sub-window.

4 Check the settings, and click [Finish].



Reference

Refer to [Data Acquisition & Processing Theory Guide] for details on the retention time calculation method.

This completes the procedure for modifying the set times in the method file's compound table.

NOTE

- Linear retention indices available for a ramped temperature measurement are used in the Automatic Adjustment of Retention Time (AART). The accuracy of the adjusted time may be lower under the measurement with a fixed temperature step or multi-ramped steps than a single ramped one.
- The modified retention times obtained here are only reference values. Before using them in actual measurement or analysis, confirm the set times with reference to ["12.7 Confirm and Adjust Setting Times"](#).

12.7 Confirm and Adjust Setting Times

The set times in the compound table modified by AART are only reference values. Before using them in actual measurement or analysis, confirm and adjust the set times with reference to a data file for target compounds.

12.7.1 Measure Target Compounds

Measure target compounds to confirm the set times modified by AART. The data file obtained here is used for confirmation and adjustment in "12.7.2 Confirm and Adjust Retention Times in the Compound Table".

(Example: Method file AART_24m.gcm, Data file AART_24m.gcd)

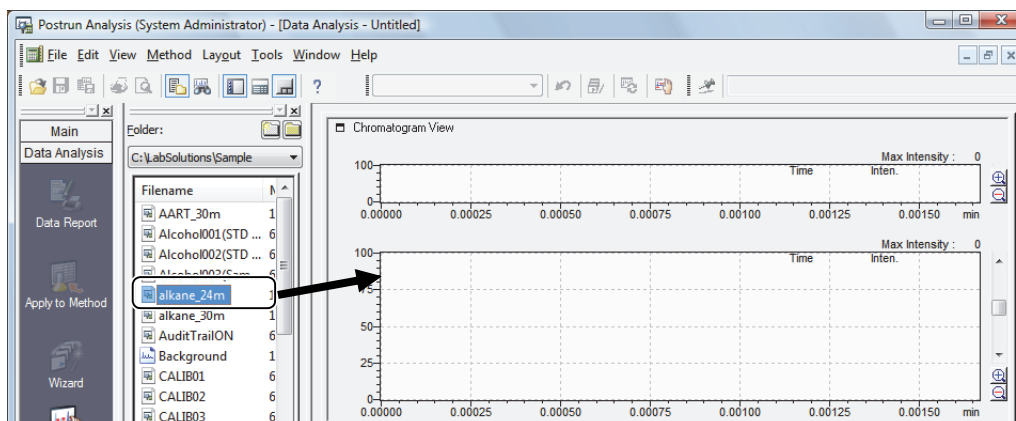
Reference

Refer to "3.4.1 Execute Single Run" P.52 for details on single run.

12.7.2 Confirm and Adjust Retention Times in the Compound Table

Perform identification processing for the target compounds using the compound table. The identified times are reflected in the compound table of the method file for measuring target compounds.

- 1 Drag-and-drop the data file (AART_24m.gcd) measured in "12.7.1 Measure Target Compounds" onto the [Data Analysis] window from the [Data Explorer] sub-window.



The data file (AART_24m.gcd) for the target compounds is opened.

2 Check whether or not the target compounds registered in the compound table have been identified correctly.

If they have not, change the retention time on the [Compound] tab in [Method View] to identify them.

The screenshot displays the Postrun Analysis software interface. The main window is titled "Postrun Analysis (System Administrator) - [Data Analysis - alkane_24m.gcd]". The interface includes a menu bar (File, Edit, View, Method, Layout, Tools, Window, Help), a toolbar, and a sidebar with navigation options like "Data Report", "Apply to Method", "Wizard", and "Manual Peak Integration".

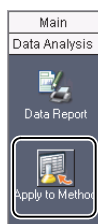
The central area shows two chromatogram views. The top view is labeled "Chromatogram View" and shows a plot of uV vs. Time (min) with a peak at 4.141 min. The bottom view is labeled "AD1" and shows a peak at 5.105 min. Both plots indicate a "Max Intensity : 1,083,153".

Below the chromatograms are two compound tables:

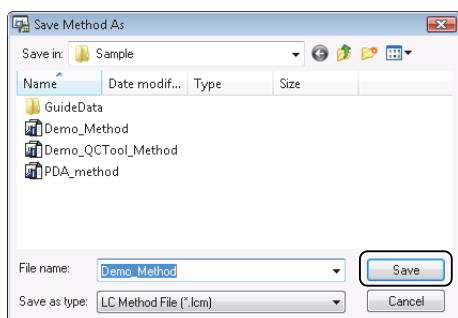
Peak Tab	Compound	Group	Calibration Curve
1	C13		
2	C14		
3	C15		
4	C16		
5	C17		

Integration	Identification	Quantitative	Compound
1	Target		
2	Target		
3	Target		
4	Target		
5	Target		

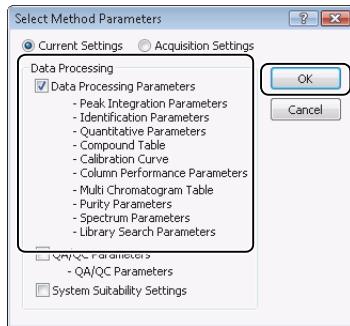
3 Click the (Apply to Method) icon on the [Data Analysis] assistant bar.



4 Select the method file (AART_24m.gcm), and click [Save].



5

 Select [Data Processing Parameters], and click [OK].

The compound table are saved to the method file (AART_24m.gcm).

13

Appendices

This chapter describes how to locate operation details on the Help menu or in the online manuals. Use this information in the event that you are having problems with software operation, and the basic operations in software screens.



13.1 Operation Problems

This software provides the Help menu and online manuals. Use the Help menu and online manuals to learn more about software operations or the terms displayed on screen.

This section describes how to use the Help menu and online manuals.

13.1.1 Help

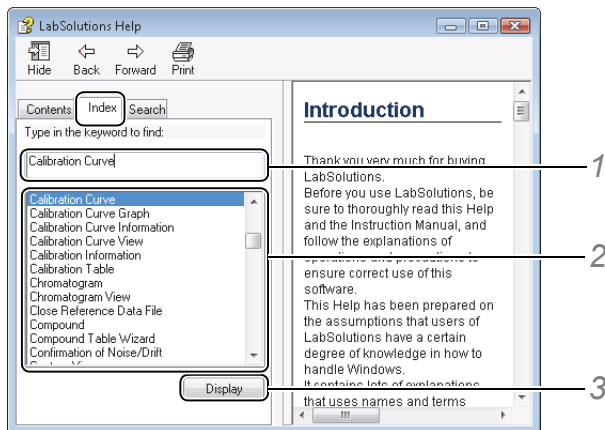
Use the following procedures to open the Help menu.

Type of Operation	Operation Procedures
[Help]	Click [Help] on the sub-window. The section Help for the current sub-window is displayed.
 (Help)	Click  (Help) on the toolbar.
[Help] menu	Click [Contents] on the [Help] menu.
[F1] key	Press the [F1] key on your keyboard. To locate the details relating to the current sub-window.

■ Keyword Search

If the term or parameter is unknown, enter a keyword to perform a search, and a list of topics that match the keyword is displayed. This allows for review of Help topics that pertain to the terms and parameters.

- 1 Open Help.
- 2 Click the [Index] tab, and execute the search.

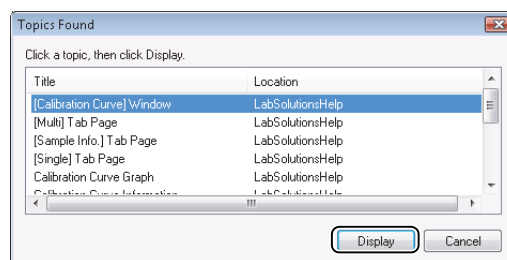


- 1 Enter the keyword to search for, and press the [Enter] key on your keyboard.
Topics matching the keyword are displayed in an alphabetical order.
- 2 Click the topic.
- 3 Click [Display].
The contents of the selected topic is displayed.



NOTE

- The [Topic Found] sub-window opens if there are multiple matching keywords. Select the desired keyword in the list in this sub-window, and click [Display].



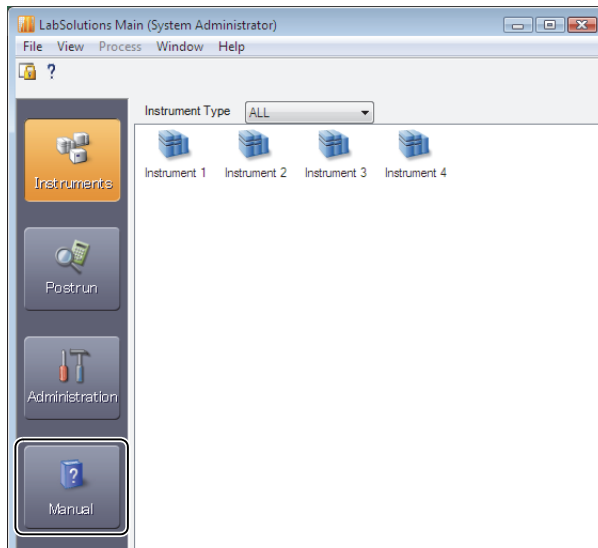
- Use the [Search] tab in the Help window to search the entire text of the Help topic for the keyword terms.

13.1.2 Online Manuals

The “Operators Guide”, “System Users Guide”, “Data Acquisition & Processing Theory Guide” and “Getting Start Guide” online manuals are installed in PDF format when this software is installed.

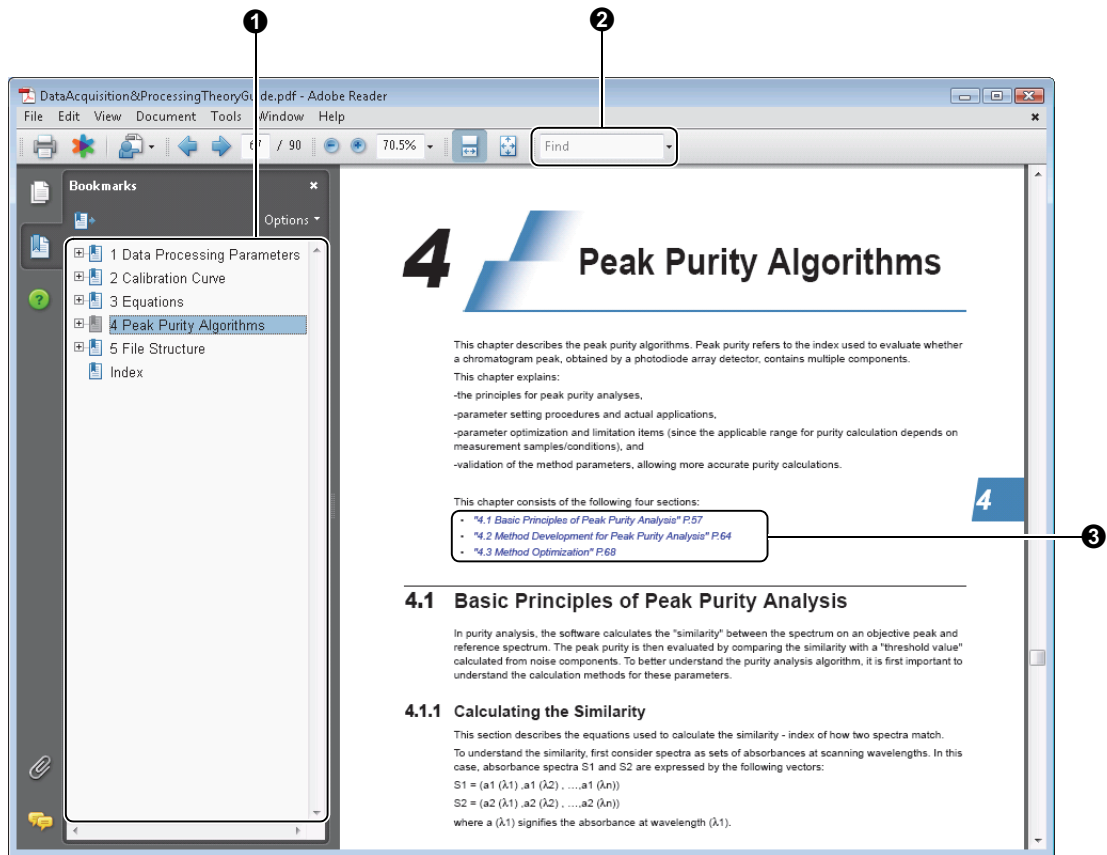
This section describes how to display online manuals.

- 1 Click the  icon in the [LabSolutions Main] window.



2 Click the icon of the desired instruction manual.

This opens Adobe Acrobat® Reader® and the instruction manual.



No.	Explanation
1	Go directly to the desired page by clicking the hierarchically structured bookmarks (table of contents).
2	Search for desired terms.
3	Go directly to a related page by clicking the references or the terms in blue.

NOTE

- The “Operators Guide” online manual can also be opened by clicking [Online Manual] on the [Help] menu in the window.
- Adobe Reader® is required to open online manuals.
- Visit Adobe's website for details on Adobe Reader®.



13.2 Common Screen Operations

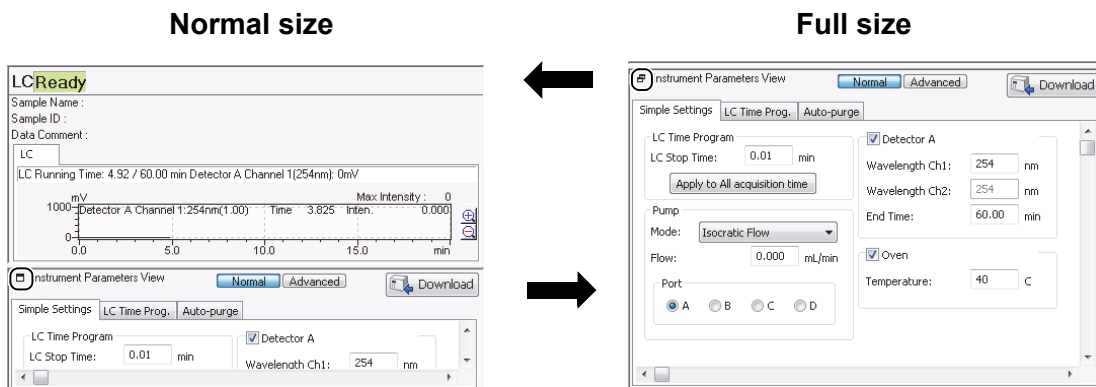
The windows, assistant bars, toolbars and other graphical user interface elements in this software can be customized.

13.2.1 Resize the View



Many of the windows such as [Data Acquisition] and [Data Analysis] are comprised of sections (views) that are separated by dividers. Drag the dividers to resize the views to make on-screen operations more efficient.

■ Resize Icons

To resize a view, click  (Full Size) in each view. This changes the normal size display to its full size. Alternatively, click  (Normal Size) to return the full size display to its normal size.

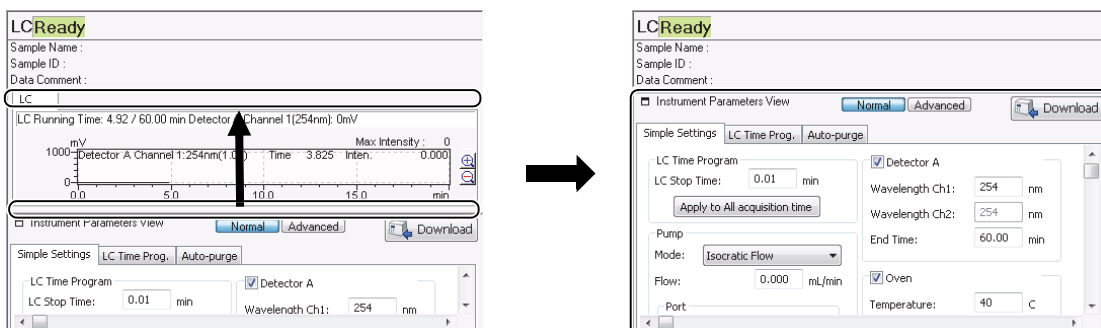


NOTE

[Results View] and [Method View] in the [Data Analysis] window contain a  (Wide Size) icon for displaying views at the full horizontal size and a  (Normal Size) icon to return the wide size view to the normal size.

■ Drag the Dividers to Resize Views

Views can be resized as desired by dragging the dividers of each view.



13.2.2 Customize Windows

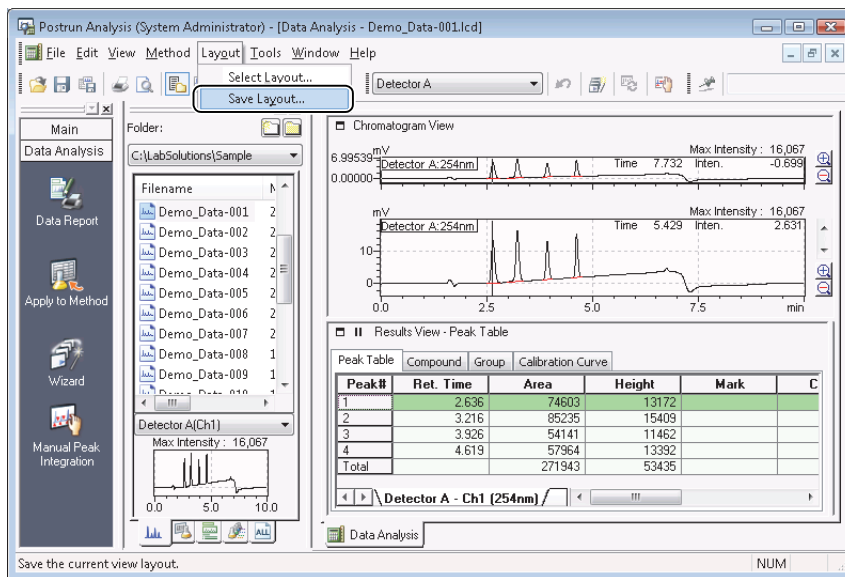
This software allows a customized view layout for a specific operation to be saved.

For example, since the [Data Analysis] and [PDA Data Analysis] windows have many views, data can be more easily analyzed by saving various layouts with unwanted views hidden.

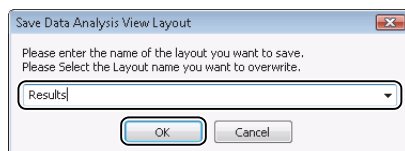
This section describes the procedure for saving the [Data Analysis] window layouts.

■ Save Layouts

1 Click [Save Layout] on the [Layout] menu.



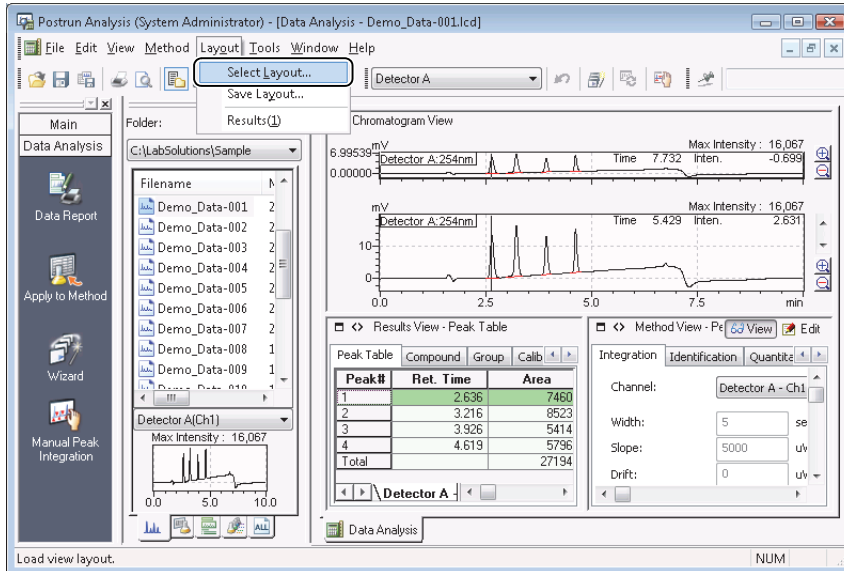
2 Enter the name of the layout, and click [OK].



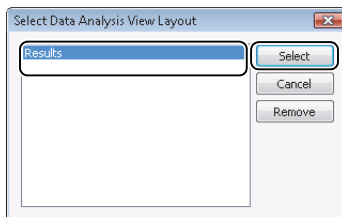
The layout of the currently open window is saved.

■ Open a Saved Layout

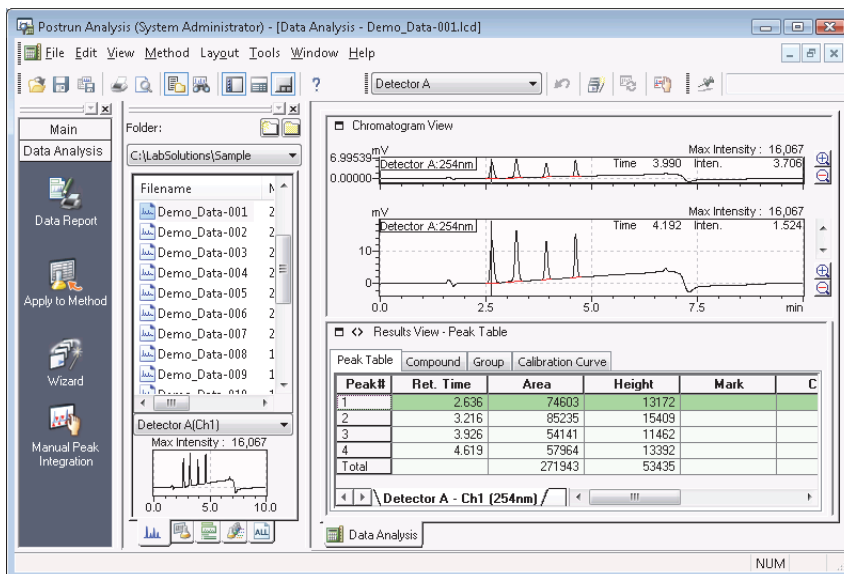
1 Click [Select Layout] on the [Layout] menu.



2 Select the name of the layout, and click [Select].



The window is opened using the selected layout.

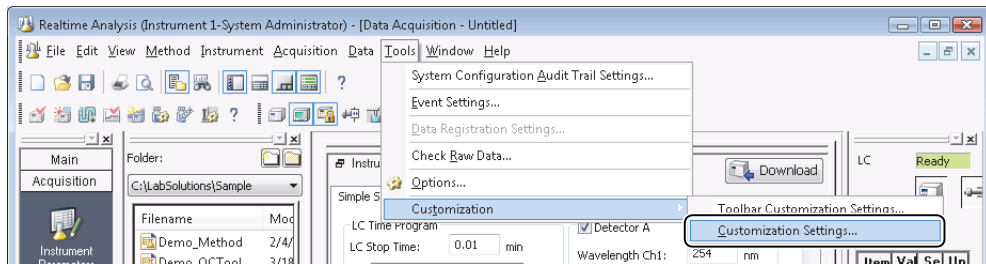


13.2.3 Customize Assistant Bars

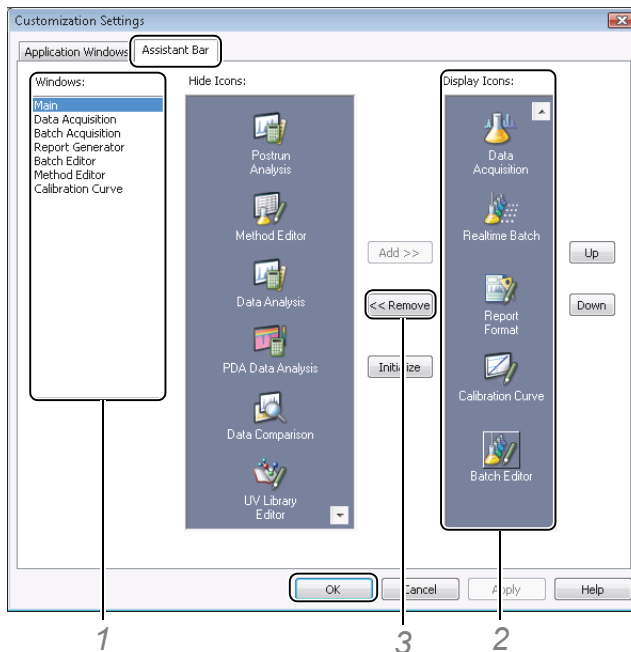
This software allows the addition or deletion of icons displayed on assistant bars to customize assistant bars for specific operations.

This section describes how to delete the [Batch Editor] icon from the [Main] assistant bar in the [Realtime Analysis] program.

- 1 Open the [Data Acquisition] window.
- 2 Select [Customization] on the [Tools] menu, and click [Customization Settings].



- 3 Click the [Assistant Bar] tab, select the icon to delete, and then click [OK].



- 1 Select [Main] at [Windows].
- 2 Select the [Batch Editor] icon at [Display Icons].
- 3 Click [Remove] to move the [Batch Editor] icon to [Hide Icons].

The [Batch Editor] icon is no longer displayed on the [Main] assistant bar in [Realtime Analysis].

NOTE

- It is only possible to customize the icons for the functions used in each window of the [Realtime Analysis], [Postrun Analysis] and [Browser] programs. Customize windows by editing [Available] on the [Application Windows] tab.

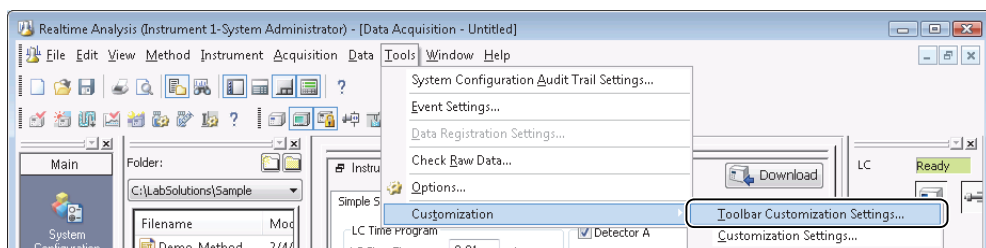
- Select the icon at [Display Icons], and click [Up] or [Down] to change the display order of icons on the assistant bar.

13.2.4 Customize Toolbars

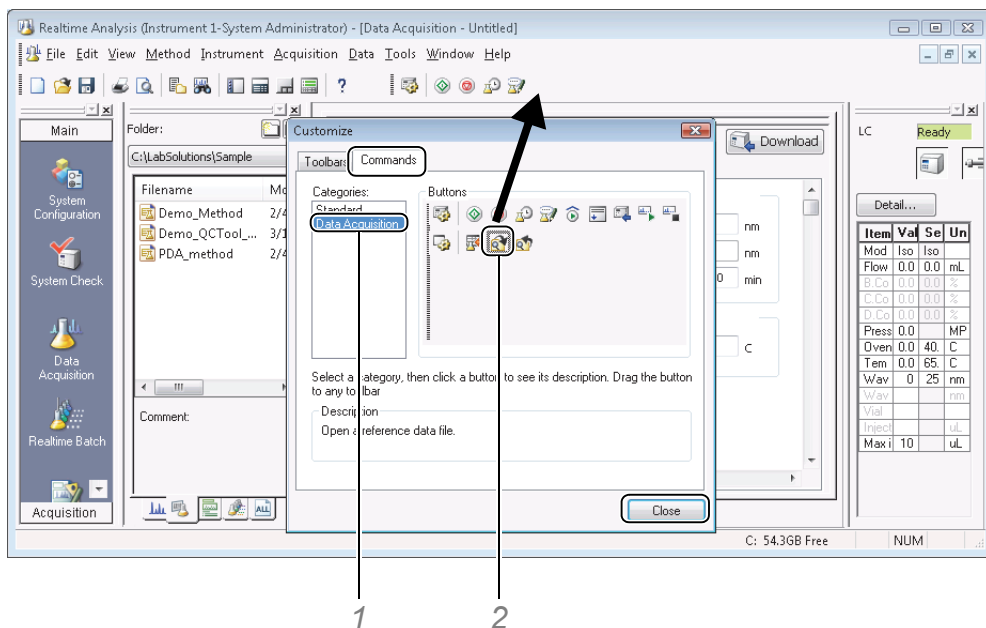
This software allows the addition or deletion of icons displayed on toolbars to customize the toolbars for specific operations.


This section describes how to add the [Open Reference Data File] icon to the [Data Acquisition] toolbar.

- 1 Open the [Data Acquisition] window.
- 2 Select [Customization] on the [Tools] menu, and click [Toolbar Customization Settings].



- 3 Click the [Command] tab, customize the [Data Acquisition] toolbar, and then click [Close].



- 1 Select [Data Acquisition] at [Categories].
- 2 Drag-and-drop  (Open Reference Data File) onto the [Data Acquisition] toolbar.

The button is added to the [Data Acquisition] toolbar.

NOTE

- Deselect the check mark of a displayed toolbar on the [Toolbar] tab to hide a toolbar.
- Drag-and-drop a button on the toolbar to an area outside of the toolbar to delete the button from the toolbar.

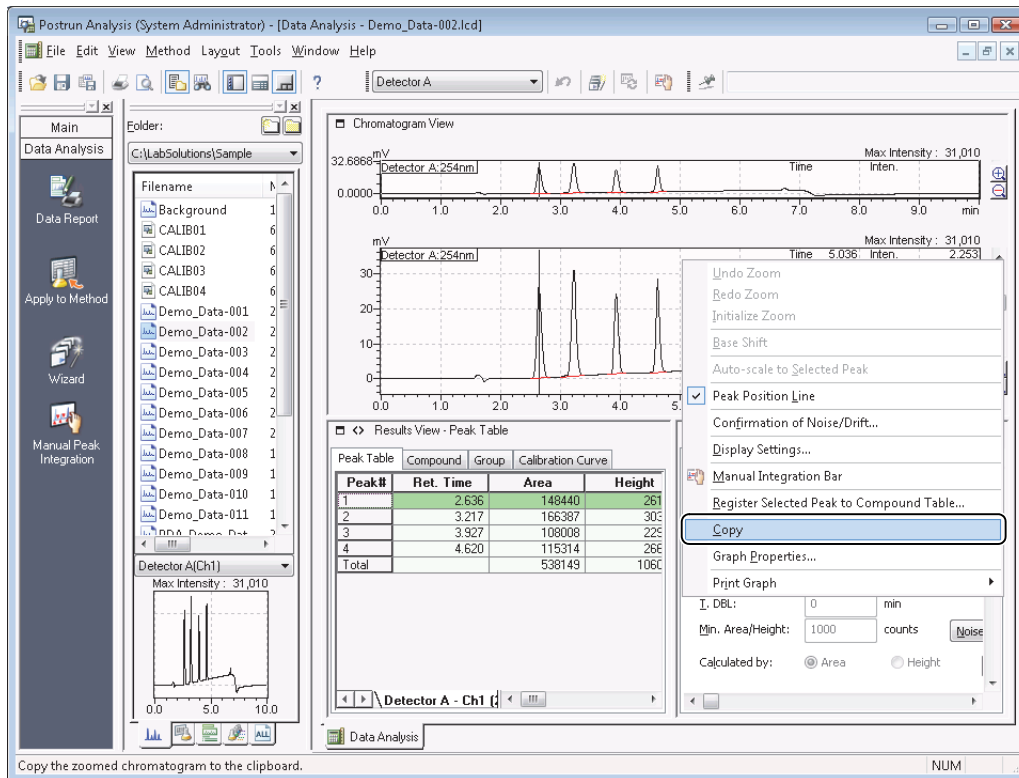
13.2.5 Copy Sub-Windows to the Clipboard

Chromatograms and Calculation Results Tables displayed in the sub-windows of this software can be copied to the Clipboard and pasted to other application software.

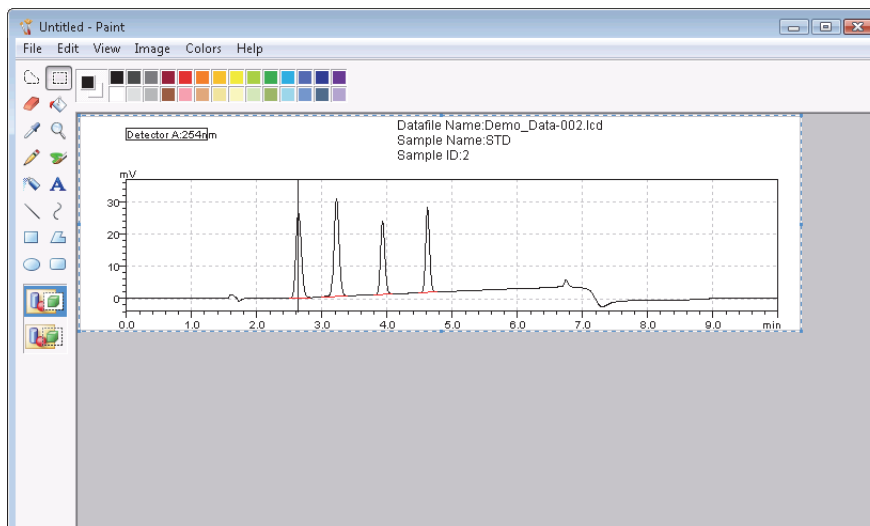
This section describes how to copy chromatograms and Calculation Results Tables displayed in the [Data Analysis] window.

■ Copy Chromatograms to the Clipboard

Right-click on the graph in [Chromatogram View], and click [Copy]. The currently displayed content of the chromatogram is copied to the Clipboard.



The chromatogram is displayed as follows when it is pasted from the Clipboard to other applications (In this example Paint is used).



■ Copy Results Tables to the Clipboard

Select and right-click on the cell or row of a Compound Table or Peak Table, and click [Copy]. The currently displayed table information is copied to the Clipboard.

Click [Copy Entire Table] to copy all of the information included in the table (displayed and hidden).

The screenshot shows the Postrun Analysis software interface. The main window displays a chromatogram view and a results view. The results view shows a peak table with the following data:

Peak#	Ret. Time	Area	Height	Mark	Conc.	Unit
1					2.000	mg/L
2					2.000	mg/L
3					2.000	mg/L
4					2.000	mg/L
Total					8.000	

A context menu is open over the peak table, showing options: Copy, Copy Entire Table, Register Selected Peak to Compound Table, Show Total, and Table Style... The 'Copy' option is selected.

At the bottom of the window, a status bar displays the text: "Copy the selection of the peak table to the clipboard." and "NUM".

13.3 Common File Operations

The contents of the files displayed in the [Data Explorer] sub-window can be displayed by double-clicking the files in the [Data Explorer] sub-window or dragging-and-dropping them onto each window.

This section describes how to open files in this software.

13.3.1 Double-Click Files in the [Data Explorer] Sub-window

This section describes the action when a file in the [Data Explorer] sub-window is double-clicked.

■ If the File Display Window Is Not Open

File Name	Program Name	Open Window
Method file	[Realtime Analysis] program	[Data Acquisition] window
	[Offline Editor] program	[Method Editor] window
	[Postrun Analysis] program	[Calibration Curve] window <ul style="list-style-type: none"> If the method file contains calibration curve information, all data files for the standard samples that make up the calibration curve are loaded in the [Data Files] tree view.
	[Browser] program	[Quant Browser] window <ul style="list-style-type: none"> If the method file contains calibration curve information, all standard sample data files that make up the calibration curve are loaded in the [Quantitative Results View].
Data file	[Realtime Analysis] program	[Data Analysis] window
	[Offline Editor] program	[PDA Data Analysis] window
	[Postrun Analysis] program	<ul style="list-style-type: none"> The [PDA Data Analysis] window opens when data acquisition was performed by a photodiode array detector.
	[Browser] program	[Quant Browser] window <ul style="list-style-type: none"> If the method file is not open in the [Quant Browser] window, the method file used to process the data files opens at the same time.
Batch file	[Realtime Analysis] program	[Realtime Batch] window
	[Offline Editor] program	[Batch Editor] window
	[Postrun Analysis] program	[Postrun Batch] window
	[Browser] program	[Quant Browser] window <ul style="list-style-type: none"> The method file in the initial row of the Batch Table and all data files in the Batch Table open at the same time.
Report format file	[Realtime Analysis] program	[Report] window
	[Offline Editor] program	
	[Postrun Analysis] program	
	[Browser] program	
Browsing file	[Browser] program	[Quant Browser] window <ul style="list-style-type: none"> The method file and data files open at the same time.
Layout file	[Browser] program	[Data Browser] window <ul style="list-style-type: none"> All data files attached to the layout file open.

NOTE

- The windows for each of the files are opened from the program according to the file relationships set during installation.
- Double-click a file to load the file in the window indicated in the "Open Window" column. If the window is already open, the file is loaded to that window.

■ If the File Display Window Is Open

File Name	Double-Clicked File Handling Window
Method file	[Data Acquisition] window
	[Method Editor] window
	[Calibration Curve] window <ul style="list-style-type: none"> If the method file contains calibration curve information, all data files for the standard samples that make up the calibration curve are loaded to the [Data Files] tree view.
	[Quant Browser] window <ul style="list-style-type: none"> If the method file contains calibration curve information, all standard sample data files that make up the calibration curve are loaded to [Quantitative Results View].
Data file	[Data Analysis] window
	[PDA Data Analysis] window <ul style="list-style-type: none"> The [PDA Data Analysis] window opens when data acquisition was performed by a photodiode array detector.
	[Data Comparison] window
	[Data Browser] window
Batch file	[Quant Browser] window <ul style="list-style-type: none"> If the method file is not open in the [Quant Browser] window, the method file used to process the data files opens at the same time. If the method file contains calibration curve information, all data files for the standard samples that make up the calibration curve are loaded to the [Data Files] tree view.
	[Report] window
Report format file	[Report] window
Browsing file	[Quant Browser] window <ul style="list-style-type: none"> The method file and data files open at the same time.
Layout file	[Data Browser] window <ul style="list-style-type: none"> All data files attached to the layout file open.



NOTE

An exclusive [Report] window opens for displaying data report format data.

13.3.2 Drag-and-Drop Files from the [Data Explorer] Sub-Window

The following table describes the operations equivalent to drag-and-drop to display the method file in a specific window.

■ Operations Equivalent To Drag-and-Drop

File Name	Drop Destination Window	Operations Equivalent to Dragging-and-Dropping
Method file	[Data Acquisition] window	[File] - [Open Method File]
	[Method Editor] window	
	[Calibration Curve] window	
	[Quant Browser] window	
	[Data Analysis] window	
	[PDA Data Analysis] window	[File] - [Load Method Parameters] • Default method parameter are set when the method file data does not match the instrument configuration.
Data file	[Data Analysis] window	[File] - [Open Data File]
	[PDA Data Analysis] window	
	[Data Comparison] window	[File] - [Open] - [Add Data File]
	[Data Browser] window	[File] - [Load Data to Cell]
	[Calibration Curve] window	[Data] - [Add] • The data file is displayed in the [Data Files] tree view.
	[Quant Browser] window	[Data] - [Add] • If the method file is not open in the [Quant Browser] window, the method file used to process the data file opens at the same time.
	[Postrun Batch] window	[Edit] - [Add Rows with Selected Data File]
	[Report] window	[File] - [Load Data File]
Batch file	[Realtime Batch] window	[File] - [Open Batch File]
	[Batch Editor] window	
	[Postrun Batch] window	
	[Quant Browser] window	
Report format file	[Report] window	[File] - [Open Report Format File]
Library file	[UV Library Editor] window	[File] - [Open Library File]
Browsing file	[Quant Browser] window	[Layout] - [Open Browsing File] • The method file and data files in the browsing file open at the same time.
Layout file	[Data Browser] window	[Layout] - [Open Layout File] • All data files in the layout file open.





NOTE

- Only the currently displayed data can be displayed in the exclusive [Report] window.
- The method file cannot be opened in a [Calibration Curve] window opened from the [Quant Browser] window.

■ Drag-and-Drop Onto a Report with the [Shift] Key Held Down

The following table describes the action when a file is dragged-and-dropped from the [Data Explorer] sub-window onto a report item with the [Shift] key held down.

File Name	Drop Destination Item	Action
Method file	[System Configuration]	The system configuration information in the method file is displayed.
	[Method]	The instrument parameters and data processing parameters in the method file are displayed.
	[Calibration Curve]	The calibration curve information in the method file is displayed.
Data file	All places where data files can be loaded	<p>Items are displayed individually. The chromatogram of the standard sample and the chromatograms of unknown samples can be displayed in a single report by dropping data files onto each item.</p> <p> NOTE</p> <ul style="list-style-type: none"> Multiple data files can be dragged-and-dropped onto the [Summary (Concentration)], [Summary (Compound)], and [Summary (Data)] items. Data files cannot be loaded in the [Line], [Arrow], [Rectangle], [Ellipse], [Picture], [UV Spectrum], and [UV Library] items.
Batch file	[Batch Table]	<p>The table and batch table information are displayed.</p> <p> NOTE</p> <p>Batch files saved in text format cannot be loaded.</p>
Library file	[UV Library]	The spectrum information in the library file is displayed.
System check result file	[System Check]	Displays the results of the system check.

13.3.3 Batch Table File Operations

This section describes the action when each cell in the method file, data files and report format files set to the Batch Table are clicked with the [Alt] key on your keyboard held down.

File Name	Program Name	Open Window
Method file	[Realtime Analysis] program	[Data Acquisition] window
	[Offline Editor] program	[Method Editor] window
	[Postrun Analysis] program	[Calibration Curve] window <ul style="list-style-type: none"> If the method file contains calibration curve information, all data files for the standard samples that make up the calibration curve are loaded to the [Data Files] tree view.
Data file	[Realtime Analysis] program	[Data Analysis] window
	[Offline Editor] program	[PDA Data Analysis] window
	[Postrun Analysis] program	<ul style="list-style-type: none"> If data acquisition was performed with a photodiode array detector, the [PDA Data Analysis] window opens.
Report format file	[Realtime Analysis] program	[Report] window
	[Offline Editor] program	
	[Postrun Analysis] program	



NOTE

While performing an operation on a file in the Batch Table, either select the file with the [Alt] key held down or double-click the file. To make changes, select [Options] on the [Tools] menu, and enter the changes on the [Batch Table Edit] tab in the [Setting Options] sub-window that opens.

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