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SHIMADZU

## Shimadzu High Performance Liquid Chromatography

# LabSolutions GPC

# Instruction Manual

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

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# Introduction

# Read this Instruction Manual thoroughly before using the product.

Thank you for purchasing the LabSolutions GPC software for Shimadzu High Performance Liquid Chromatography Workstation (hereafter referred to as "the software" or "LabSolutions GPC").

LabSolutions GPC works as an extension of LabSolutions, and enables you to conduct GPC analysis on data acquired by LabSolutions under various conditions.

LabSolutions GPC operates on Window 7. Other PC hardware requirements conform to those for LabSolutions.

This manual explains the basic operations of LabSolutions GPC. Read this manual thoroughly before using the product and operate the product in accordance with the instructions in this manual.

Keep it in a safe place so that it can be referred to whenever you have questions regarding the operation of this product.

This manual assumes that readers are knowledgeable of basic operation of the LC workstation software, LabSolutions. Refer to 'Operation Manual' of LabSolutions for points that are not explained in this manual.

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.

This manual includes contents that are common across the LabSolutions series. Note that the screen captures inserted in the text may be those of the similar product if there are no significant discrepancies in the explanation.

# 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 reinstallation (after the product is moved) is required.

# Notice

- Information in this manual is subject to change without notice and does not represent a commitment on the part of the vendor.
- Any errors or omissions which may have occurred in this manual despite the utmost care taken in its production will be corrected as soon as possible, although not necessarily immediately after detection.
- 
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  Adobe, Adobe logo and Adobe Reader are trademarks or registered trademarks of Adobe Systems Incorporated in the United States and/or other countries.
  Other company names and product names mentioned in this manual are trademarks or registered trademarks of their respective companies. The TM and ® symbols are omitted in this manual.
- Microsoft® Windows® 7 Operating System is referred to as "Windows 7".
- Replacement parts for this product will be available for a period of seven (7) years after the product is discontinued. Thereafter, such parts may cease to be available. Note, however, that the availability of parts not manufactured by Shimadzu shall be determined by the relevant manufacturers.

# Instruction Manuals

## ■ List of Instruction Manuals

| Name | Content |
|---|---|
| Notice Before Using | Explains the information necessary to use the LabSolutions GPC, such as how to update, how to convert the data and caution about the specification of GPC. |
| Instruction Manual (This document) | Explains data acquisition and analysis procedures of LabSolutions GPC for various purposes. |
| Quick Manual | Explains basic analysis excerpted from the Instruction Manual. |
| 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.<br>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.<br>For information on how to use it, refer to "8.1.1 Using Help" on page 111 in this manual. |

**NOTE**

Also, refer to the manuals for LabSolutions if necessary. For details, refer to the manuals for LabSolutions.

**Reference**

"8 Appendix"

## ■ 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 |
|---|---|
| NOTE | Emphasizes additional information that is provided to ensure the proper use of this product. |
| Reference | Indicates the location of related reference information. |
| ' ' | The names of the instruction manuals. |
| " " | The names of programs and products. |
| [ ] | Indicates the names of buttons, menu options, setting options, windows/sub-windows, and icons that are displayed in a window.<br>Example: Click [OK]. |
| [ ] - [ ] | When several operations are performed one after another, hyphens are used to show the sequence.<br>Example: Select [File] - [Print].<br>Click the [File] menu and select [Print]. |

# Warranty

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.

3. Limitation of Liability:

(1) In no event will Shimadzu be liable for any lost revenue, profit or data, or for special, indirect, consequential, incidental or punitive damages, however caused regardless of the theory of liability, arising out of or related to the use of or inability to use the product, even if Shimadzu has been advised of the possibility of such damage.

(2) In no event will Shimadzu's liability to you, whether in contract, tort (including negligence), or otherwise, exceed the amount you paid for the product.

4. Exceptions:

Failures caused by the following are excluded from the warranty, even if they occur during the warranty period.

1) Improper product handling

2) Repairs or modifications performed by parties other than Shimadzu or Shimadzu designated companies

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.

# Contents

# 3 Generating Calibration Curves



# 4 GPC Calculation

# 7 GPC File Converter



# 8 Appendix

# 1 Overview of LabSolutions GPC



LabSolutions GPC is software that runs on LabSolutions platform. Data acquisition and analysis can be performed using operations similar to LabSolutions.

This document describes only those items different from LabSolutions. See 'Operation Manual' of LabSolutions for descriptions on "data acquisition", "peak integration" and "batch processing".

## 1.1 What is GPC?

GPC is short for Gel Permeation Chromatography, and is also called Size Exclusion. Chromatography. This is a type of separation method used in liquid chromatographs, in which sample compounds are physically separated by the size of molecules, regardless of any chemical interaction between sample components and the stationary phase.

## 1.2 Functions of LabSolutions GPC

LabSolutions GPC is optional software for LabSolutions that calculates molecular weight distribution and various average molecular weight values from the data acquired by a gel permeation chromatograph. It enables you to generate parameters and graphs for evaluating characteristics of a polymer sample using the similar operations with LabSolutions. Furthermore, statistical calculation of those values and their comparison by overlaying graphs are possible.

### ■ Configuration of the LabSolutions GPC Software

LabSolutions GPC consists mainly of the following three applications:

- **GPC Data Analysis**
  Calculates the molecular weight distribution and average molecular weight values of an unknown sample from a calibration curve generated by "GPC Calibration Curve".
- **GPC Calibration Curve**
  Generates a calibration curve* that is used to calculate the molecular weight and molecular weight distribution of an unknown sample.
  * A graph showing the relationship between the logarithm of the molecular weight of the samples and the elution time (eluent volume)
- **GPC Data Comparison**
  Enables you to compare chromatograms and differential and integral molecular weight curves of multiple unknown samples by overlaying the graphs.
- **Batch Postrun**
  GPC data analysis can be performed for data from multiple samples.
- **Report Creation**
  In addition to the usual report items, report items for outputting GPC analysis results, including molecular weight distribution calculation results, are added.

### ■ File Compatibility

- GPC method files of CLASS-LC10/CLASS-VP can be imported and used.
- LCsolution GPC data files and method files can be read as they are. However, files created with LabSolutions GPC cannot be read by LCsolution GPC.

# 1.3 Description of Terms

Following are descriptions on terms used in LabSolutions GPC:

| Term | Description |
|---|---|
| **Mn** | A number average molecular weight, which is calculated based on the total number of molecules |
| **Mw** | A weight average molecular weight, which is calculated based on the total weight of molecules |
| **Mz** | A Z average molecular weight |
| **Mz1** | A Z+1 average molecular weight |
| **Mv** | A viscosity average molecular weight |
| **Q factor** | A molecular weight per unit chain length of a polymer |

# 2 Starting the Analysis

This chapter describes the basic operation of LabSolutions GPC. For better understanding, it is recommended that you actually operate LabSolutions GPC and work through the analysis procedure of this chapter.

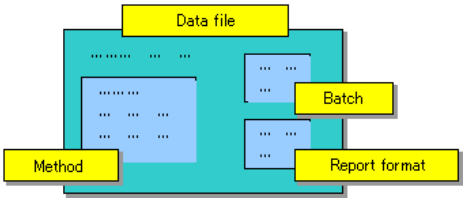
To specify the instrument control parameters for data acquisition and the peak integration parameters, refer to "LabSolutions Operation manual". This manual primarily describes the procedures particularly required for operating LabSolutions GPC.



## 2.1 Before Reading This Chapter

### 2.1.1 The Data Structure of LabSolutions GPC

This section gives a brief explanation about the data structure of LabSolutions GPC.
Adding to method parameters for LC Analysis and LC Postrun, the GPC data file also stores various data, such as GPC calibration curve information and GPC calculation parameters.
This ensures the traceability of data since the analysis conditions and parameters can be referenced from the data file itself. In addition, you can reanalyze the data using only the data file.




**NOTE**

The method information stored in the data file is the duplicate of the method file used during the acquisition and analysis of data. Therefore, when modifying the method parameter in the data file, only the "method in data" is modified and no changes are made to the original method file. But the original method file can be updated accordingly with the modified method in the data file by using "Apply to the Method File" (save as a method file) function.

### 2.1.2 LabSolutions GPC Operation Flow

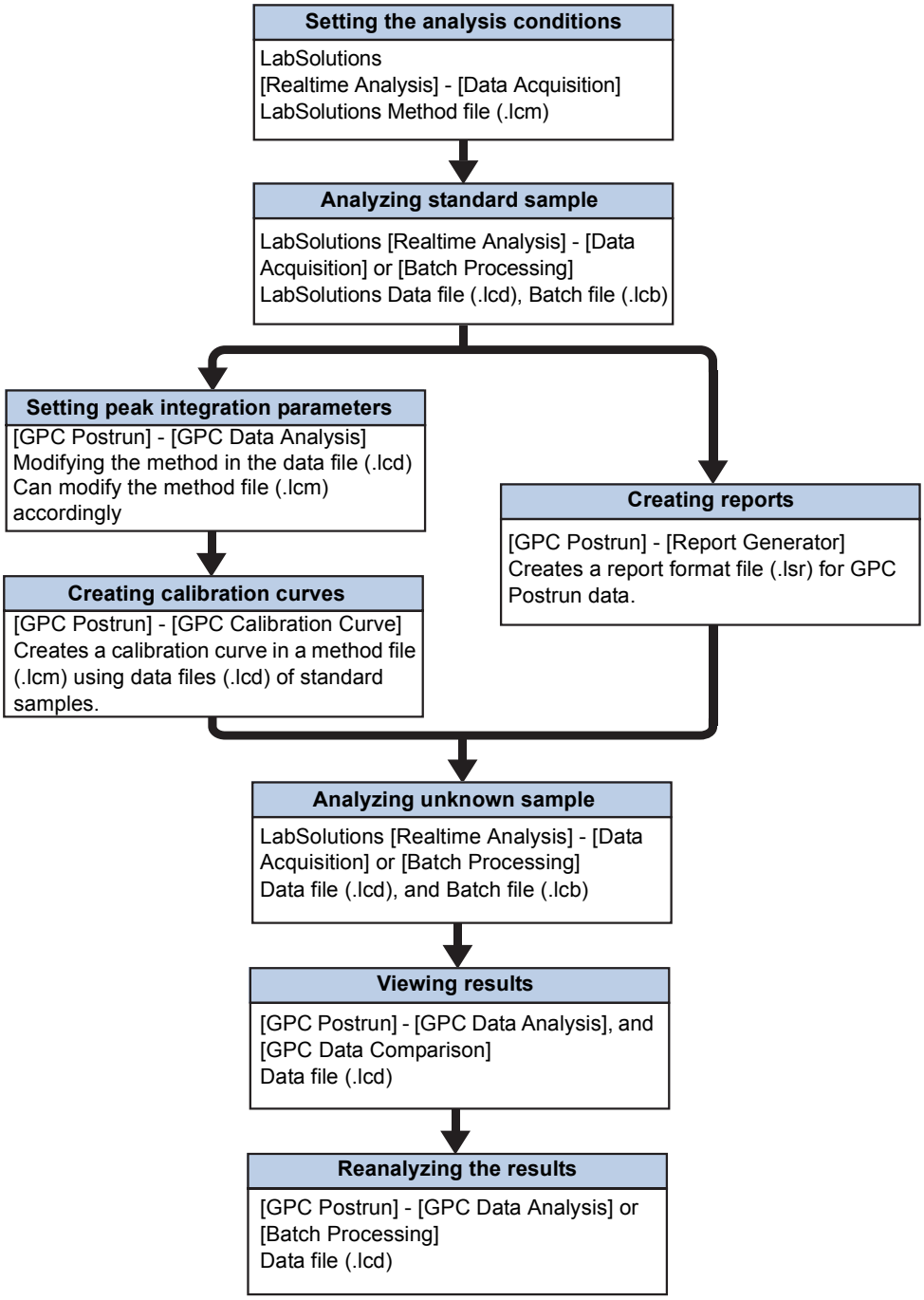
In this chapter, the operation flow of LabSolutions GPC is explained as shown in the following chart.
In LabSolutions GPC, adding to the parameters for LabSolutions, you set parameters for calibration curve, molecular weight calculation, etc. in a method file. You can create calibration curves in the [GPC Postrun] program, and once you have set all these parameters, you can perform GPC calculation, such as molecular weight calculation, while performing data acquisition by using the method file.

**Explanation on how to view the following chart:**

| Operation |
|---|
| Application<br>Target files<br>(Their file name extensions) |

File Names

| File Names | extension | contents |
|---|---|---|
| Method file | .lcm | Analysis conditions, postrun analysis conditions, calibration curve conditions |
| Report format file | .lsr | Report format |
| Batch file | .lcb | Batch table, batch settings |
| Data file | .lcd | Chromatogram, Peak table, Report format (Report format in data), Method (copy), Batch table (copy) |



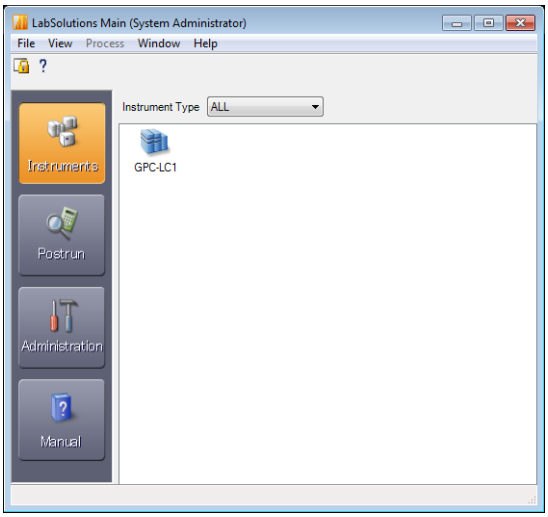
**NOTE**

- In a batch table, the method file (.lcm) and the report format file (.lsr) are specified for each particular data file (.lcd). When the batch analysis is completed, it creates a data file (.lcd) containing the same information stored in the batch table (.lcb) and .lcm and .lsr (when a report is output) set for each line of the batch table.
- When you open a method file (.lcm) in the [GPC Calibration Curve] window, the data files (.lcd) for all levels in the calibration curve are loaded simultaneously. If the method file (.lcm) is edited here, the data can be recalculated using the new analysis conditions for each data file (.lcd) that has been imported. You can also optimize the quantitative method and the calibration curve type beside adding or deleting calibration level data.

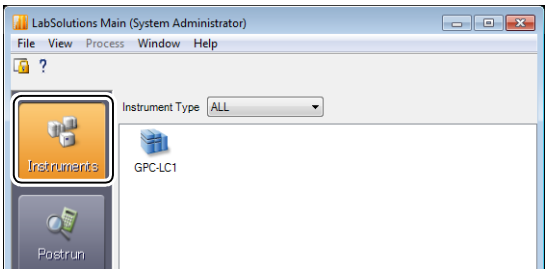


# 2.2 Starting LabSolutions Analysis

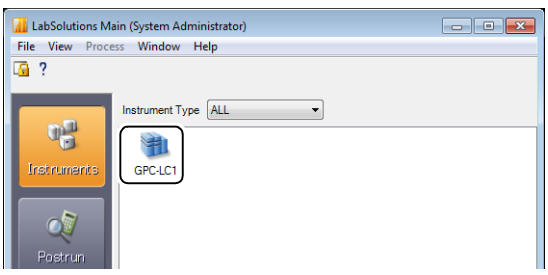
**1** **Display the [LabSolutions Main] window.**




**2** **Click**  **(Instruments).**




**3** **Double-click on the instrument to use for analysis.**



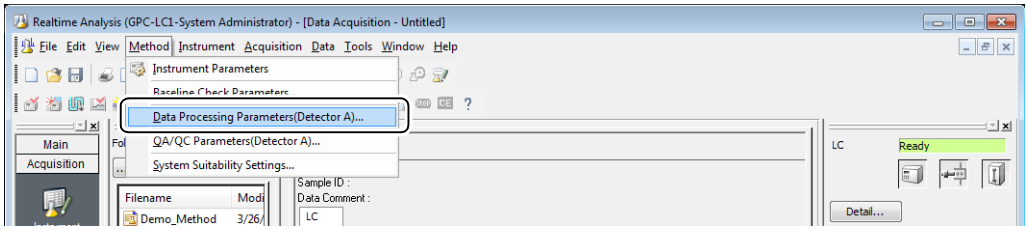

The [Realtime Analysis] program will start.

# 2.3 Preparing for Analysis

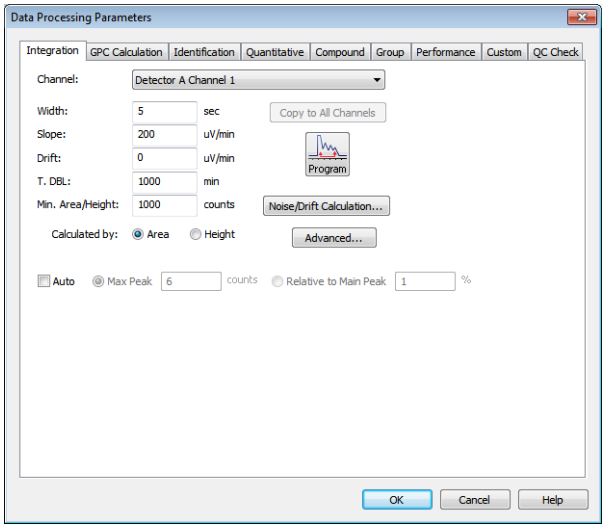
Referring to "LabSolutions Operation Manual", complete the system configuration and the preparation of analytical instruments, and specify the instrument parameters as required. This section primarily explains how to set parameters necessary for LabSolutions GPC analysis, such as the integration parameters, etc. You can also set the parameters when creating calibration curves in the [GPC Postrun] program after completing standard sample analysis.

## 2.3.1 Setting Data Analysis Parameters

**1** **Click [Data Processing Parameters] from the [Method] menu in the [Realtime Analysis] program.**




The [Data Processing Parameters] screen appears.

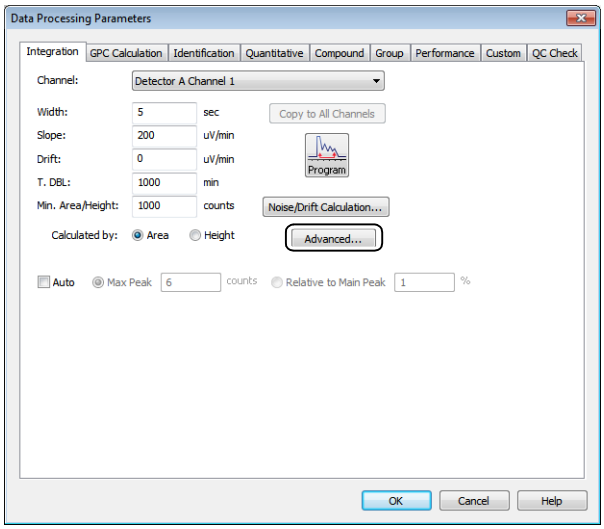



LabSolutions GPC performs the molecular weight calculation, etc., using "slice data". The "slice data" refers to the height values obtained by separating chromatograms by a certain time interval. Therefore, in addition to configuring the usual integration parameters in LabSolutions, the following settings must also be configured in the [Data Processing Parameters] screen.

## ■ Setting the Maximum Number of Slices

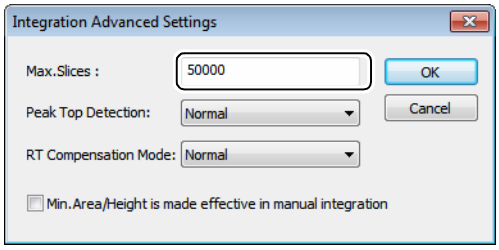
The maximum number of slices corresponds to the maximum number of "slice data" that can be stored in a data file. You can set this value up to [50000].

### 1 Click [Advanced] in the [Integration] tab.




### 2 Enter the number of slices in [Max.Slices].

Set the maximum value: [50000].




**NOTE**

Each slice interval is 1/10 of the time (sec) specified as [Width] in the integration parameters. The interval information is stored for each area detected as a peak. If a width of a detected peak is quite long and the number of slices exceeds [50000], an error message appears. In this case, set the larger value for [Width].

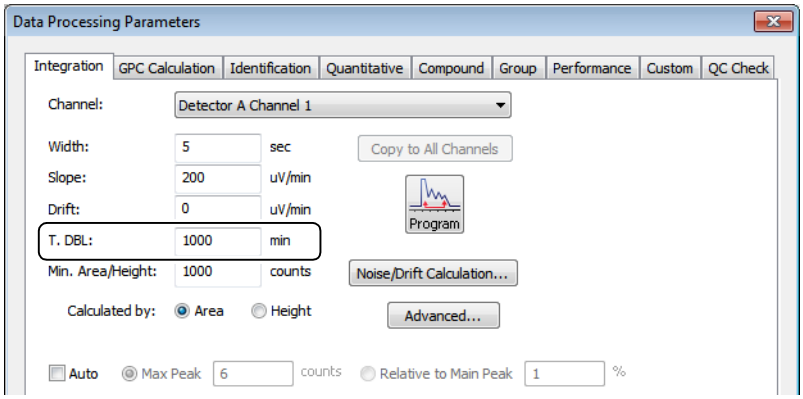
### 3 Click [OK].

This confirms the setting of the maximum number of slices.

## ■ Setting T.DBL

T.DBL is a parameter that is used to automatically integrate peaks which broaden with time by increasing [Width] and decreasing [Slope] according to the time specified.

**1** **Enter [1000] in [T.DBL].**



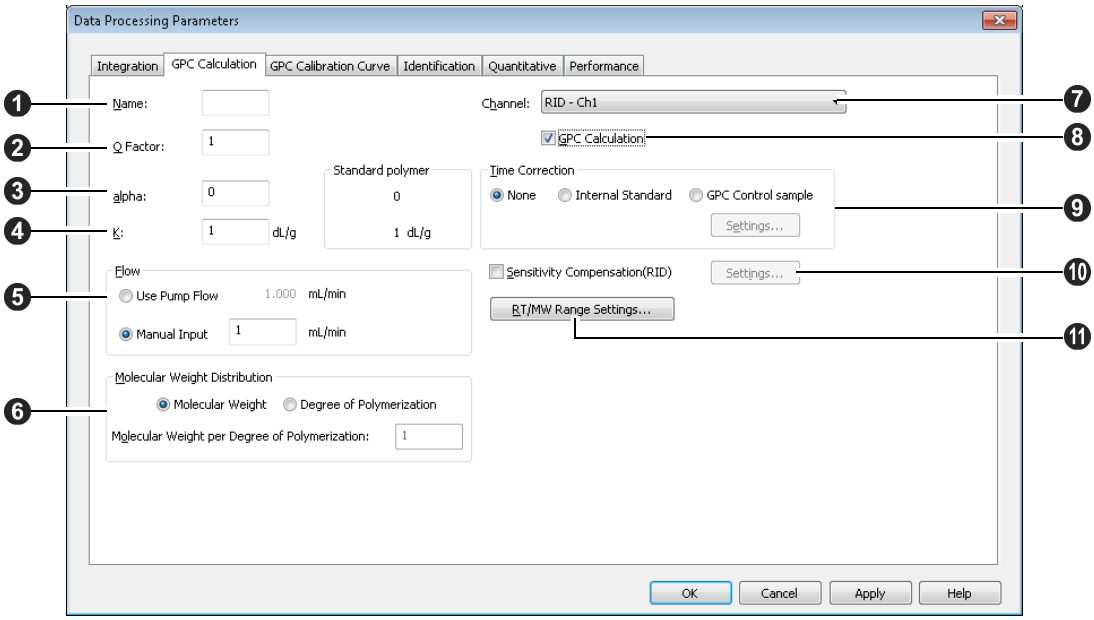

**2** **Click [OK].**

**NOTE**

If [T.DBL] is enabled in molecular weight distribution calculation, [Width] increases with time as a function of the parameter. It follows the increase of intervals of slice data, and consequently the molecular weight calculation may not be performed properly. To avoid this, you set [T.DBL] to [1000] to disable this parameter.

## ■ Setting GPC Calculation Parameters

### 1 Click the [GPC Calculation] tab and configure the settings.




| No. | Description |
|---|---|
| ❶ | Enter the element name. Up to 64 characters can be entered. The initial value is blank. |
| ❷ | Enter the Q factor. A positive real number can be entered. The initial value is [1]. |
| ❸ | Enter the alpha value used for Mark Houwink conversion, etc. The initial value is [0].<br>(Alpha to be displayed for standard polymer are those specified in the [GPC Calibration Curve] tab.) |
| ❹ | Enter the K value used for Mark Houwink conversion, etc. The initial value is [1].<br>(K to be displayed for standard polymer are those specified in the [GPC Calibration Curve] tab.) |
| ❺ | Select whether you use the pump flow or a manually input value for the flow calculation. If you use a manually input value, set the flow quantity per minute. |
| ❻ | Select the molecular weight or the degree of polymerization for the display unit of the Y axis. [Molecular weight] is selected initially. By selecting [Degree of Polymerization], you can enter [Molecular Weight] per degree of polymerization. |
| ❼ | Select a channel of the detector. |
| ❽ | Specify whether to perform the GPC calculation for each channel. |
| ❾ | Select a method of the time correction. [None] is selected initially. |
| ❿ | Specify whether to perform the sensitivity compensation of the RI detector. When performing compensation, click [Settings] and set the sensitivity compensation of the RI detector. |
| ⓫ | Click this to display the [RT/MW range setting] screen. |

### 2 Click [OK].

**Reference**

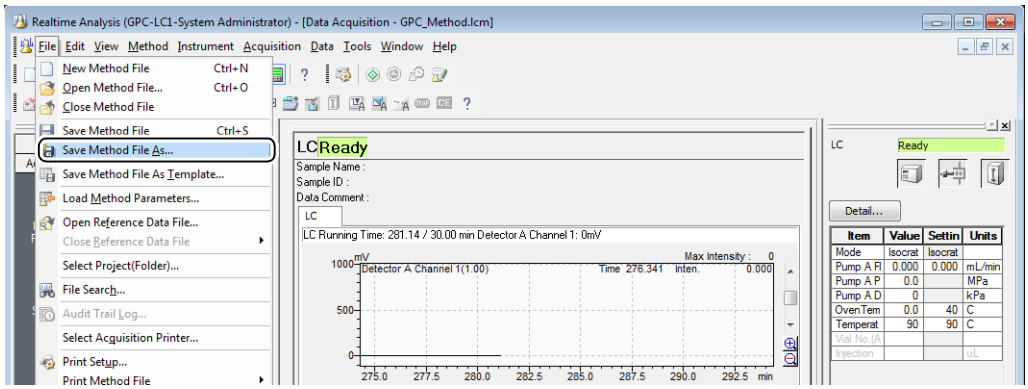
"4.4.3 Setting Data Analysis Parameters"

**NOTE**

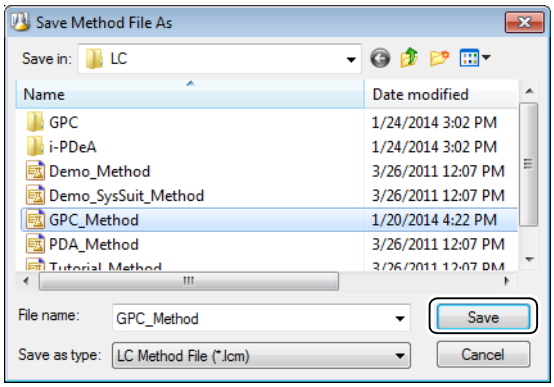
- Configure the settings in the [GPC Data Analysis] window or in the [GPC Calibration Curve] window.
- If you have set these parameters in the [GPC Data Analysis] window, you need to apply the "method inside data file" to the original method file by using "Apply to Method" function. Also, you can create calibration curves in the [GPC Calibration Curve] window.

### 2.3.2 Saving Method Files

**1** **Click [Save Method File As] from the [File] menu.**




**2** **Input the file name and click [Save].**




**NOTE**

You can specify the default location for saving files by selecting the project folder in [File] -[Select Project (Folder)].

## 2.4 Analyzing Standard Samples

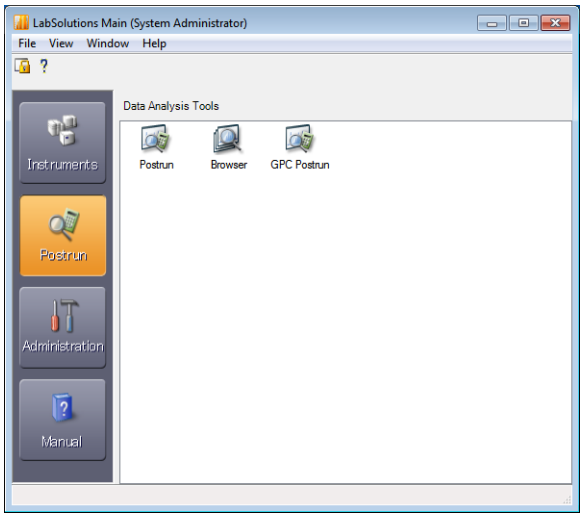
When creating a calibration curve based on the analysis results of standard sample data, you need to complete the data acquisition prior to the calibration curve creation. Referring to "LabSolutions Operation Manual", analyze the standard sample through the single or batch analysis to acquire the sample data.

## 2.5 Creating Calibration Curve

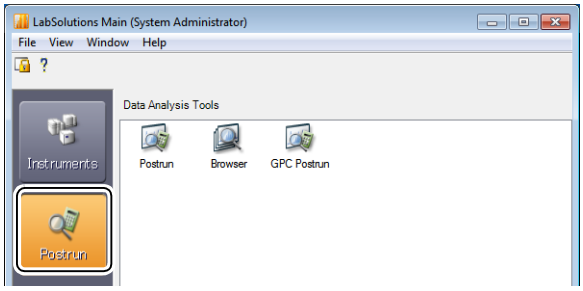
In LabSolutions GPC, you create calibration curves in the [GPC Calibration Curve] window of the [GPC Postrun] program. Prior to that, you need to set [Integration Parameters] and [GPC Calculation Parameters].
This section describes how to create the calibration curve using the data already acquired.
The following is the brief explanation for the procedures:

## 2.5.1 Displaying the [GPC Calibration Curve] Window

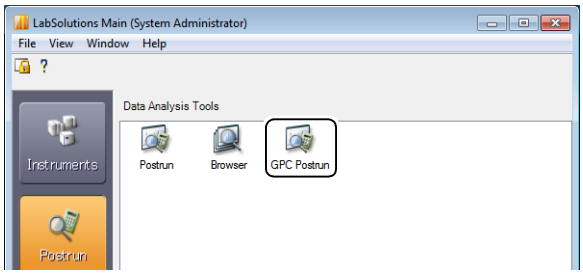
**1** **Display the [LabSolutions Main] window.**




**2** **Click**  **(Postrun).**




**3** **Double-click**  **(GPC Postrun).**




The [GPC Postrun] program will start.

**NOTE**

- Click 

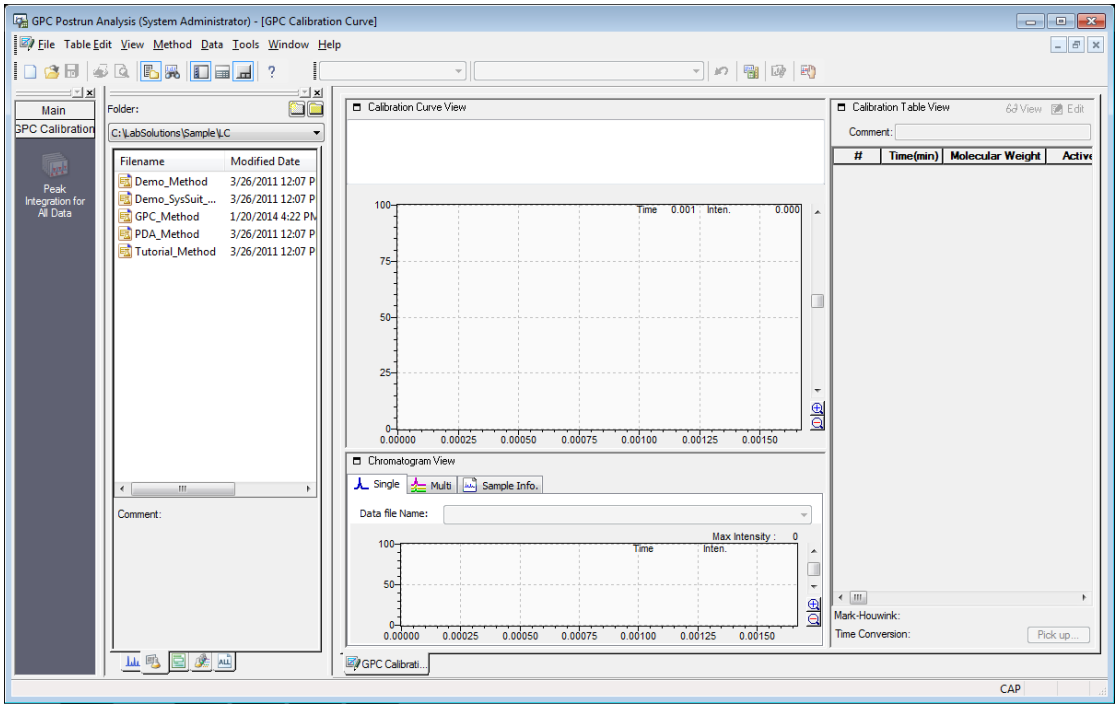
(GPC Postrun) for GPC data analysis, including molecular weight distribution calculation, as you click 

(Postrun) for the regular data analysis.
- If 

(GPC Postrun) is not displayed on the menu, the license for LabSolutions GPC is not recognized in your system. Use the USB dongle that stores the license.

## 4 Click GPC Calibration Curve (GPC Calibration Curve) from the [Main] assistant bar in the [GPC Postrun] program.


The [GPC Calibration Curve] window appears.



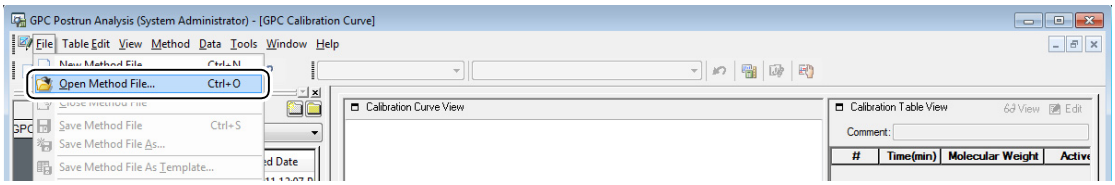

**NOTE**

When the [GPC Calibration Curve] window is displayed, no data has been loaded yet.

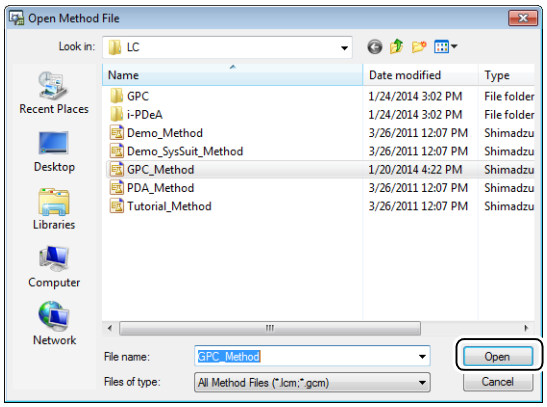
## 2.5.2 Opening Method File

Open the method file used for analyzing the standard sample.

**1** **Click [Open Method File] from the [File] menu.**




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

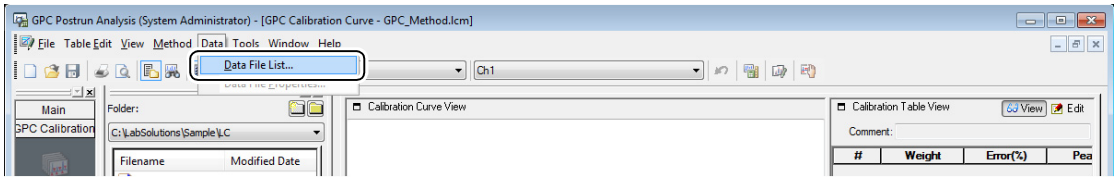



**NOTE**

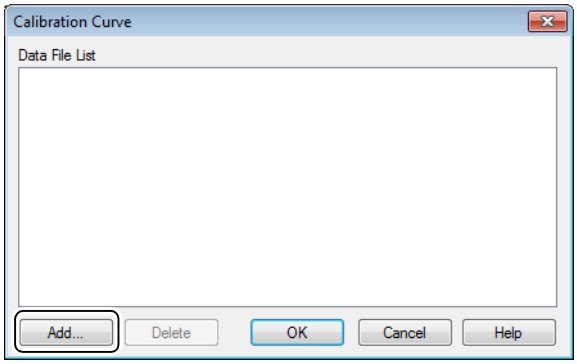
You can select either LabSolutions method files or those from older software versions.

## 2.5.3 Displaying Data Files

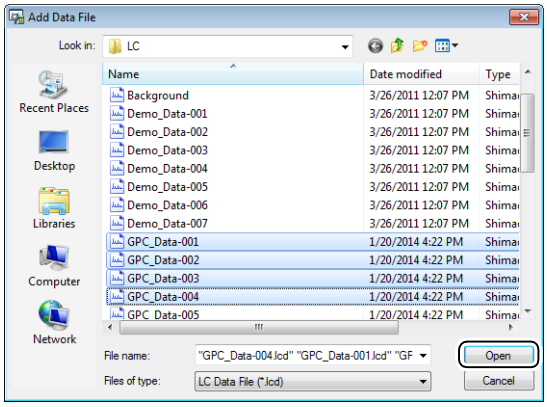
**1** **Click [Data File List] from the [Data] menu.**



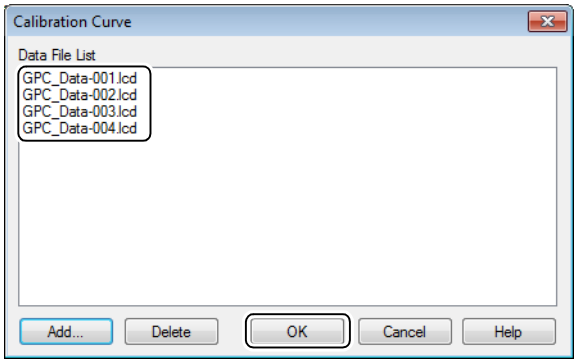
**2** **Click [Add].**




**3** **Select the standard sample data you wish to use for creating calibration curve, and click [Open].**




**4** **Verify that the data file of the standard sample is displayed in the data file list, and click [OK].**

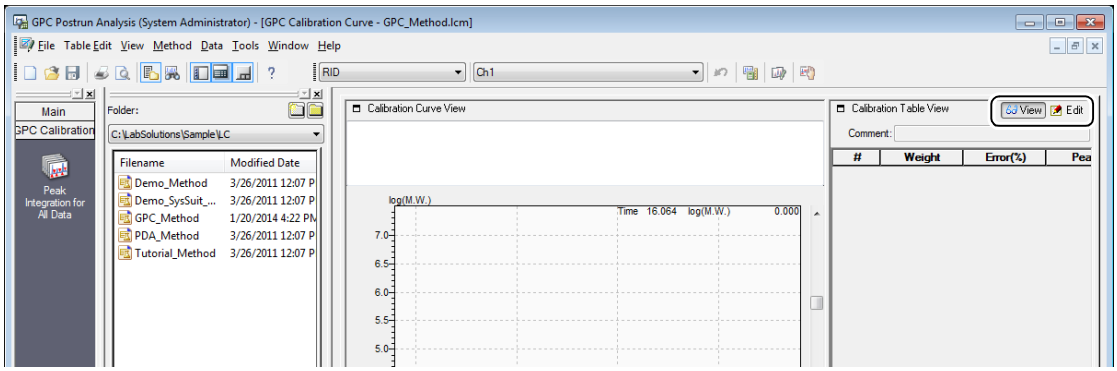



**NOTE**

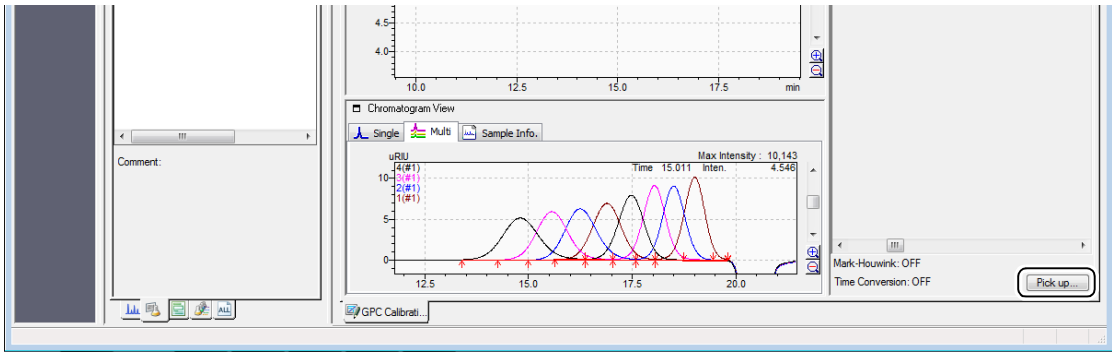
To select multiple sample data, repeat this procedure as necessary.

## 2.5.4 Picking up Retention Time

**1** **Click [Edit] in the [Calibration Table View] screen.**

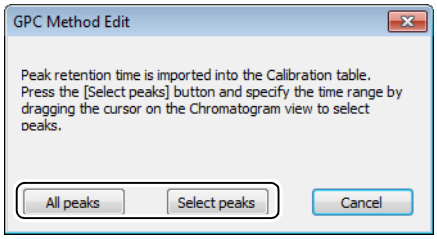



**2** **Click [Pick up] in the [Calibration Table View] screen.**



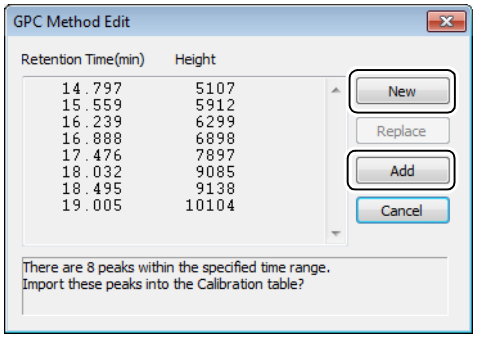

**3** **Click [All peaks] or [Select peaks].**

Select [All peaks] when importing data of the whole retention time, and select [Select peaks] when importing data for a certain time range. When [Select peaks] is selected, use the mouse to specify the range on the chromatogram.

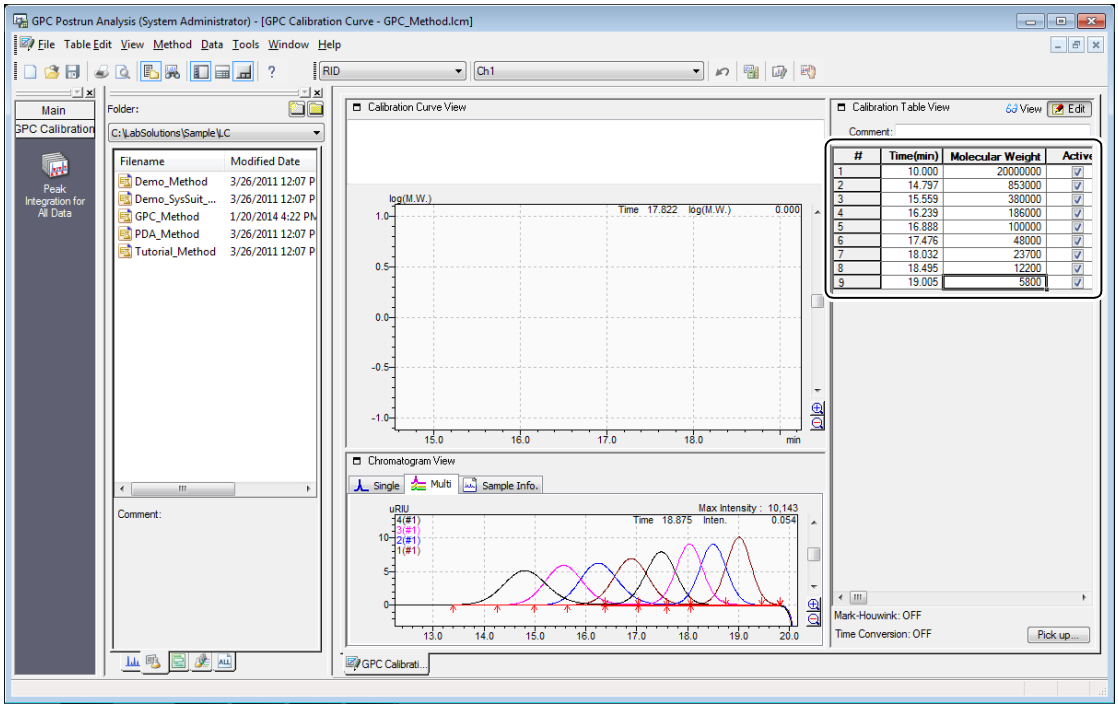


## 4 Click [New] or [Add].

Select [New] when importing peak data after deleting an existing calibration curve. Select [Add] when adding peak data to existing calibration points.




## 5 Set the parameters not yet defined in the calibration curve table, such as molecular weight values.

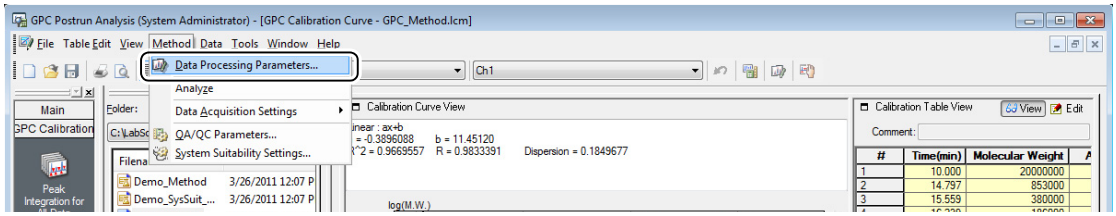



### NOTE

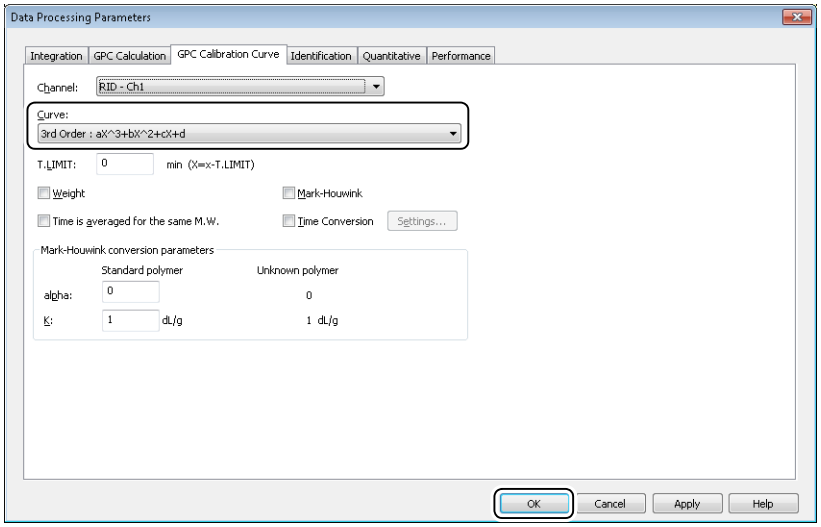
- You can import parameter values from the [Table Edit] menu or by right-clicking and opening the [Import Calibration Table] screen from the menu. When importing a method file, pick up the [retention time] after importing. To do so, click [Retention Time Refresh] in the [GPC Method Edit] screen.
- In the edit mode of Calibration Table View, you can delete unnecessary calibration points by selecting the row of the calibration point and selecting [Delete Row] from the right-click menu.
- Peak data is sorted by the retention time when switching the edit mode to the view mode.

## 2.5.5 Setting Calibration Curve Parameters

**1** **Select [Data Processing Parameters] from the [Method] menu.**




**2** **Select the [Curve] type in the [GPC Calibration Curve] tab, and click [OK].**

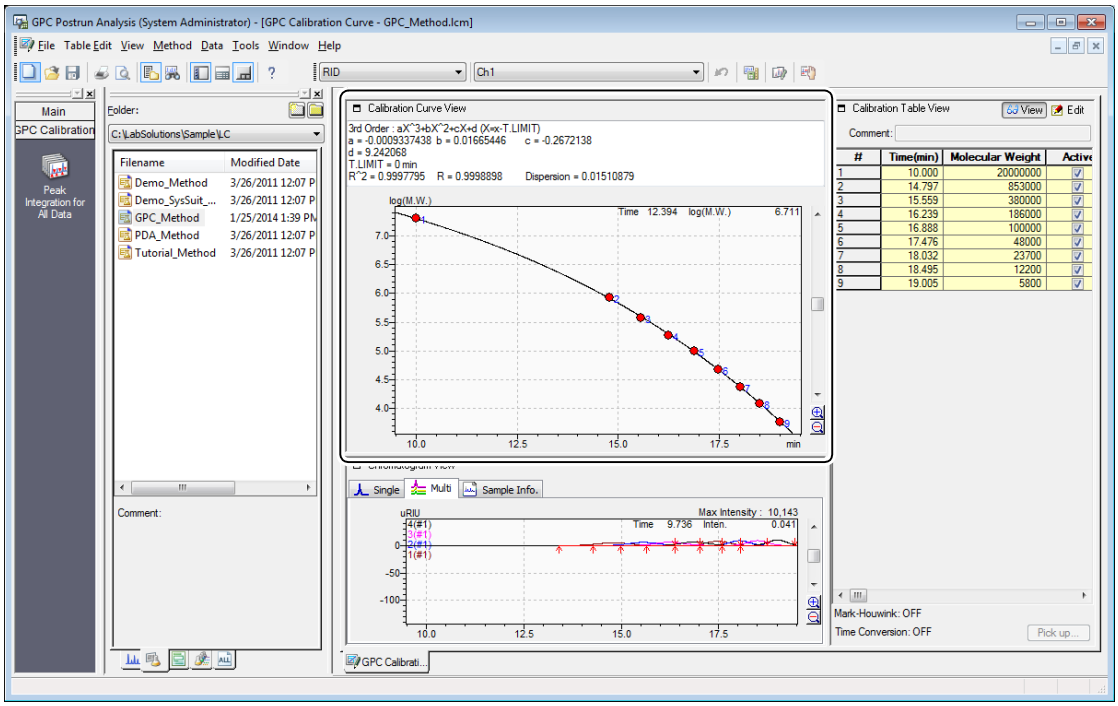



**NOTE**

If the number of calibration points is not enough, the calculation for high order calibration curve may not be performed.

## 2.5.6 Saving Calibration Curves

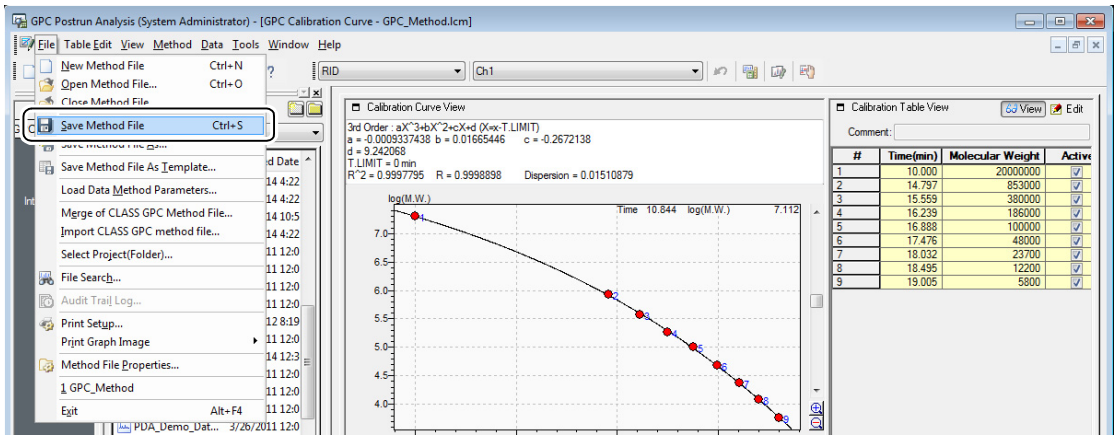
**1** **Verify the calibration curve created in the [Calibration Curve View] screen.**




**NOTE**

To modify the calibration curve, configure the settings again in the [Data Processing Parameters] - [GPC Calibration Curve] tab.

**2** **Click [Save Method File] from the [File] menu.**




The calibration curve is saved in the method file.

# 2.6 Creating Report Format

The procedures on creating a report format or summary report format of GPC analysis data are similar to those for LabSolutions. Refer to "LabSolutions Operation Manual".
In LabSolutions GPC, the report items for outputting the results of GPC analysis, such as molecular weight distributions, are newly added to the existing items. For more details, refer to "6 Report Function".

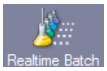
# 2.7 Analyzing Unknown Samples



This section describes the procedures for analyzing unknown samples through batch processing, using a method file where the integration parameters and calibration curve are set in procedures "2.3 Preparing for Analysis" and "2.5 Creating Calibration Curve".

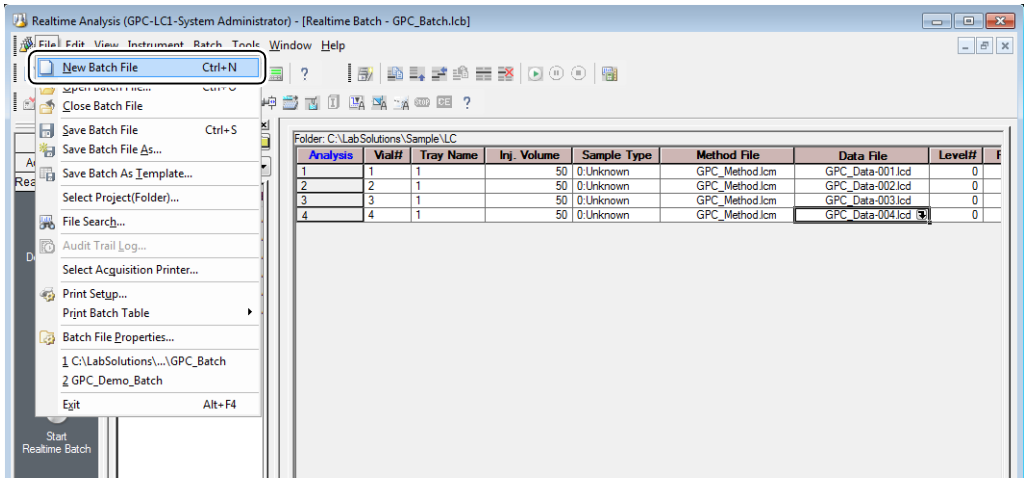
## 2.7.1 Performing Batch Analysis

Set the schedule for continuous analysis.

**1** **Click** 

**(Realtime Batch) from the [Main] assistant bar in the [Realtime Analysis] program.**


**2** **Select [New Batch File] from the [File] menu.**



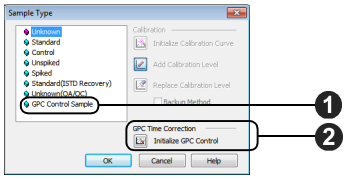
## 3 Enter the batch analysis schedule in the batch table.

The main items to be entered into the batch table are as follows:

Folder: C:\LabSolutions\Sample\LC

| Analysis | Vial# | Tray Name | Inj. Volume | Sample Type | Method File | Data File | Level# | F |
|---|---|---|---|---|---|---|---|---|
| 1 | 5 | 1 | 50 | 0:Unknown | GPC_Method.lcm | GPC_Data-005.lcd | 0 | |
| 2 | 6 | 1 | 50 | 0:Unknown | GPC_Method.lcm | GPC_Data-006.lcd | 0 | |
| 3 | 7 | 1 | 50 | 0:Unknown | GPC_Method.lcm | GPC_Data-007.lcd | 0 | |
| 4 | 8 | 1 | 50 | 0:Unknown | GPC_Method.lcm | GPC_Data-008.lcd | 0 | |

| Parameter | Description |
|---|---|
| Vial# | Enter the vial number of the sample injected by the autosampler. If no sample is being injected, enter "-1". |
| Tray Name | Enter the tray number of the sample injected by the autosampler. No entry is necessary when using an autosampler without multiple tray settings. |
| Inj. Volume | Enter the injection volume (unit: µL). |
| Sample Type | Select the sample type.<br>In LabSolutions GPC, [GPC Control Sample] is added in the list in order to specify the correction according to the control sample.<br>When you analyze an unknown sample first, enable [Initialize GPC Control] to initialize the correction factor. |
| Method File | Specify the method file to be used for the analysis. |
| Data File | Name the data that is to be saved as the analysis results.<br>When the file name is entered without a path, the data is created in the currently browsed project folder (as previously specified). |




| No. | Description |
|---|---|
| 1 | The GPC Control Sample is used for correction of retention time. |
| 2 | Initializes the parameter for the time correction by GPC Control Sample. |

**NOTE**

If an item is not displayed in the table, right-click on [Batch Table] and click [Table Style] from the menu to set [Display Items].

## 4 Click (Save) in the toolbar, and save under a new name.

The content of the batch table is saved.

## 5 Click (Start) in the toolbar to start batch analysis.

**NOTE**

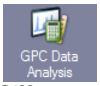
The correction factor is not updated when the correction peaks of the control sample cannot be identified. The control sample is corrected using the correction factor before the analysis.

# 2.8 Performing GPC Calculation

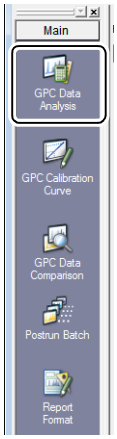
This section describes how to view the results of analyzing molecular weight distribution of unknown samples, etc., and how to set the GPC calculation parameters used for calculating molecular weight distributions. By applying the GPC parameters optimized here to a method file and performing [Batch Processing] in the [GPC Postrun] program, you can reanalyze multiple unknown sample data in the same conditions.

## 2.8.1 Displaying the GPC Data Analysis Results

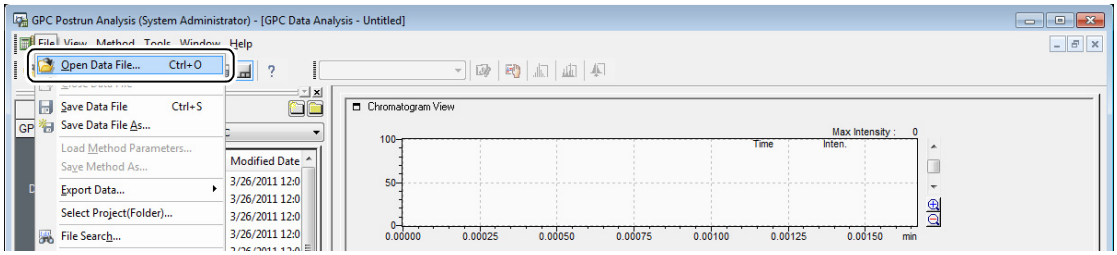


**1** **Click** 

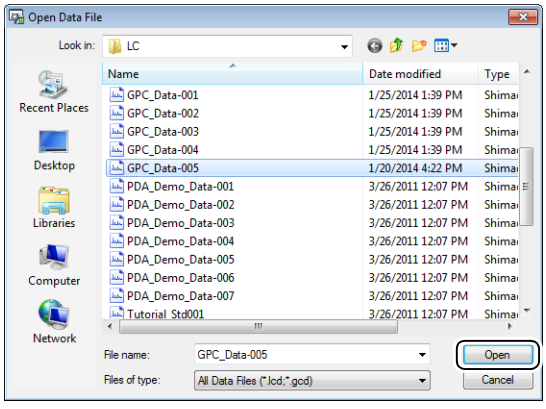
**(GPC Data Analysis) from the [Main] assistant bar in the [GPC Postrun] program.**



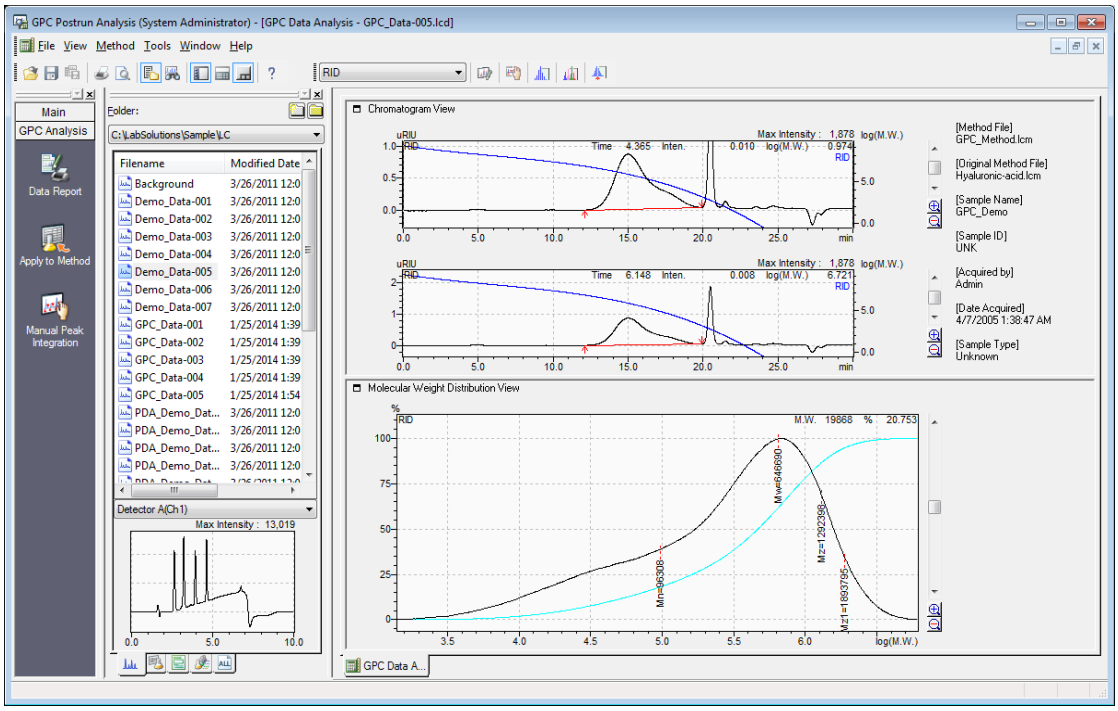

**2** **Click [Open Data File] from the [File] menu.**




**3** **Select the data file, and click [Open].**

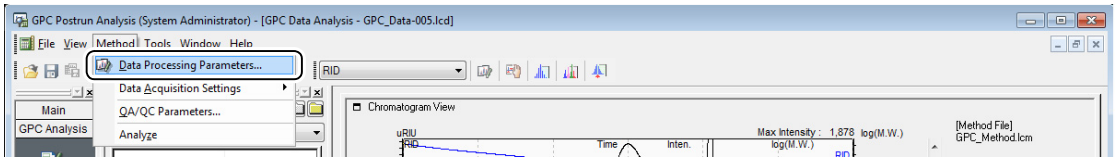


The data file of unknown sample is loaded, and the chromatogram view displays the chromatogram, the calibration curve, and the molecular weight distribution curve.

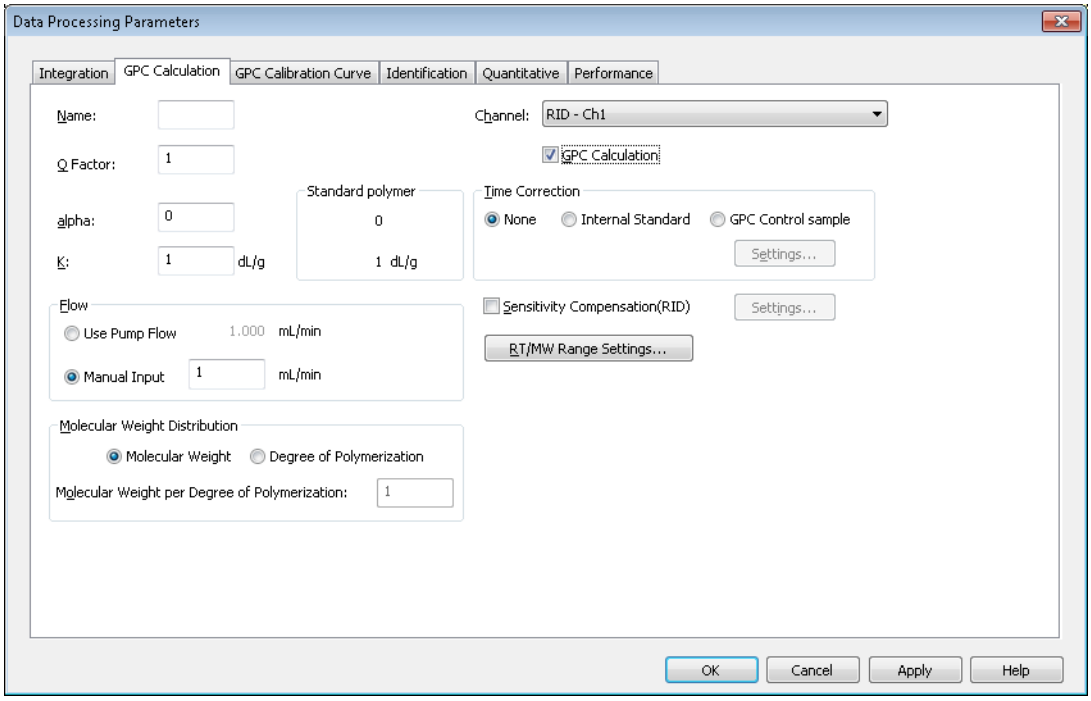


## 2.8.2 Setting the Parameters for Molecular Weight Calculation

**1** **Select [Data Processing Parameters] from the [Method] menu.**

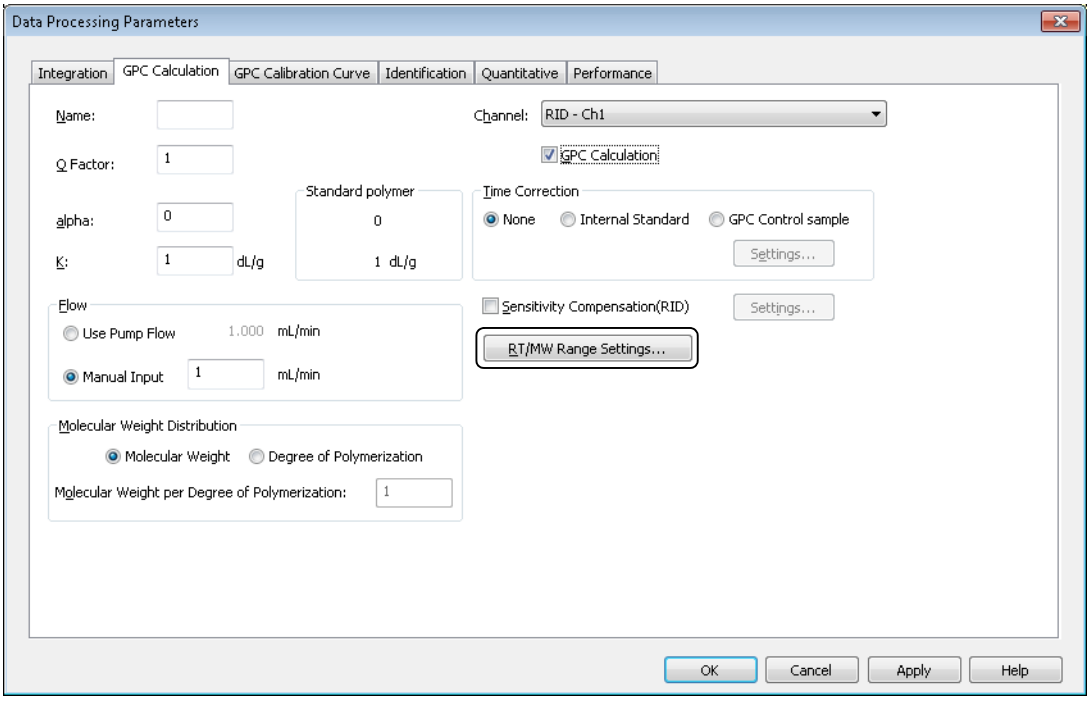



**2** **Click the [GPC Calculation] tab to verify the parameters.**

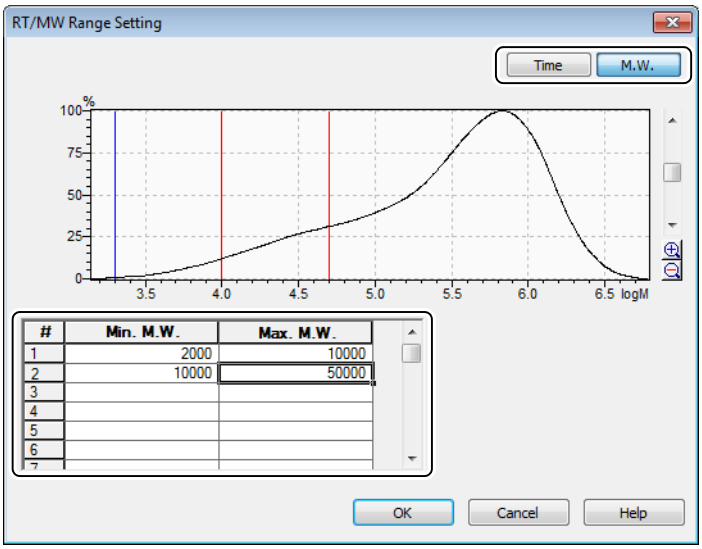


## ■ Setting RT/MW Range

**1** **Click [RT/MW Range Settings] in the [GPC Calculation] tab.**




**2** **Select [Time] or [M.W.], and input the RT/MW range.**

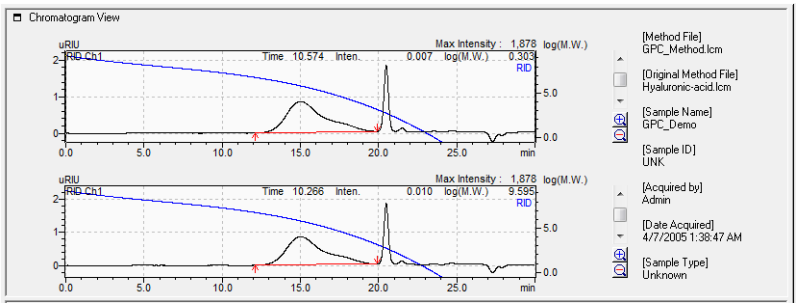



**3** **Click [OK].**

## 2.8.3 Performing GPC Calculation

**1** **Click [OK] in the [Data Processing Parameters] screen.**

The data is analyzed, and the chromatogram view displays the molecular weight distribution curve and the integrated molecular weight distribution curve.




**2** **View the analysis results.**

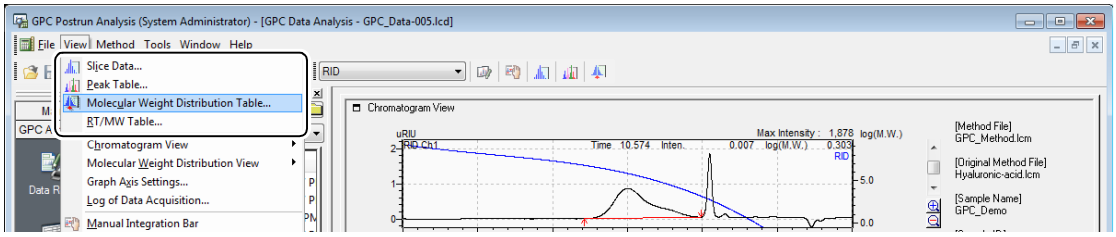
**NOTE**

When reanalyzing the data, click the [GPC Calculation] tab from the [Data Processing Parameters] screen, and modify the calculation parameters.

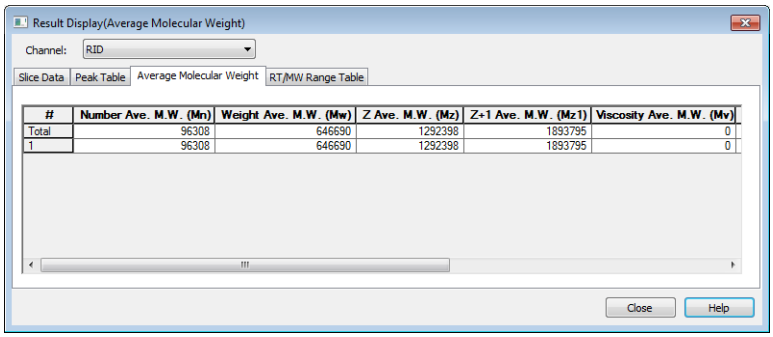
## 2.8.4 Viewing Calculation Results

The calculation results for the slice data, peak table, average molecular weight table, and RT/MW range table can be checked.

**1** **Click the appropriate item from the [View] menu.**




**2** **Click the appropriate tab in the [Result Display] screen to check the contents.**



# 2.9 Comparing GPC Data

You can overlay multiple results of GPC molecular weight calculation in one view, and also perform the statistical calculation.

## 2.9.1 Displaying the [GPC Data Comparison] Window

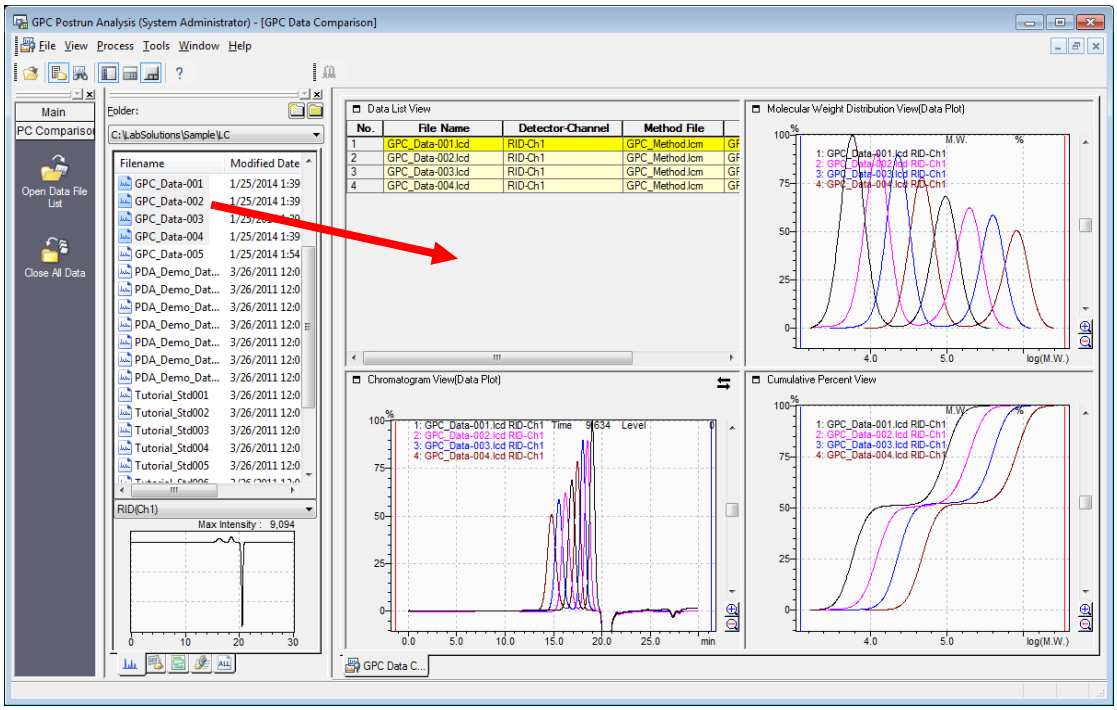
**1** **Click** 

**(GPC Data Comparison) from the [Main] assistant bar in the [GPC Postrun] program.**


**NOTE**

See "5 GPC Data Comparison" for details on the [GPC Data Comparison] window.

**2** **Drag and drop data files to compare from Data Explorer to the [GPC Data Comparison] window view.**




The chromatogams and molecular weight distribution curves appear.

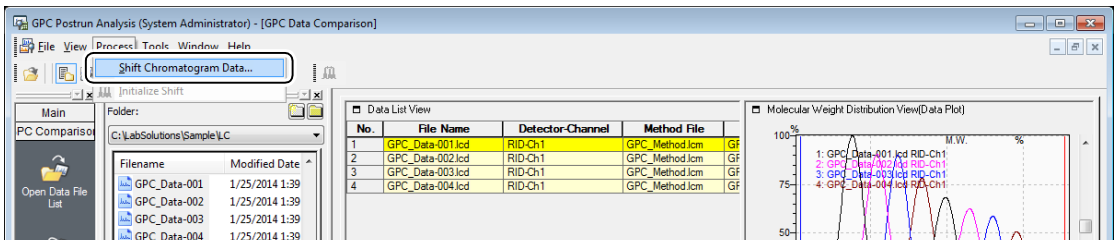
**NOTE**

When different channels are used for GPC calculation in the drag-and-dropped files, the data file list appears so that you can select a detector channel.

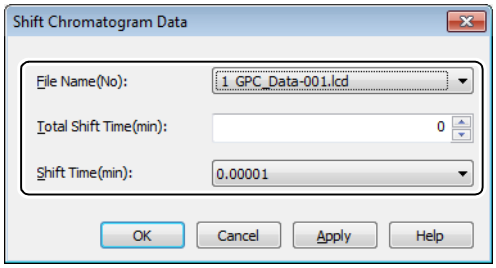
## ■ Shifting Chromatograms

As you shift chromatograms, the molecular weight distribution curve and the integrated molecular weight distribution curve shift accordingly.

**1** **Click [Shift Chromatogram Data] from the [Process] menu.**



**2** **Configure the settings.**



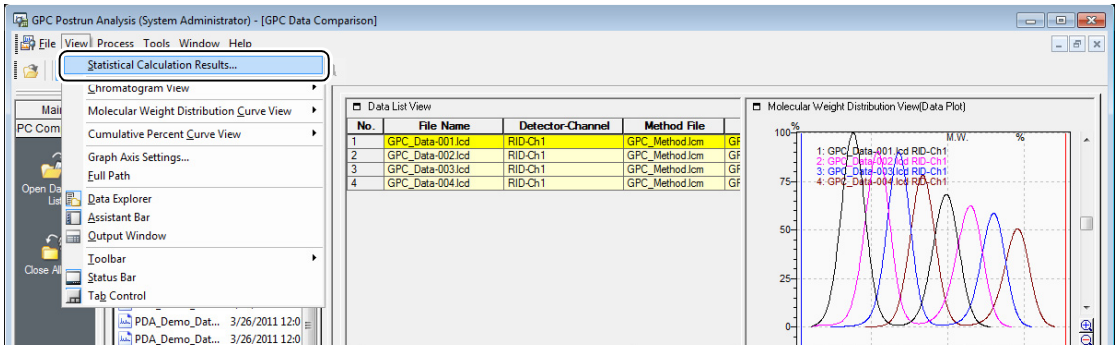

**3** **Click [OK].**

**NOTE**

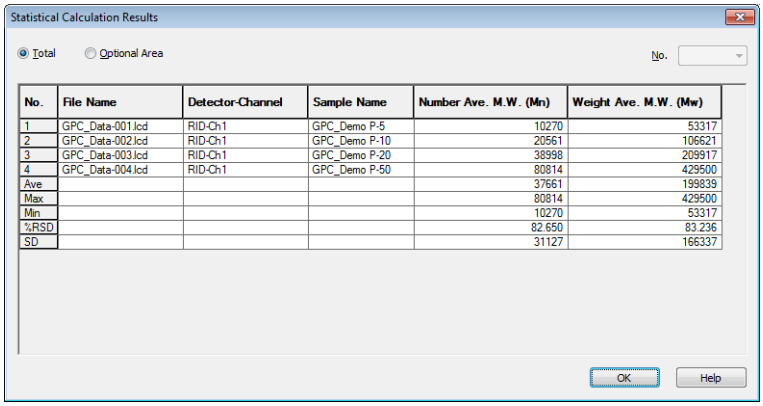
Chromatograms can be shifted as follows: Select the target data in the data list view, click (Move Left/Right) in the chromatogram view, then drag the chromatogram.

## ■ Statistical Calculation Results

**1** **Select [Statistical Calculation Results] from the [View] menu.**




The [Statistical Calculation Result] screen appears.




| No. | File Name | Detector-Channel | Sample Name | Number Ave. M.W. (Mn) | Weight Ave. M.W. (Mw) |
|---|---|---|---|---|---|
| 1 | GPC_Data-001.lcd | RID-Ch1 | GPC_Demo P-5 | 10270 | 53317 |
| 2 | GPC_Data-002.lcd | RID-Ch1 | GPC_Demo P-10 | 20561 | 106621 |
| 3 | GPC_Data-003.lcd | RID-Ch1 | GPC_Demo P-20 | 38998 | 209917 |
| 4 | GPC_Data-004.lcd | RID-Ch1 | GPC_Demo P-50 | 80814 | 429500 |
| Ave | | | | 37661 | 199839 |
| Max | | | | 80814 | 429500 |
| Min | | | | 10270 | 53317 |
| %RSD | | | | 82.650 | 83.236 |
| SD | | | | 31127 | 166337 |

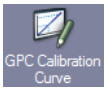
# 3 Generating Calibration Curves

Calibration curves are registered in a method file by detector or channel. The molecular weight is calculated besed on the eluent volume of analysis sample by a formula using the eluent volume and the molecular weight of the standard sample.

To create calibration curves, check the [GPC Calculation] box on the [GPC Calculation] tab of the [Data Processing Parameters] window.



## 3.1 Displaying the [GPC Calibration Curve] Window

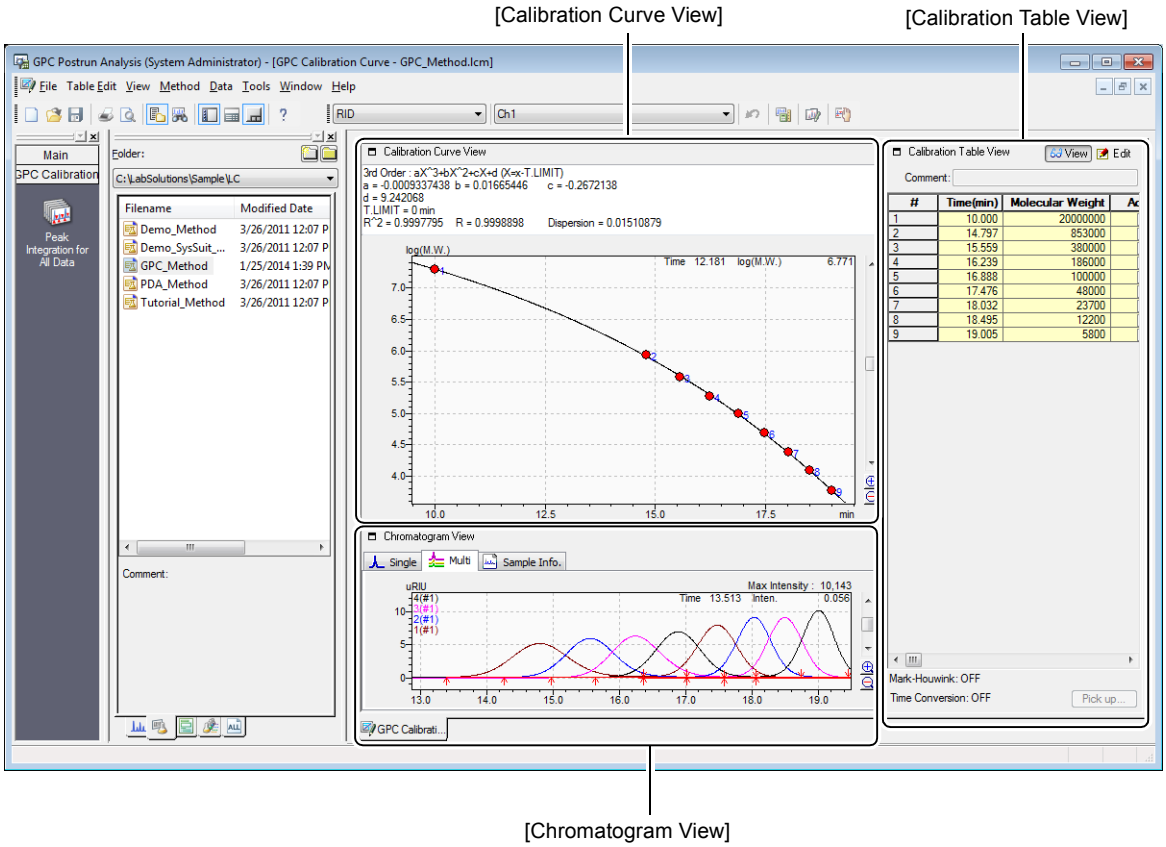
**1** **Click** 

**(GPC Calibration Curve) in the [Main] assistant bar of the [GPC Postrun] program.**


The [GPC Calibration Curve] window appears.

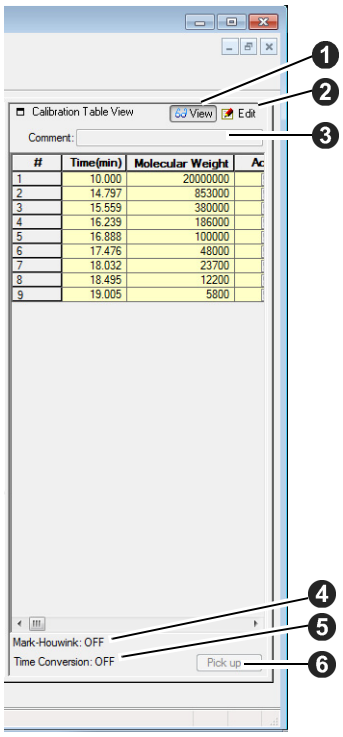
# 3.2 Using and Viewing the [GPC Calibration Curve] Window

The [GPC Calibration Curve] window has [Calibration Curve View], [Chromatogram View], and [Calibration Table View]. (The areas sectioned by splitters (frames) are called "Views". You can customize the layout and adjust the display area by dragging the splitters.)



# 3.3 Calibration Table View

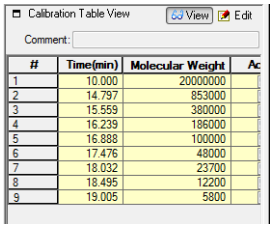
In this view, you can set information about calibration points for creating a calibration curve.




| No. | Description |
|---|---|
| ❶ | Click this to switch the calibration table into the view mode. |
| ❷ | Click this to switch the calibration table into the edit mode. |
| ❸ | Enter comments for the calibration curve. You can enter up to 64 characters. |
| ❹ | Displays the setting of Mark Houwink conversion that is set in the data analysis parameters. |
| ❺ | Displays the setting of time conversion that is set in the data analysis parameters. |
| ❻ | Click this to import the peak data of the chromatogram displayed in the Chromatogram View into the calibration table. |

## 3.3.1 Calibration Table

A calibration table displays information of calibration points in the table format. It can be entered and modified only in the edit mode. The calibration point information includes the following items.




**NOTE**

If an item is not displayed in the table, right-click on [Calibration Table], click [Table Style] from the menu, and set [Display Items].

| Name | Description |
|---|---|
| # | Displays the numbers (1 - 64). |
| Time (min.) | Enter the time of a calibration point (peak position). The value larger than the filtration limit time should be entered. Enter the time after conversion when the time conversion is enabled. |
| Molecular Weight | Enter the molecular weight of a calibration point (peak position). Enter the molecular weight after the conversion when the Mark Houwink conversion is enabled. |
| Active | Check this to make the calibration point active. If unchecked, the calibration point is not used to calculate a calibration curve, and it is not displayed on the calibration curve graph in the calibration curve view. |
| Virtual | Check this to make the calibration point virtual. Virtual points are used as a supplement when a calibration curve cannot be properly calculated using only the peak data. |
| Weight | Select the weight from among [1000], [100], [10], [1], [1/10], [1/100], and [1/1000]. This can be entered when the [Weight] box is checked in the [Calibration Curve] tab of the [Data Processing Parameters] screen. |
| Error (%) | Displays errors between the calculated value of the calibration curve and the molecular weight. An error is calculated by the following formula.<br>Error = (Molecular Weight - Calculated Value of Calibration Curve) * 100 / Molecular Weight |
| The following items display information about the peaks when the peak data is picked up from a chromatogram. Values cannot be entered manually to these items in the table. [-] is displayed unless peak data is picked up. | |
| Peak# | Displays the peak numbers in a data file from which the time information is picked up. |
| Acquired by | Displays who acquired the data file from which the time information is picked up. |
| Date Acquired | Displays the data acquired date of the data file from which the time information is picked up. |
| Time Acquired | Displays the data acquired time of the data file from which the time information is picked up. |
| Sample Name | Displays [Sample Name] of the data file from which the time information is picked up. |
| Sample ID | Displays [Sample ID] of the data file from which the time information is picked up. |
| Tray Name | Displays [Tray Name] of the data file from which the time information is picked up. |
| Vial Number | Displays [Vial Number] of the data file from which the time information is picked up. |
| Data File | Displays [Data File Name] of the data file from which the time information is picked up. |
| Original Data File (Full Path) | Displays [Original Data File] of the data file from which the time information is picked up. |
| Original Method File (Full Path) | Displays [Original Method File] of the data file from which the time information is picked up. |
| Background Data File | Displays [Background Data File] of the data file from which the time information is picked up. |
| Report Format File | Displays [Report Format File] of the data file from which the time information is picked up. |
| Original Batch File (Full Path) | Displays [Original Batch File] of the data file from which the time information is picked up. |
| Description | Displays [Description] of the data file from which the time information is picked up. |
| Processed by | Displays [Processed by] of the data file from which the time information is picked up. |
| Date Processed | Displays [Date Processed] of the data file from which the time information is picked up. |
| Time Processed | Displays [Time Processed] of the data file from which the time information is picked up. |

**NOTE**

When generating a calibration curve with chain lengths, enter chain lengths for molecular weights, and set the Q factor correctly. When generating a calibration curve with molecular weights, set the Q factor to 1 (the default value).

**Reference**

"4.4.3 Setting Data Analysis Parameters", "■ The Use of the Q Factor"

## ■ Pop-up Menu

The following menus are displayed when right-clicking on the calibration table view. Displayed menus differ when [Calibration Table View] is in the view or edit mode. Unavailable menu items are grayed.

### In the view mode

| Name | Description |
|---|---|
| Copy | Copies the selected cells into the clipboard. |
| Copy Entire Table | Copies the entire table into the clipboard. |
| Select All | Selects the entire table. |
| View Mode | A check is displayed in front because the screen is in [View Mode]. |
| Edit Mode | Switches to the edit mode. |
| Export Calibration Table | Outputs the calibration table into an ASCII file. |
| Table Style | Allows setting the table style. |

### In the edit mode

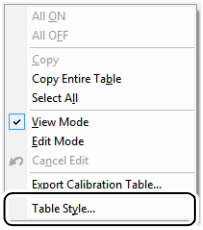
The different menu items from the view mode are described.

| Name | Description |
|---|---|
| Pickup Peak Data | Picks up retention time information from the data file into the calibration table. |
| All ON | When the selected column is Active or Virtual, all the cells of that column are checked. |
| All OFF | When the selected column contains checkboxes, all the cells are unchecked. |
| Cut | Cuts the selected cells into clipboard. |
| Copy | Copies the selected cells into the clipboard. |
| Paste | Pastes the contents of the clipboard. |
| Clear | Clears the selected cells. |
| Copy Entire Table | Copies the entire table into the clipboard. |
| Select All | Selects the entire table. |
| Add Row | Adds a row at the end of the table. |
| Insert Row | Inserts a row into the current cursor position. |
| Delete Row | Deletes the selected rows. |
| Sort by Save Time | Sorts the table contents by save time. |
| Data Analysis Parameters | Displays the [Data Processing Parameters] dialog. |
| View Mode | Switches to the view mode. |
| Edit Mode | This item is preceded by a check mark because you are in the edit mode. |
| Cancel Edit | Cancels the edit and switches to the view mode. |
| Import Calibration Table | Imports calibration points from an ASCII file into the calibration table. |
| Export Calibration Table | Outputs the calibration table to an ASCII file. |
| Table Style | Allows you to configure the table style. |

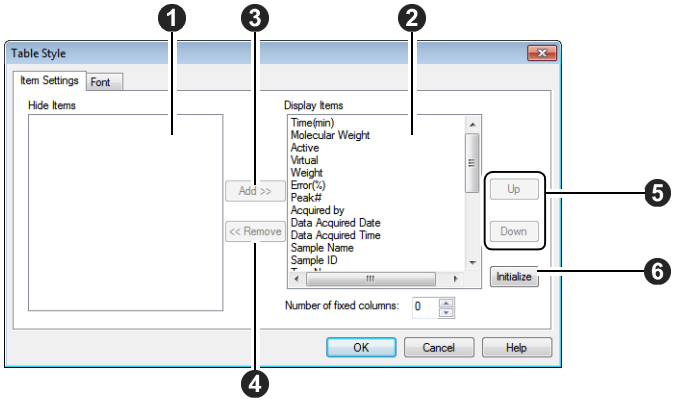
## ■ Display Items and Their Order in the Calibration Table

The display items and the font of the calibration table can be set.

**1** **Right-click in the calibration table view and click [Table Style] from the menu.**

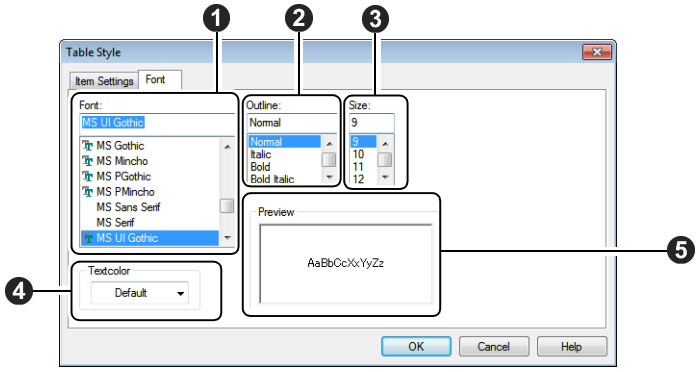


## 2 Click the [Item Settings] tab, and set display items and their order.




| No. | Description |
|---|---|
| ❶ | Shows items not displayed on the calibration table. |
| ❷ | Shows items displayed on the calibration table. Items displayed here are displayed in the calibration table starting from the left. |
| ❸ | Moves items selected in [Hide Items] to [Display Items]. |
| ❹ | Moves items selected in [Display Items] to [Hide Items]. |
| ❺ | Moves the selected [Display Items] up or down. |
| ❻ | Returns to the default for [Display Items] and [Hide Items]. |

## 3 Click the [Font] tab and set font.




| No. | Description |
|---|---|
| ❶ | Enter or select a font name. |
| ❷ | Enter or select a style. |
| ❸ | Enter or select a size. |
| ❹ | Select the text color. |
| ❺ | Displays a text preview based on the configured settings. |

## 4 Click [OK].

## 3.3.2 Importing Calibration Points from an ASCII File

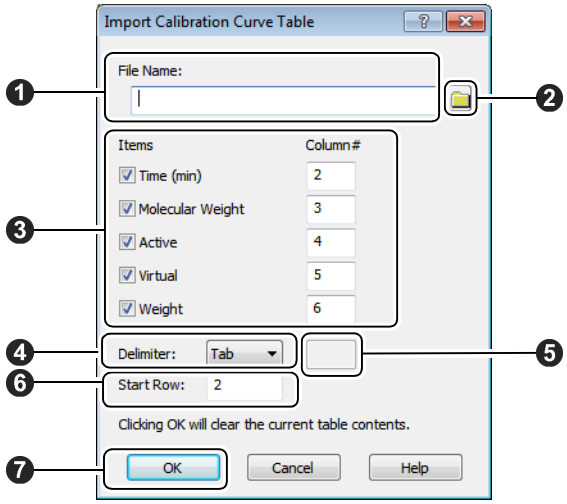
You can import information including molecular weight and retention time into a calibration table from a file that are saved in the ASCII format (such as the CSV format).

**1** **Click [Edit] in the calibration table view.**

**2** **Right-click in the calibration table view and click [Import Calibration Table] from the menu.**

The [Import Calibration Curve Table] screen appears.

**3** **Specify the input file name and items to be imported.**




| No. | Description |
|---|---|
| ❶ | Enter the file name to be imported. |
| ❷ | Click this to display the file selection screen. |
| ❸ | Select items to be imported. Check the items to be imported from ASCII files and enter the column number. |
| ❹ | Select a delimiter for items in the input file. |
| ❺ | Enter a delimiter when [Other] is selected for [Delimiter]. |
| ❻ | Specify the row number of the file to be imported where data start. |
| ❼ | Click [OK] to import the specified file into [Calibration Table] using above settings. |

**4** **Click [OK].**

Calibration points are imported from the ASCII file based on the specified setting.

**NOTE**

The current content of [Calibration Table] is replaced with the content of the ASCII file.

## 3.3.3 Exporting Calibration Table into an ASCII File

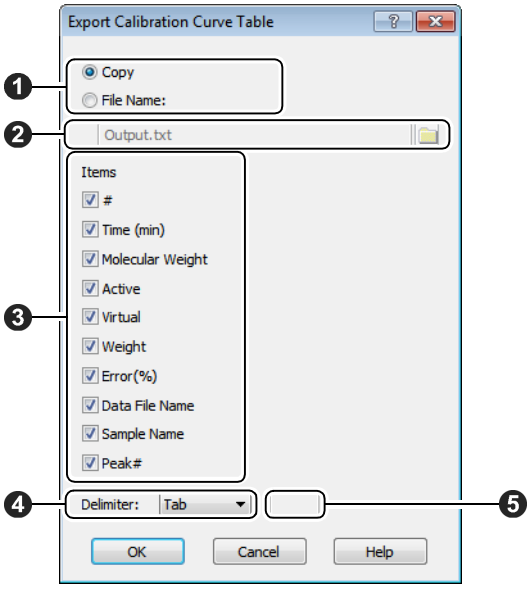
You can output the Items that have to be repeatedly entered, such as molecular weight, into an ASCII file from the calibration table.

**1** **Click [Edit] in the calibration table view.**

**2** **Right-click in the calibration table view and click [Export Calibration Table] from the menu.**

The [Export Calibration Curve Table] screen appears.

**3** **Set the name and items for the output file.**




| No. | Description |
|---|---|
| ❶ | Select where to output. |
| ❷ | Enter an output file name when you selected [File Name]. |
| ❸ | Select items to be exported. |
| ❹ | Select a delimiter for items in the output file. |
| ❺ | Enter a delimiter when [Other] is selected for [Delimiter]. |

**4** **Specify an output file name and items to be output, and click [OK].**

Data is output into an ASCII file from the calibration table based on the specified setting.

**NOTE**

Titles of the specified items are output in the first row. Values for Active and Virtual are in the ON/OFF format.

## 3.3.4 Picking Up Time of Peak Data from Chromatogram

You can pick up the time of the peak data in a data file into [Calibration Table].

1. **Click [Edit] in the calibration table view.**
2. **Click [Pick up] in [Calibration Table View] in [Edit] mode in the chromatogram view.**
   The time of the peak data in a data file is copied into [Calibration Table].

**Reference**

"2.5.4 Picking up Retention Time"



## 3.3.5 Calculating Calibration Curve

When you switch the calibration table from the edit mode to the view mode, the content of the calibration table is confirmed, and then the calibration curve is calculated.
The data is sorted by time, and then the calibration curve information is calculated.

1. **Set information required for calculation of the calibration curve in the [Data Processing Parameters] screen.**

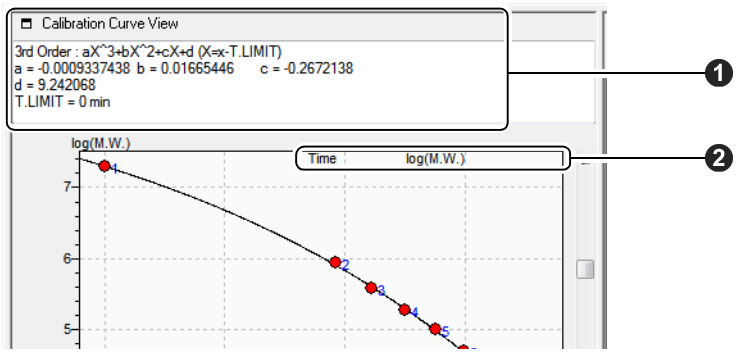
**Reference**

"3.7 Data analysis parameter"

2. **Click [Edit] in the calibration table view.**
3. **Enter [Time], [Molecular Weight], [Active], [Virtual], and [Weight] in the calibration table.**
4. **Click [View] in the calibration table view.**
   The calibration table is confirmed, and the calibration curve information is calculated.

# 3.4 Calibration Curve View

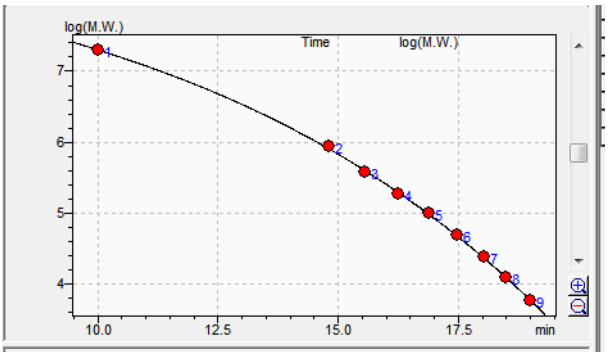
Displays calibration curves registered in method files.




| No. | Description |
|---|---|
| ❶ | Displays factors and identity ($R^2$, R, Dispersion) of the calibration curve. |
| ❷ | Displays the time or elution volume and log(M.W.) of the coordinates in real time when placing the mouse on the calibration curve graph.<br>The time and the elution volume can be switched by the axis configuration of the graph. |

## 3.4.1 Calibration Curve Graph

A calibration curve is displayed in this graph.




Calibration curve graph legend
●: Calibration point
▲: Calibration point (Average value [Note])
■: Calibration point (Virtual)
Filtration limit value line (Default shown in blue)

**NOTE**

This is a calibration point of the molecular weight of which the average is calculated when [Time is averaged for the same M.W.] on the [GPC Calibration Curve] tab in the [Data Analysis Parameters] screen is checked.

**Zooming in graph**

When specifying a range by dragging a square on the calibration curve graph, the graph is zoomed in according to the specified range.

**Adding virtual points**

Double-click on the calibration curve graph to register the coordinate in the calibration table as a virtual point.

**Right-click menu**

Right-click on the calibration curve graph to display the menu.

| Name | Description |
|---|---|
| Undo Zoom | Cancels the previous zooming action. |
| Redo Zoom | Zoom again. |
| Initialize Zoom | Returns the display to the initial state. |
| Data Processing Parameters | Displays the calibration curve tab of the [Data Processing Parameters] screen. |
| Copy | Copies the calibration curve graph image to the clipboard. |
| Scale Settings | Displays the [Scale Setting] screen. |
| Properties | Sets display attributes such as graph color. |

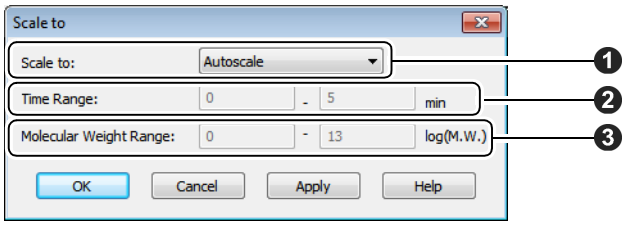


## ■ Setting the Scale of the Graph

Set the scale of the calibration curve graph.

**1** **Right-click on the calibration curve graph and click [Scale Settings] from the menu.**

**2** **Configure the settings.**

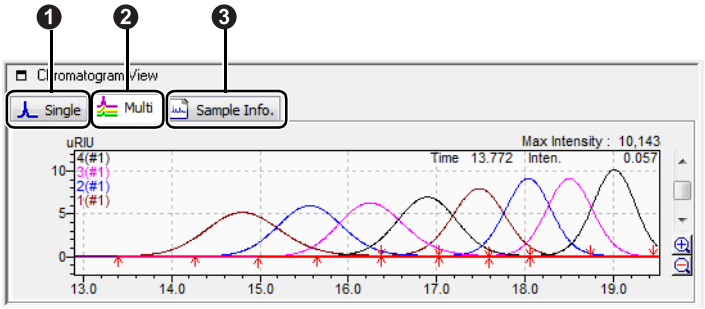



| No. | Description |
|---|---|
| ❶ | Select between [Autoscale] and [User Defined] for the scale of the calibration curve graph. |
| ❷ | Enter the X axis range of the calibration curve graph. |
| ❸ | Enter the Y axis range of the calibration curve graph. |

**3** **Click [OK].**

# 3.5 Chromatogram View

This view displays chromatograms of data files used to create a calibration curve. The data files are registered in the data file list. The chromatogram view has the following three tabs.



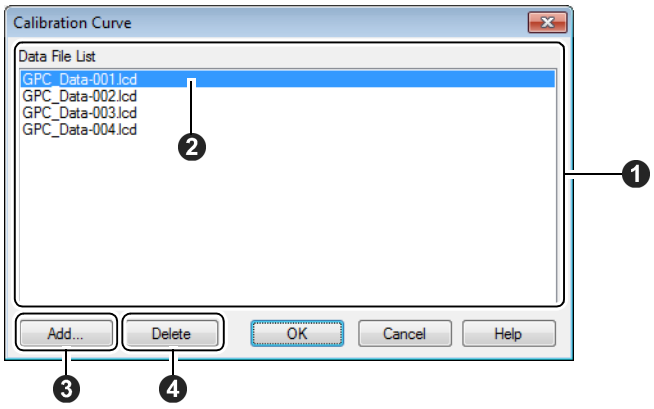

| No. | Description |
|---|---|
| ❶ | Displays a chromatogram of the selected data. |
| ❷ | Overlays all chromatograms in the data file list. |
| ❸ | Displays sample information of the selected data. |

## 3.5.1 Data File List

Data files used when creating calibration curves are displayed in a list. Data files can be added or deleted.

**1** **Right-click on the chromatogram and click [Data File List] from the menu.**

**2** **Configure the settings.**




| No. | Description |
|---|---|
| ❶ | Lists the data files registered in the method file. |
| ❷ | Click a file name to make the file selected. |
| ❸ | Adding a data file. |
| ❹ | Click this button to delete the registration of the data file selected in the data file list. |

**3** **Click [OK].**

**NOTE**

Select [View] - [Full Path] from the menu on the [Calibration Curve] screen to display file names in full path.

## ■ Adding Data Files

Data files to create the calibration curve are added in the data file list.

**1** **Click [Add] on the [Calibration Curve] screen.**

The [Add Data File] screen appears.

**2** **Select data file to be added, and click [Open].**

The selected data file is added to the data file list.

**NOTE**

Data files can be added if you drag-and-drop them from Data Explorer into the chromatogram view.

## ■ Deleting Data Files

Data files to create the calibration curve are deleted from the data file list.

**1** **Select a data file to be deleted from the data file list.**

**2** **Click [Delete].**

The message [Do you remove data file from data file list?] appears.

**3** **Click [OK].**

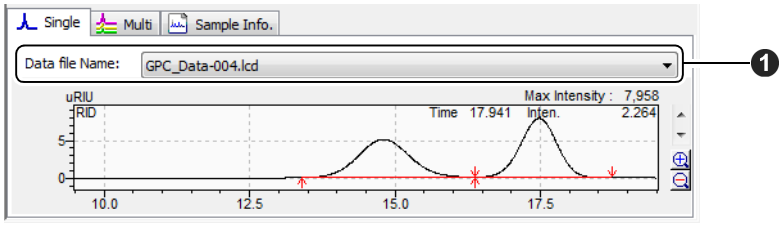
The selected data file is deleted from the data file list.

**NOTE**

When swiching file name display, adding or deleting data files, clicking [OK] and closing the [Calibration Curve] screen reflect the change.

## 3.5.2 [Single] Tab

This tab displays an entire chromatogram of the data file selected from the data files used to create the calibration curve.




| No. | Description |
|---|---|
| ❶ | Select a data file to display. |

### ■ Zooming the Graph

When specifying a range by dragging a square on the chromatogram, the graph is zoomed in according to the specified range.

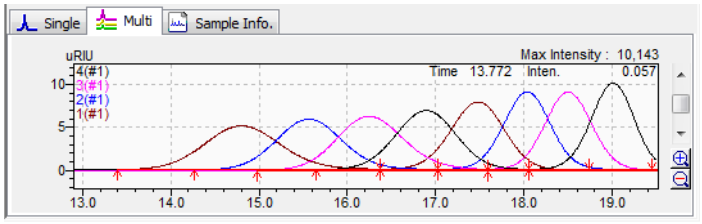
### ■ Displaying the Right-click Menu

Right-click on the chromatogram to display the menu.
The displayed menu is as follows:

| Name | Description |
|---|---|
| Undo Zoom | Cancels the previous zooming action. |
| Redo Zoom | Zoom again. |
| Initialize Zoom | Returns the display to the initial state. |
| Peak Table | Displays the peak table of the selected data file. |
| Manual Integration Bar | Displays or hides the manual peak integration bar. |
| Data File List | Displays the [Calibration Curve] screen. |
| Copy | Copies the chromatogram image to the clipboard. |
| Properties | Sets display attributes such as graph color. |

## 3.5.3 [Multi] Tab

Multiple data files registered in the data file list are overlayed in one graph.




### ■ Zooming the Graph

When specifying a range with the mouse on the chromatogram, graph is zoomed in according to the specified range.

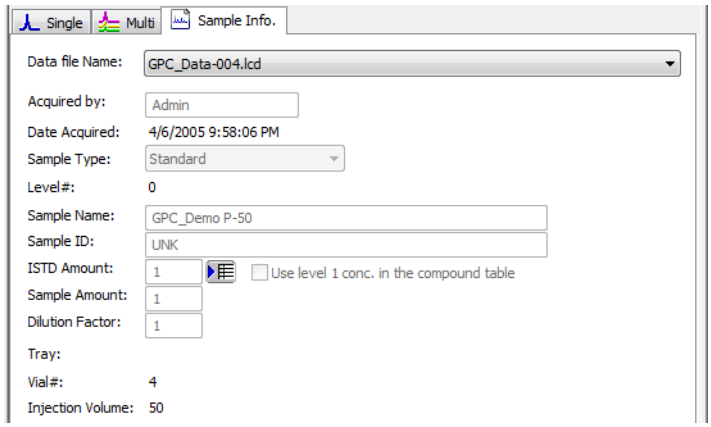
### ■ Displaying the Right-click Menu

Right-click on the chromatogram to display the menu.
The displayed menu is as follows:

| Name | Description |
|---|---|
| Undo Zoom | Cancels the previous zooming action. |
| Redo Zoom | Zoom again. |
| Initialize Zoom | Returns the display to the initial state. |
| Base Shift | Displays or hides the base shift. |
| Data File List | Displays the [Calibration Curve] screen. |
| Copy | Copies the chromatogram image to the clipboard. |
| Properties | Sets display attributes such as graph color. |

## 3.5.4 [Sample Info.] Tab

Sample information of data files is displayed.

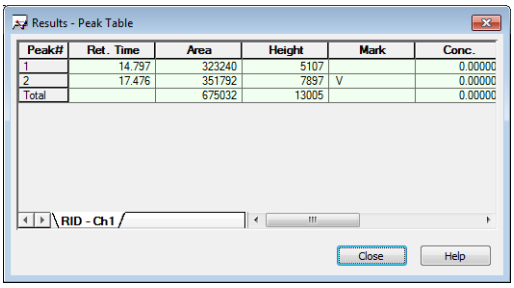


# 3.6 Peak table

Peak table of the selected data in the data file list is displayed.

**1** **Right-click on the chromatogram and click [Peak Table] from the menu.**

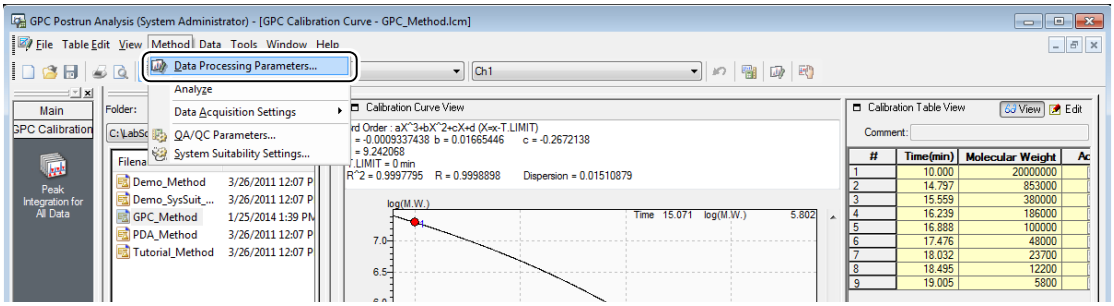
The peak table is displayed.



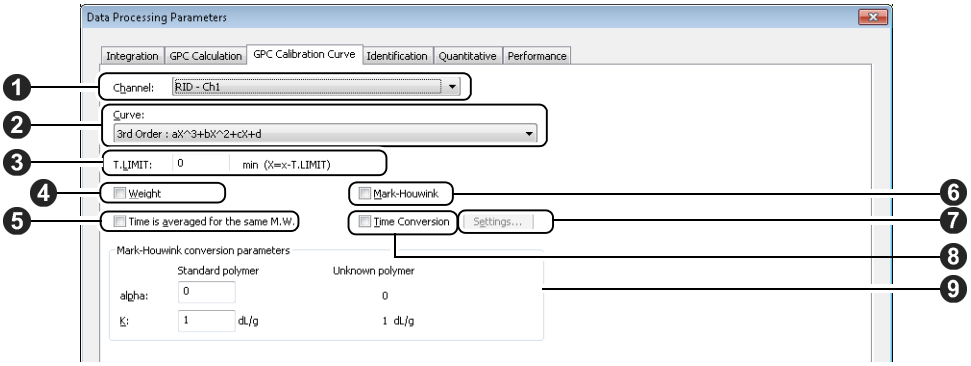

# 3.7 Data analysis parameter

Parameters related to calculations of calibration curve or molecular weight are set.

**1** **Click [Data Processing Parameters] from the [Method] menu.**




**2** **Click the [GPC Calibration Curve] tab, and configure the settings.**



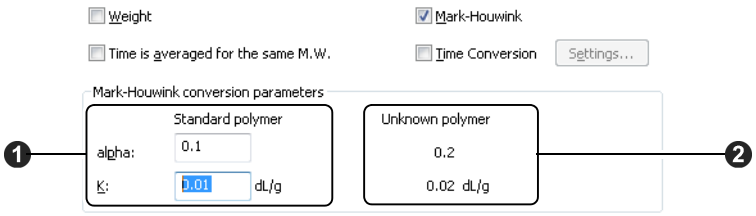
| No. | Description |
|---|---|
| ❶ | Select a channel to set the calibration curve information. |
| ❷ | Select a calibration curve type. |
| ❸ | Enter the filtration limit time. |
| ❹ | Check this box to enable the weight setting so that calibration curves are weighted in the calculation. |
| ❺ | Check this box to calculate an average value of times of calibration points having the same molecular weight in the calibration table and treat it as a single calibration point. |
| ❻ | Check this box to enable the Mark-Houwink conversion. |
| ❼ | Click this button to open the setting screen for the time conversion. |
| ❽ | Check this box to enable the time conversion. |
| ❾ | Set parameters used in Mark-Houwink conversion. |

## ■ Setting Mark Houwink Conversion



**1** **Check [Mark-Houwink] on the [GPC Calibration Curve] tab.**

**2** **Set the [Mark-Houwink Conversion Parameters] fields.**




| No. | Description |
|---|---|
| ❶ | Set the alpha and K of the standard polymer |
| ❷ | Displays the alpha and K of the unknown polymer.<br>(Values set in [GPC Calculation] tab in Data Processing Parameters are fixedly displayed.) |

**3** **Click [OK].**

**NOTE**

Mark Houwink conversion is performed with the following formula.

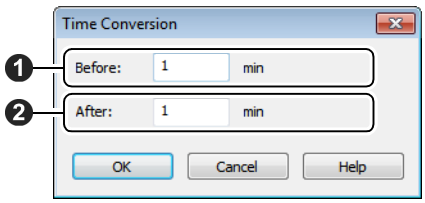
$\log Mb = (1 / (1 + \alpha b)) \log (Ka / Kb) + ((1 + \alpha a) / (1 + \alpha b)) \log Ma$

Ma: Molecular weight of the standard polymer
Mb: Molecular weight of the unknown polymer
$\alpha a$: Alpha of the standard polymer
$\alpha b$: Alpha of the unknown polymer
Ka : K of the standard polymer
Kb : K of the unknown polymer

## ■ Setting Time Conversion

**1** **Check [Time Conversion] in the [GPC Calibration Curve] tab, and click [Settings].**

**2** **Configure the settings.**




| No. | Description |
|---|---|
| ❶ | Enter time before conversion. |
| ❷ | Enter time after conversion. |

**3** **Click [OK].**

**NOTE**

Time conversion is performed with the following formula.
RTc = (time after conversion / time before conversion) RT

# 4 GPC Calculation

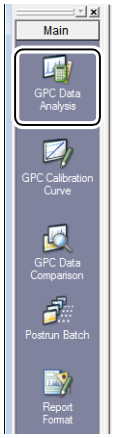
This chapter explains the GPC calculation.

In the GPC calculation, a molecular weight distribution and an average molecular weight of samples are calculated from acquired chromatograms and calibration curves.

## 4.1 Displaying the [GPC Data Analysis] Window

**1** **Click the** 

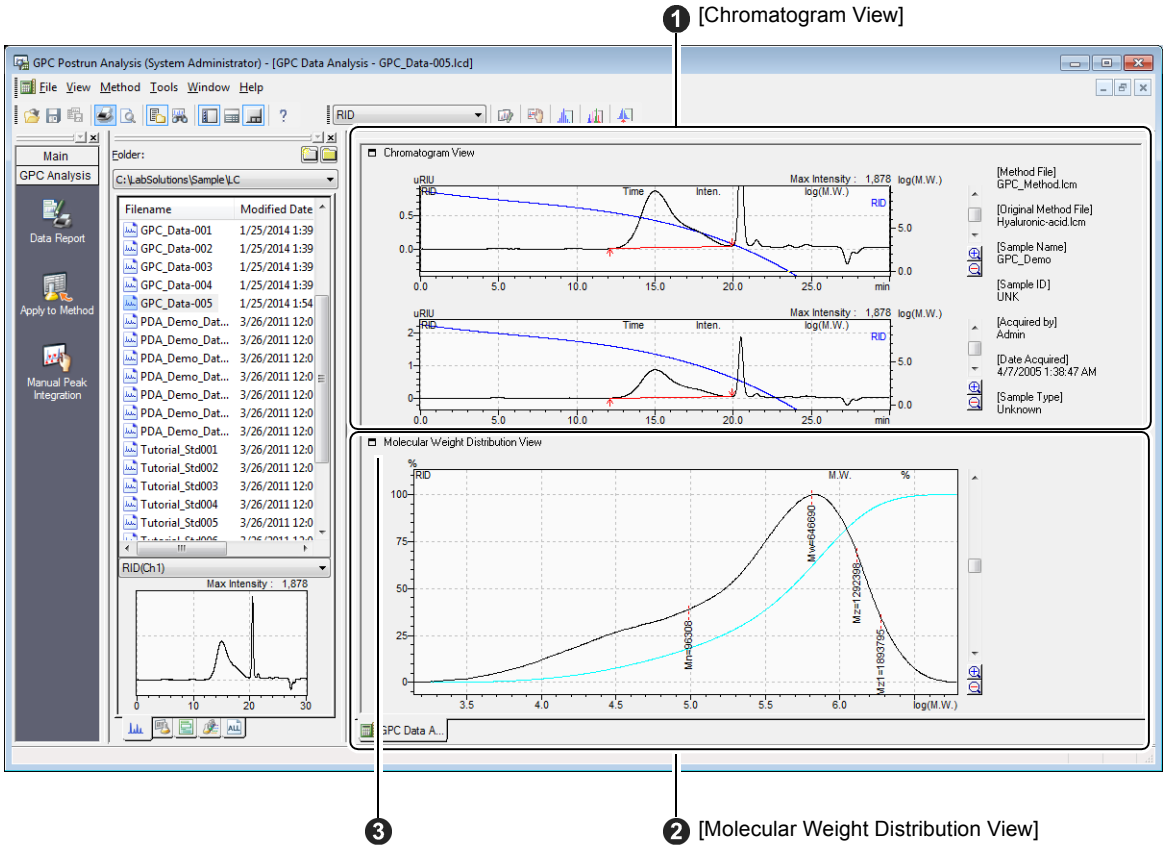
**(GPC Data Analysis) icon in the [Main] assistant bar of the [GPC Postrun] program.**




The [GPC Data Analysis] window appears.

# 4.2 Using and Viewing the [GPC Data Analysis] Window

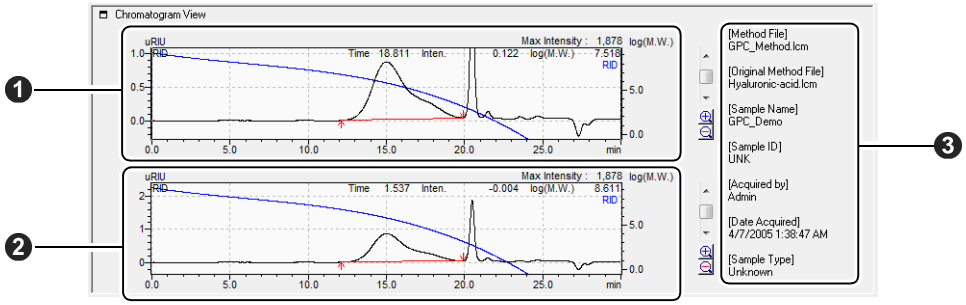
The [GPC Data Analysis] window has [Chromatogram View] and [Molecular Weight Distribution View].




| No. | Description |
|---|---|
| ❶ | Chromatograms and calibration curves are displayed. |
| ❷ | Differential and integral molecular weight curves calculated from the chromatogram and the calibration curve are displayed. |
| ❸ | Click this button (change size button) to switch between the full screen and standard displays. |

# 4.3 Chromatogram View

In [Chromatogram View], the chromatogram and the calibration curve are displayed in layers.




| No. | Description |
|---|---|
| ❶ | Displays the full chromatogram. An area to be zoomed in can be specified by dragging a mouse. |
| ❷ | Zooms into a specified area on the chromatogram. An area to be zoomed into can be specified by dragging a mouse. |
| ❸ | Displays the sample information. |

### ■ Right-click Menu

When right-clicking on the chromatogram, a menu appears. You can select various operations and settings for the chromatogram from the displayed menu.

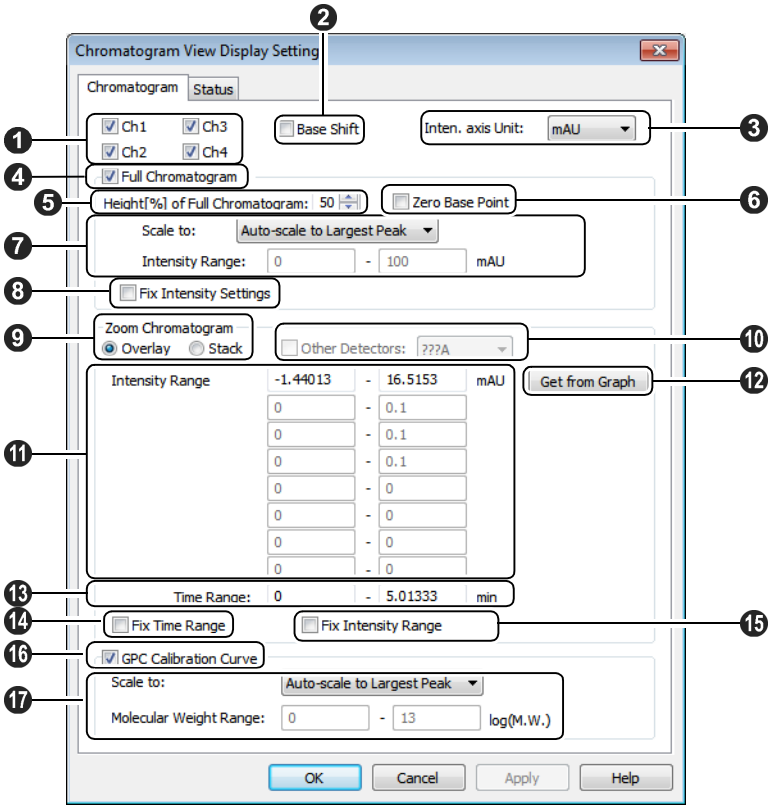
## 4.3.1 Display Settings of Chromatograms

### ■ Display of Chromatograms

Set the display of the chromatograph.

**1** **Right-click on the chromatogram, and click [Display Settings] from the displayed menu.**

## 2 Click the [Chromatogram] tab and set the display of the chromatogram.




| No. | Description |
|---|---|
| ❶ | Displays or hides Ch1 through Ch4 chromatograms when the detector is of the dual mode or the PDA detector. |
| ❷ | Displays or hides the base shift. |
| ❸ | Set the intensity axis unit. The contents and default values displayed in the list vary according to the detector. |
| ❹ | Displays or hides the full chromatogram. |
| ❺ | Set the height of the full chromatogram on the screen. |
| ❻ | When checked, the chromatogram is displayed by adjusting the scale of the intensity axis to 0 V or more. |
| ❼ | Select the chromatogram scale on the intensity axis. [Auto-scale to Largest Peak] is selected initially. When selecting [User Defined], the [Intensity Range] can be set. |
| ❽ | When checked, the intensity axis range displayed for all data will be fixed to the set value. |
| ❾ | Sets the zoom chromatograms to either an overlaid display or a stacked display. |
| ❿ | Displays or hides the chromatogram of another detector. When checked, select the other detector. |
| ⓫ | Allows you to set the upper and lower limits of the intensity axis of the zoom chromatogram for each detector. |
| ⓬ | When this button is pressed, the display range of the current graph is applied to the range of the zoom chromatograms. |
| ⓭ | Set the upper and lower limits of the time axis of the zoom chromatogram. |
| ⓮ | Fixes the time axis range displayed for all data to the set value or releases it. |
| ⓯ | Fixes the intensity axis range displayed for all data to the set value or releases it. |
| ⓰ | Displays or hides the GPC calibration curve. |
| ⓱ | Select the GPC calibration curve scale on the intensity axis. When selecting [User Defined], the [Molecular Weight Range] can be set. |

**NOTE**

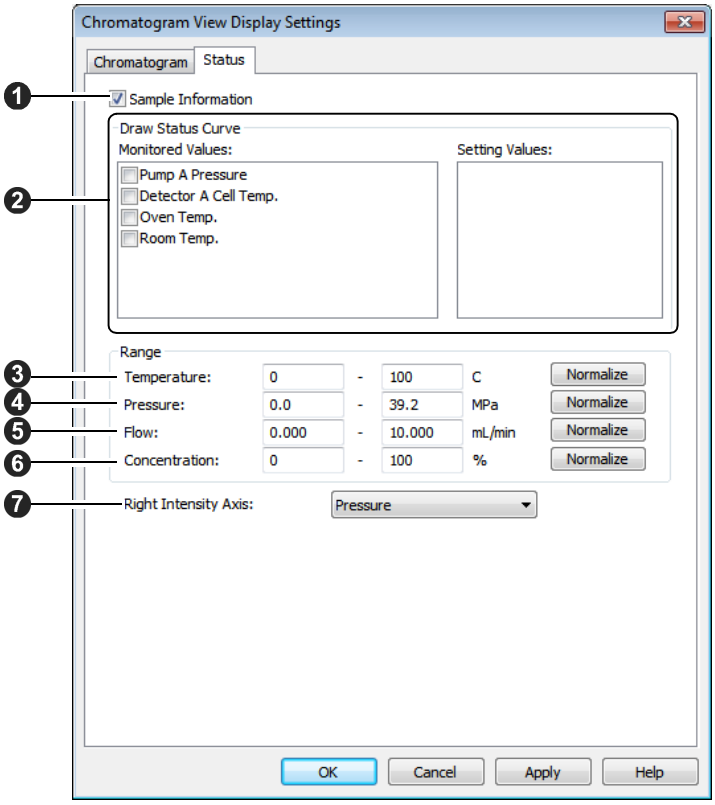
The range of the horizontal axis of the zoom chromatogram is specified with (min) when the display unit is time, and with (mL) when it is the eluent volume.

## ■ Display of Status Graphs

Sets the display of the status graphs.

**1** **Right-click on the chromatogram and click [Display Settings] from the menu.**

**2** **Click the [Status] tab, and set the display of the status graphs.**

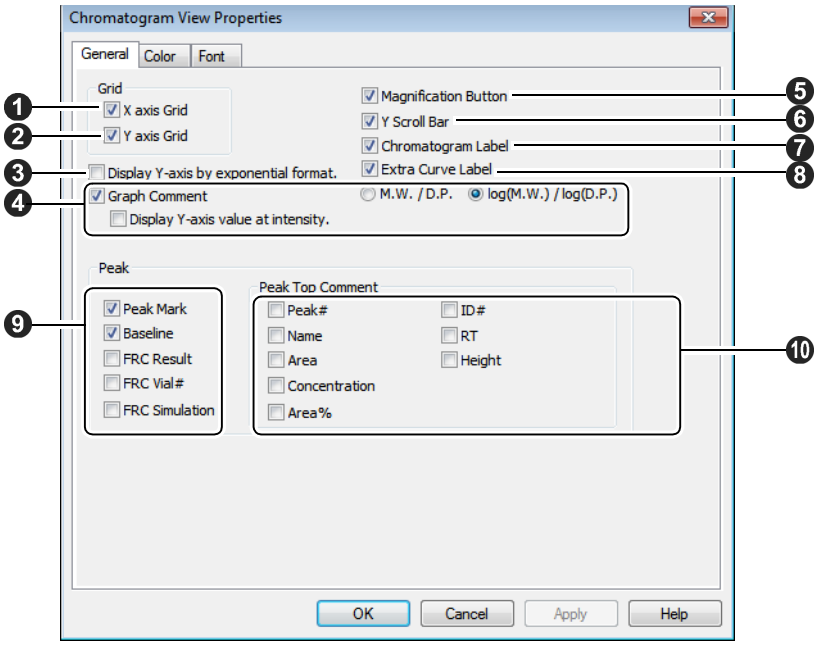



| No. | Description |
|---|---|
| ❶ | Displays or hides the sample information. |
| ❷ | Check items to draw the status curve. |
| ❸ | Set the upper and lower limits of the temperature. Click [Normalize] to set the temperature range automatically. |
| ❹ | Set the upper and lower limits of the pressure. Click [Normalize] to set the pressure range automatically. |
| ❺ | Set the upper and lower limits of the flow. Click [Normalize] to set the flow range automatically. |
| ❻ | Set the upper and lower limits of the concentration. Click [Normalize] to set the concentration range automatically. |
| ❼ | Select the unit of measure for the intensity axis on the right-hand side. |

## 4.3.2 Setting View Properties

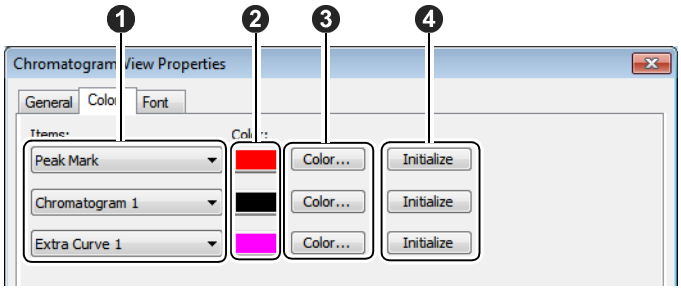
**1** **Right-click on the chromatogram and click [Graph View Properties] from the menu.**

**2** **Click the [General] tab and configure the settings.**



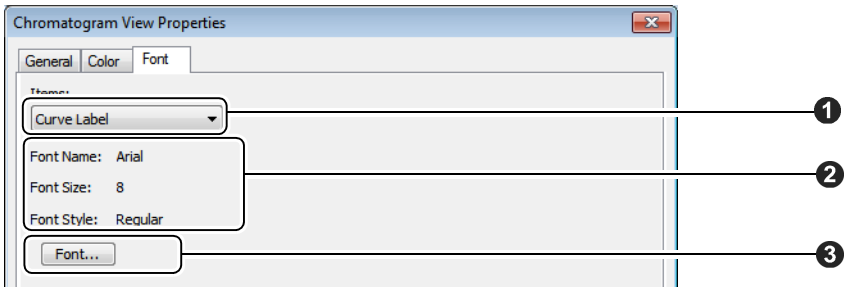

| No. | Description |
|---|---|
| ❶ | Displays or hides the X axis grid. |
| ❷ | Displays or hides the Y axis grid. |
| ❸ | Displays or hides the Y axis intensity value in the exponential format (such as x10 or x100). |
| ❹ | Displays or hides the graph comment.<br>Select either [M.W./D.P] or [log (M.W.) /log (D.P.)] for the scale display when displaying the molecular weight information (molecular weight or degree of polymerization) in a graph comment.<br>When [Show Mouse Position] is checked, the Y-axis coordinate of the mouse will be displayed in the intensity value. |
| ❺ | Displays or hides the magnification buttons (zoom-in and zoom-out). |
| ❻ | Displays or hides the Y axis scroll bar. |
| ❼ | Displays or hides the detector and channel names. |
| ❽ | Displays or hides the extra curve labels, such as of temperature and pressure. |
| ❾ | Displays or hides the peak mark, baseline, fraction collector result and simulation. |
| ❿ | Select items to display as peak top comments. |

## 3 Click the [Color] tab and configure the settings.




| No. | Description |
|---|---|
| 1 | Select a display item for color setting. |
| 2 | Displays the currently set colors. |
| 3 | Click these to set the color of the display item. |
| 4 | Click these to Initialize the color of the display item. |

## 4 Click the [Font] tab and configure the settings.




| No. | Description |
|---|---|
| 1 | Allows you to select an item for the font setting. |
| 2 | Displays the selected [Font Name], [Font Size], and [Font Style]. |
| 3 | Displays the [Font] screen for selecting the font. |

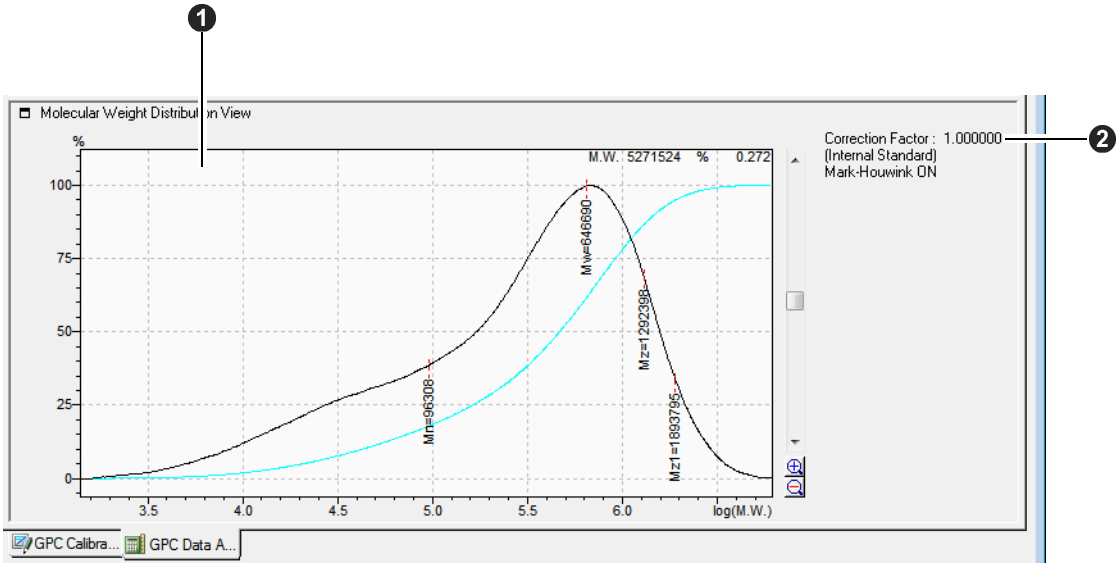
**NOTE**

The X axis of chromatogram is displayed in time (min) or eluent volume (mL) depending on the setting. The Y axis of chromatogram is displayed in log of the molecular weight (M.W.) or log of the degree of polymerization (D.P.) depending on the setting.

## 5 Click [OK].

# 4.4 Molecular Weight Distribution View

In [Molecular Weight Distribution View], the molecular weight distribution curves calculated from the chromatograms and the calibration curves are displayed. There are two types of molecular weight distribution curves: differential and integral.

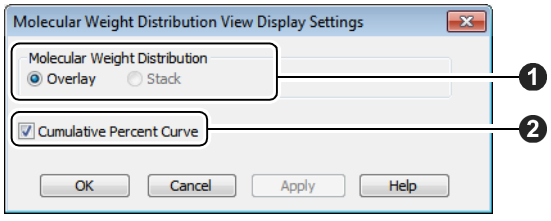



| No. | Description |
|---|---|
| 1 | Displays molecular weight distribution curves. |
| 2 | Displays the correction factor. |

## 4.4.1 Display Settings of the Molecular Weight Distribution Curves

**1** **Right-click on the molecular weight distribution curve graph and click [Display Settings] from the menu.**

**2** **Configure the settings.**



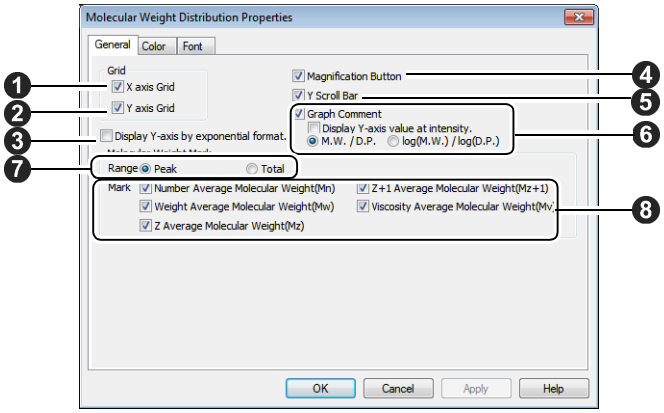

| No. | Description |
|---|---|
| 1 | Select either [Overlay] or [Stack] for the display of the molecular weight distribution graphs (differential and integral). These displays are available for multiple detectors or a detector supporting the dual mode. |
| 2 | Displays or hides the integral molecular weight distribution. |

**3** **Click [OK].**

## 4.4.2 Setting Properties of Molecular Weight Distribution Curve

**1** **Right-click on the molecular weight distribution curve graph and click [Properties] from the menu.**

**2** **Click the [General] tab and configure the settings.**




| No. | Description |
|---|---|
| ❶ | Displays or hides the X axis grid. |
| ❷ | Displays or hides the Y axis grid. |
| ❸ | Switches the display of the Y axis intensity value in the exponential format (such as x10 or x100). |
| ❹ | Displays or hides the magnification buttons (zoom-in and zoom-out). |
| ❺ | Displays or hides the Y axis scroll bar. |
| ❻ | Displays or hides the graph comment.<br>Select either [M.W./D.P] or [log (M.W.) /log (D.P.)] for the scale display when displaying the molecular weight information (molecular weight or degree of polymerization) in a graph comment.<br>When [Display Y-axis value at intensity.] is checked, the Y-axis coordinate of the mouse will be displayed in the intensity value. |
| ❼ | Select whether to display the average molecular weight mark for the entire graph or for each peak. |
| ❽ | Select the items to be displayed. |

**NOTE**

The X axis of the molecular weight distribution graph is displayed in the molecular weight log(M.W.) or the degree of polymerization log(D.P.) depending on the setting.

**3** **Click the [Color] tab and configure the settings.**

**Reference**

For details, see step 3 (P.53) in "4.3.2 Setting View Properties".

**4** **Click the [Font] tab and configure the settings.**

**Reference**

For details, see step 4 (P.53) in "4.3.2 Setting View Properties".

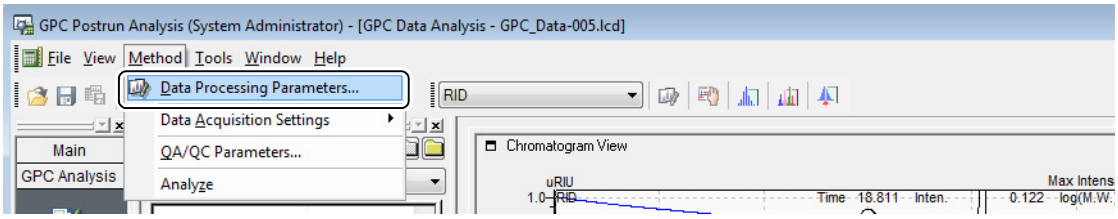
**5** **Click [OK].**

## 4.4.3 Setting Data Analysis Parameters

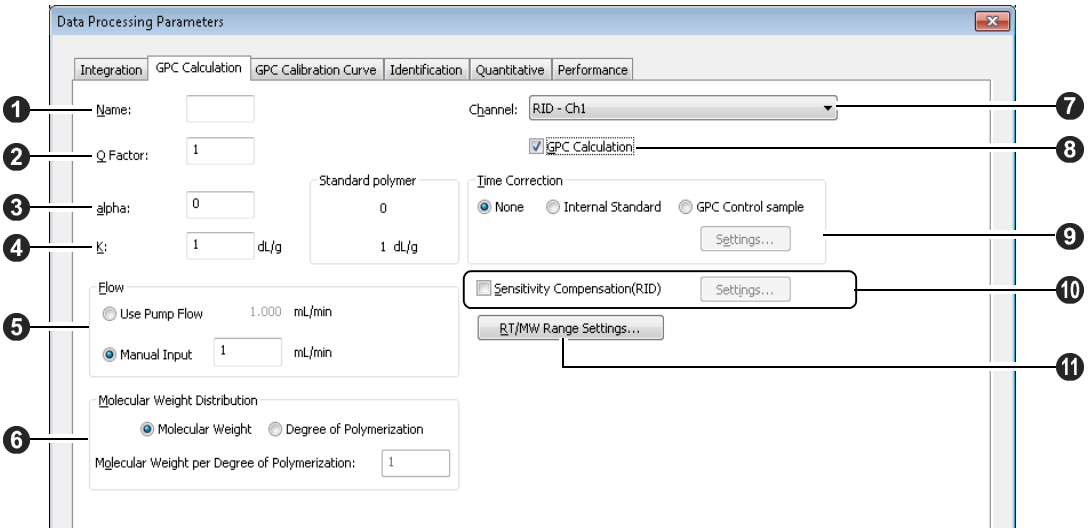
Molecular weight distribution is calculated and displayed by setting the data analysis parameters.
Set the following parameters:

- Parameters for samples (Q factor, alpha value, K value)
- Data for GPC calculation (detector, channel)
- Whether or not to perform time correction, its type and necessary factors
- Sensitivity compensation of the RI detector

### 1 Click [Data Processing Parameters] from the [Method] menu.




### 2 Click the [GPC Calculation] tab and configure the settings.




| No. | Description |
|---|---|
| ❶ | Enter the element name. Up to 64 characters can be entered. The initial value is blank. |
| ❷ | Enter the Q factor. A positive real number can be entered. The initial value is 1. |
| ❸ | Enter the alpha value used for Mark Houwink conversion, etc. The initial value is 0.<br>(Alpha to be displayed for standard polymer are those specified in the [GPC Calibration Curve] tab.) |
| ❹ | Enter the K value used for Mark Houwink conversion, etc. The initial value is 1.<br>(K to be displayed for standard polymer are those specified in the [GPC Calibration Curve] tab.) |
| ❺ | Select whether you use the pump flow or a manually input value for the flow calculation. If you use a manually input value, set the flow quantity per minute. |
| ❻ | Select the molecular weight or the degree of polymerization for the display unit of the Y axis. [Molecular weight] is selected initially. By selecting [Degree of Polymerization], you can enter the molecular weight per degree of polymerization. |
| ❼ | Select a channel of the detector. |
| ❽ | Specify whether to perform the GPC calculation for each channel. |
| ❾ | Select a method of the time correction. [None] is selected initially. |
| ❿ | Specify whether to perform the sensitivity compensation of the RI detector. When performing compensation, click [Settings], and set the sensitivity compensation of the RI detector. |
| ⓫ | Click this to display the [RT/MW Range Setting] screen. Enter the start and end time. |

## ■ The Use of the Q Factor

- What is Q factor?

  In GPC, components are separated based on the molecular size and a relationship between the elution position and the molecular size is set by a formula. When equations differ between the standard sample (from which a calibration curve is created) and the unknown sample (for which you want to find out the molecular weight), correction is required to obtain accurate molecular weight. The Q factor is used in such case.

- How to use the Q factor

  Q factor is "molecular weight of each monomer divided by the stretched chain length of each monomer". When this value is set, GPC data analysis, such as molecular weight distribution calculation, is done using stretched chain length in LabSolutions. Using the default value of 1 means that the calculation is done using molecular weight.

- Notational reminder for the use of Q factor

  When you use the conversion with the Q factor, you need to interpret the values as [Stretched Chain Length] even though they are discrbed as [Molecular Weight] in the following items in LabSolutions.

  - Molecuar weight in a calibration curve table
  - Molecuar weight in a slice data
  - Molecuar weight in a calibration curve graph
  - Molecuar weight in a molecular weight distribution curve

  Only average molecular weights displayed in a GPC calculation result are expressed in molecular weight that is corrected using the Q factor, not in stretched chain length.

- Reminder on setting when using the Q factor

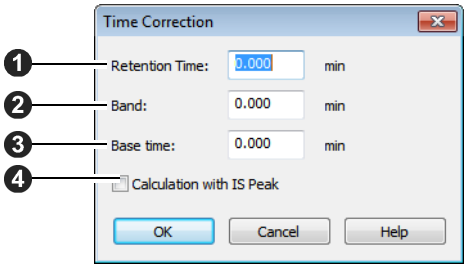
  As explained above, you need interpret values described as molecular weight in a calibration curve table as stretched chain length when you use correction with the Q factor. Therefore, specify strethced molecular chain length values in the molecular weight cells when creating a calibration curve table.

## ■ Setting the Time Correction

Set the time correction to compensate for variations in the molecular weight distribution calculation due to changes in elution time.

**1** **Check [Internal Standard] or [GPC Control sample] in [Time Correction], and click [Settings].**

**2** **Configure the settings.**




| No. | Description |
|---|---|
| ❶ | Set the retention time of the standard peak used for the time correction.<br>Standard peak refers to the internal standard peak when using "Internal Standard Method". When using "GPC Control Sample", it refers to the peak for data whose batch processing sample type is set to “GPC Control Sample”. |
| ❷ | Set the band of the standard peak. |
| ❸ | Set the base time (T0) used for the time correction calculation. Usually, zero or T.LIMIT (filtration limit time) is set. |
| ❹ | Select whether to also calculate the internal standard peak in the molecular weight calculation. |

**3** **Click [OK].**

**Reference**

"4.5.4 Time Correction Using the Internal Standard Method" on page 67

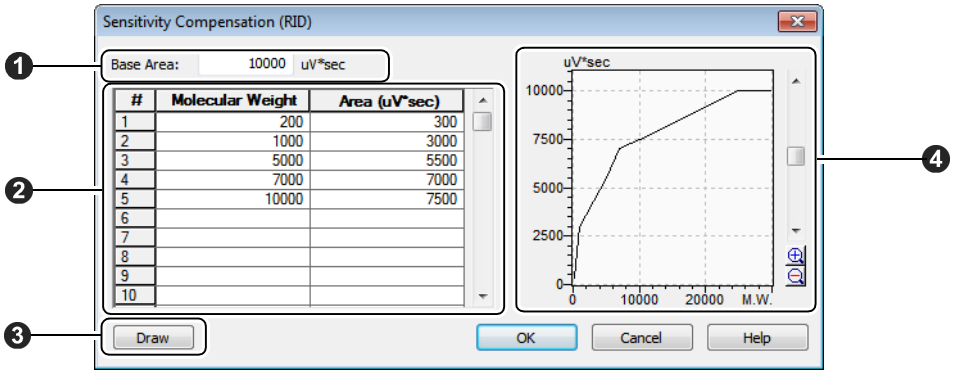
"4.5.5 Time Correction Using the Control Sample" on page 68

## ■ Sensitivity Compensation Setting of RI Detectors

Since the RI detector has a characteristic that the sensitivity lowers if the molecular weight of analyzed sample is low, perform the sensitivity compensation by setting the sensitivity compensation parameters. To use this function, it is necessary to ascertain the relationship between the molecular weight and the response sensitivity (area) as described in "4.5.6 Sensitivity Compensation of RI Detectors".

**1** **Check [Sensitivity Compensation (RID)] and click [Settings].**

**2** **Configure the settings.**




| No. | Description |
|---|---|
| ❶ | Set the base area. Set a value equal to or greater than the maximum value of the sensitivity compensation table area.<br>The area value correction factor is calculated with the following:<br>• Correction factor = (base area) / (Area value of the molecular weight on the graph) |
| ❷ | This is the mapping table of the molecular weight and the area values. A maximum of 20 lines can be entered and must monotonically increase. |
| ❸ | When clicked, the contents of the sensitivity compensation table are drawn in the graph in ❹. |
| ❹ | Displays the sensitivity compensation graph. |

**3** **Click [OK].**

**NOTE**

The table contents can be copied and cut using the right-click menu.

## ■ Setting the RT/MW Range

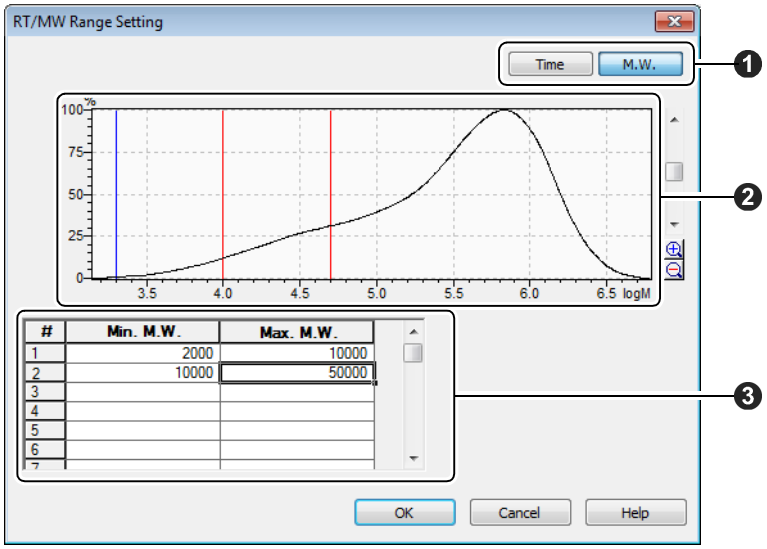
Specify ranges for performing GPC calculation.

- You can specify multiple (up to 20) ranges in the chromatogram or the molecular weight distribution graph.
- You can specify time (molecular weight) by entering numbers or clicking on the graph.

### 1 Click [RT/MW Range Setting].

The [RT/MW Range Setting] screen appears.

### 2 Configure the settings.




| No. | Description |
|---|---|
| ❶ | Switches the graph to the chromatogram or the molecular weight distribution curve. |
| ❷ | Displays the chromatogram or the molecular weight distribution curve. |
| ❸ | Displays the set RT/MW ranges. Enter values in [Start Time] and [End Time] or [Min. Molecular Weight] and [Max. Molecular Weight] to specify the RT/MW range settings. |

### 3 Click [OK].

**NOTE**

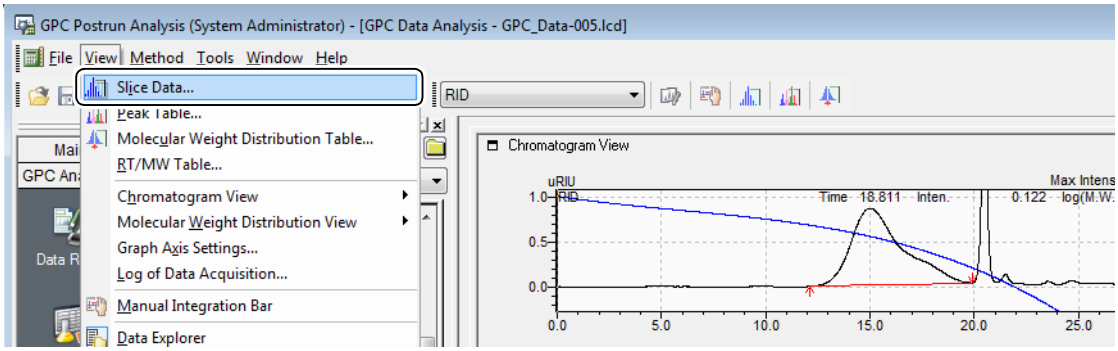
- When the RT/MW ranges are already set in the calibration curve screen, the setting is reflected by default.
- The table contents can be copied and cut using the right-click menu.

# 4.4.4 Displaying Slice Data

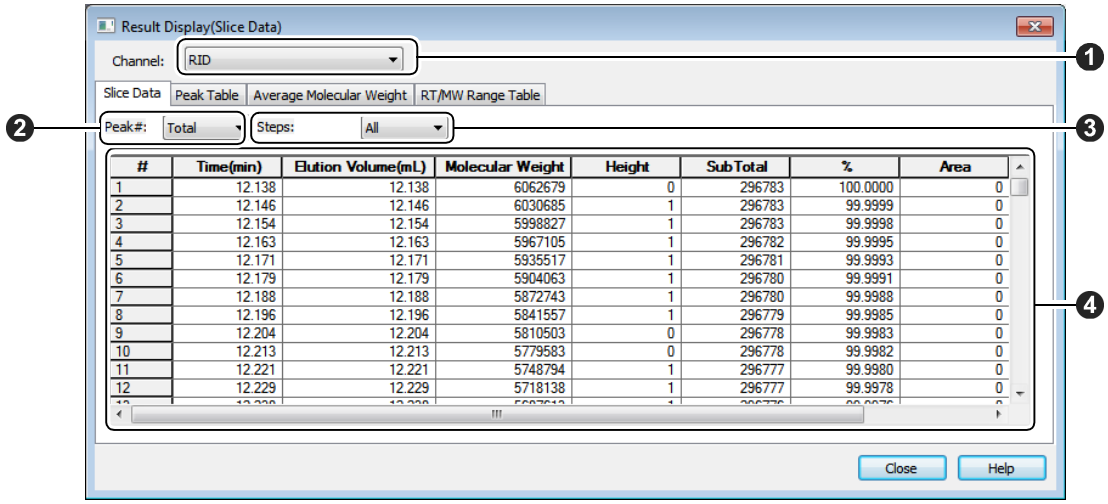
The slice data, an intermediate step of the molecular weight calculation, is displayed.

- The slice information of the specified peak is displayed at a specified interval.
- Items to be displayed and their order can be customized in the table style setting.
- Selected items can be transferred to the clipboard.

## 1 Click [Slice Data] from the [View] menu.




## 2 Configure the settings.




| No. | Description |
|---|---|
| ❶ | Select a channel of the detector. |
| ❷ | Select [Total] or any of the peak numbers. |
| ❸ | Specify an interval to display the slice data. |
| ❹ | Displays data of each slice at the specified interval. |

## 3 Click [Close].

### NOTE

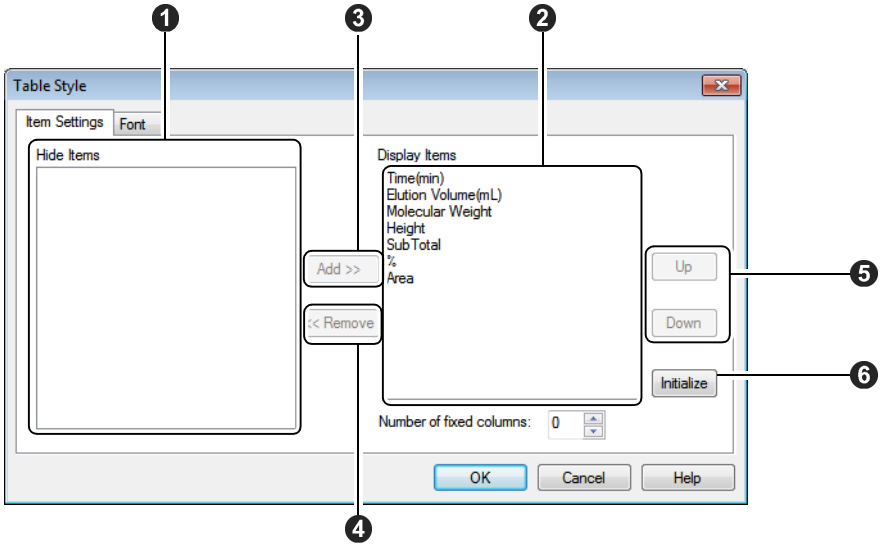
- [Slice Data] can be selected from the [View] menu only when [Calculate GPC] is checked in the [GPC Calculation] tab of the [Data Processing Parameters] screen.
- Changing the output interval ([Steps]) of the slice data does not alter the numbers displayed in the left-most [#] column.

## ■ Setting the Table Style

The table style of the slice data is set as follows:

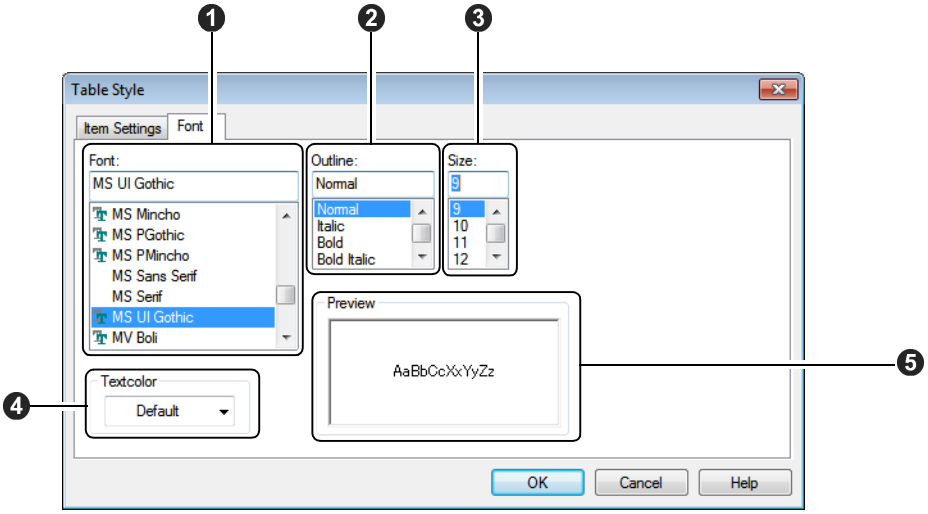
**1** **Right-click on the data table in the [Slice Data] tab, and click [Table Style] from the menu.**

**2** **Click the [Item Settings] tab and configure the settings.**




| No. | Description |
|---|---|
| ❶ | Hidden items are displayed. |
| ❷ | Displayed items are displayed. |
| ❸ | Moves items selected in [Hide Items] to [Display Items]. |
| ❹ | Moves items selected in [Display Items] to [Hide Items]. |
| ❺ | Click these to move a selected item in [Display Items] up or down. |
| ❻ | Returns [Display Items] and [Hide Items] to their default status. |

**3** **Click the [Font] tab and configure the settings.**



| No. | Description |
|---|---|
| ❶ | Enter or select a font name. |
| ❷ | Enter or select a font style. |
| ❸ | Enter or select a font size. |
| ❹ | Select a text color. |
| ❺ | Character display sample based on the setting is displayed. |

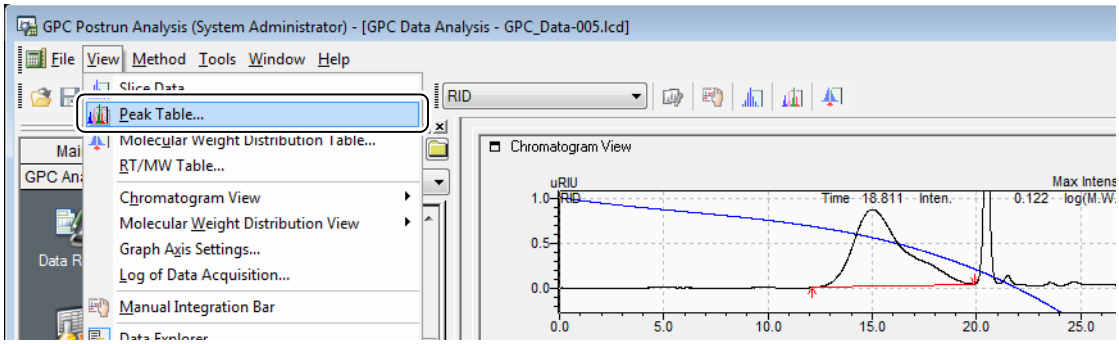
## 4.4.5 Displaying the Results from the Peak Table

The peak information or the detailed information for individual peaks are displayed.

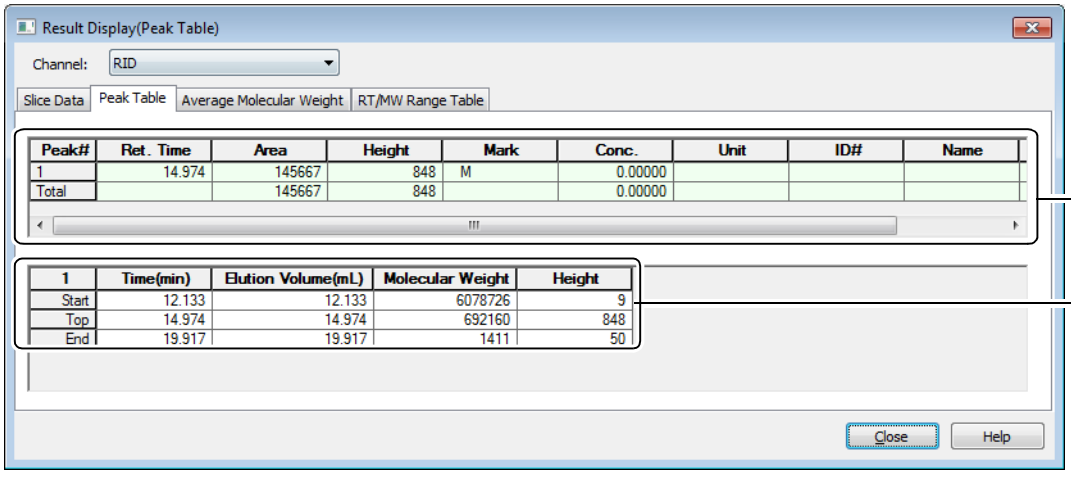
- The peak information (retention time, height, etc.) is listed.
- Detailed information (values at the start, top, and end) of the selected peak is displayed.
- Items to be displayed and their order can be customized in the table style setting.
- Selected items can be transferred to the clipboard.



### 1 Click [Peak Table] from the [View] menu.




### 2 Check the items.




| No. | Description |
|---|---|
| ❶ | Lists the peak information of the currently selected detectors and channels. |
| ❷ | Displays the detailed information of the selected peak. |

## ■ Setting the Table Style

**Reference**

"4.4.4 Displaying Slice Data", "■ Setting the Table Style"

**NOTE**

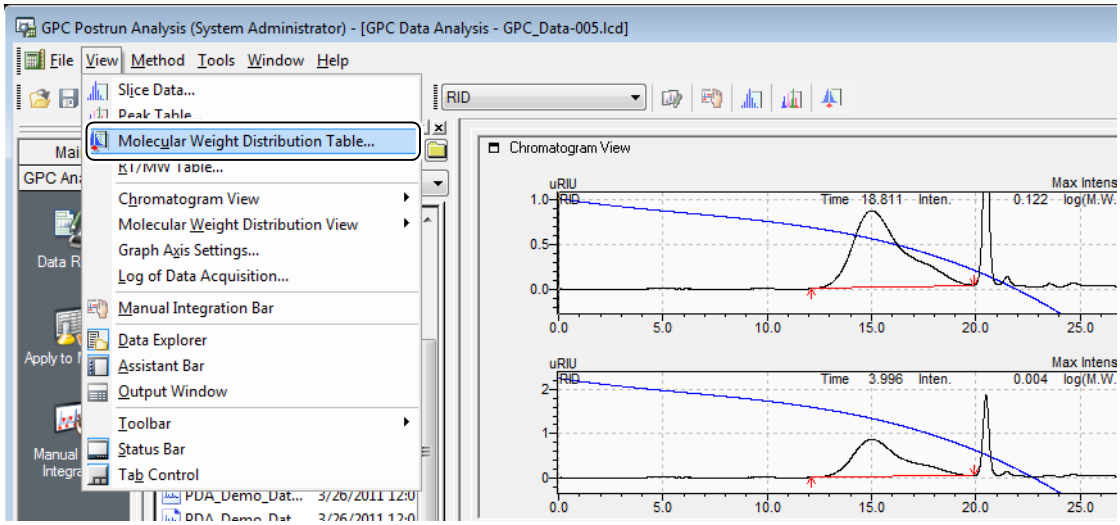
Operations are the same for any table, but the displayed items and hidden items are different.

# 4.4.6 Displaying the Result of the Average Molecular Weight

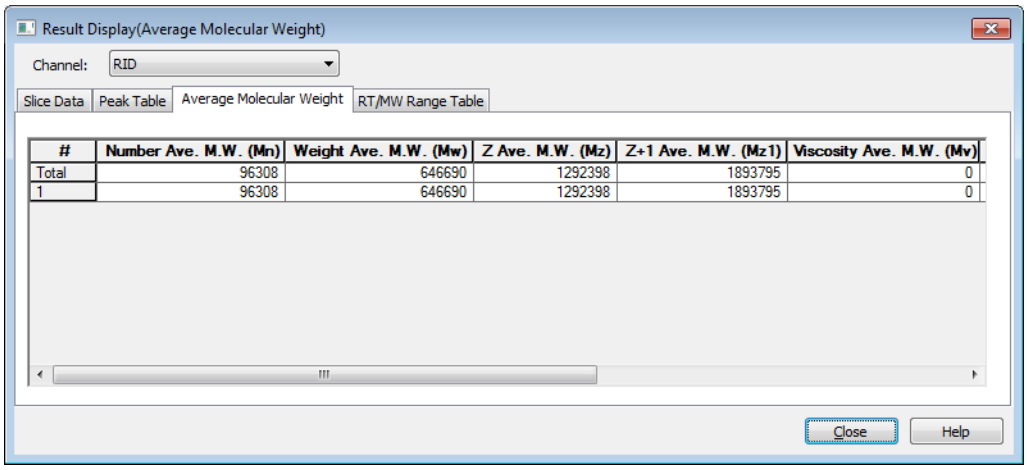
The average molecular weight is displayed by each peak.

- Average molecular weight of all the peaks and of individual peaks can be calculated.
- Items to be displayed and their order can be customized in the table style setting.
- Selected items can be transferred to the clipboard.

**1** **Click [Molecular Weight Distribution Table] from the [View] menu.**




**2** **Check the items.**




| # | Number Ave. M.W. (Mn) | Weight Ave. M.W. (Mw) | Z Ave. M.W. (Mz) | Z+1 Ave. M.W. (Mz1) | Viscosity Ave. M.W. (Mv) |
|---|---|---|---|---|---|
| Total | 96308 | 646690 | 1292398 | 1893795 | 0 |
| 1 | 96308 | 646690 | 1292398 | 1893795 | 0 |

The average molecular weight, the polydispersity, and the intrinsic viscosity of the all the peaks and of individual peaks is listed. Items to be displayed and their order can be customized in the table style setting.

## ■ Setting the Table Style

**Reference**

"4.4.4 Displaying Slice Data", "■ Setting the Table Style"

**NOTE**

Operations are the same for any table, but the displayed items and hidden items are different.

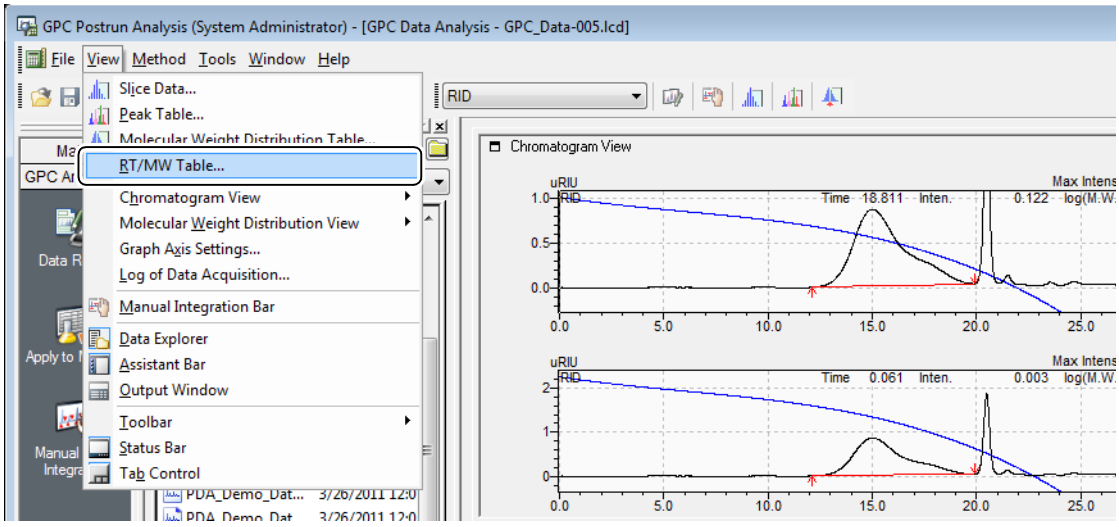
# 4.4.7 Displaying the Result of the Average Molecular Weight of the RT/MW Ranges

The average molecular weight values of the RT/MW ranges are displayed.

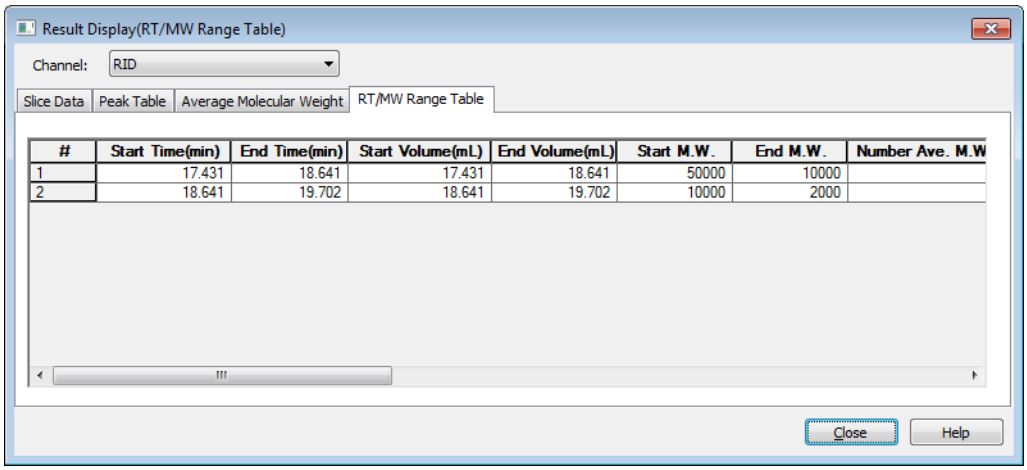
- Average molecular weight can be calculated for each specified RT/MW range.
- Items to be displayed and their order can be customized in the table style setting.
- Selected items can be transferred to the clipboard.



### 1 Click [RT/MW Table] from the [View] menu.




### 2 Check the items.




| # | Start Time(min) | End Time(min) | Start Volume(mL) | End Volume(mL) | Start M.W. | End M.W. | Number Ave. M.W |
|---|---|---|---|---|---|---|---|
| 1 | 17.431 | 18.641 | 17.431 | 18.641 | 50000 | 10000 | |
| 2 | 18.641 | 19.702 | 18.641 | 19.702 | 10000 | 2000 | |

The average molecular weight, the polydispersity, and the intrinsic viscosity of each RT/MW range is listed.
Items to be displayed and their order can be customized in the table style setting.

### ■ Setting the Table Style

**Reference**

"4.4.4 Displaying Slice Data", "■ Setting the Table Style"

**NOTE**

Operations are the same for any table, but the displayed items and hidden items are different.

# 4.5 GPC Calculation

A chromatogram is converted into a molecular weight distribution using an approximate equation, and various average molecular weight values are calculated from the molecular weight distribution.
The following time corrections are performed in the conversion to the molecular weight distribution.

- Correction using the internal standard method
- Correction using the control sample
- Sensitivity compensation of RI detectors

## 4.5.1 Approximate Equations for Calibration Curves

The following approximate equations are used for obtaining molecular weights from the chromatograms.

| Type | Equation |
|---|---|
| Point-to-point | Linear interpolation between calibration points |
| Linear (Straight line) | $\log M = aX + b$ |
| 3rd order | $\log M = aX^3 + bX^2 + cX + d$ |
| 3rd order + Hyperbolic curve | $\log M = aX^3 + bX^2 + cX + d + e/X^2$ |
| 5th order | $\log M = aX^5 + bX^4 + cX^3 + dX^2 + eX + f$ |
| 5th order + Hyperbolic curve | $\log M = aX^5 + bX^4 + cX^3 + dX^2 + eX + f + g/X^2$ |
| 7th order | $\log M = aX^7 + bX^6 + cX^5 + dX^4 + eX^3 + fX^2 + gX + h$ |
| 7th order + Hyperbolic curve | $\log M = aX^7 + bX^6 + cX^5 + dX^4 + eX^3 + fX^2 + gX + h + i/X^2$ |

X = x(elution duration) - T.LIMIT(filtration limit time)
M: the molecular weight or the chain length

## 4.5.2 Equations for Calculating Average Molecular Weight

| Type | Equation |
|---|---|
| Number average Mn | $Mn = \frac{\Sigma Hi}{\Sigma(Hi/Mi)} \times QF$ |
| Weight average Mw | $Mw = \frac{\Sigma(Mi \times Hi)}{\Sigma Hi} \times QF$ |
| Z Average Mz | $Mz = \frac{\Sigma(Mi^2 \times Hi)}{\Sigma(Mi \times Hi)} \times QF$ |
| Z+1 Average Mz1 | $Mz1 = \frac{\Sigma(Mi^3 \times Hi)}{\Sigma(Mi^2 \times Hi)} \times QF$ |
| Viscosity average Mv | $Mv = \left( \Sigma(Hi \times Mi^{\alpha}) / \Sigma Hi \right)^{1/\alpha} \times QF$ |
| Intrinsic viscosity | $I.VISC = K \times (Mv)^{\alpha}$ |

Hi: Peak height
Mi: Molecular weight or chain length
$\alpha$/*K* : Constant and Index of the viscosity equation
QF: Q factor (1 for molecular weight)

## 4.5.3 Time Correction

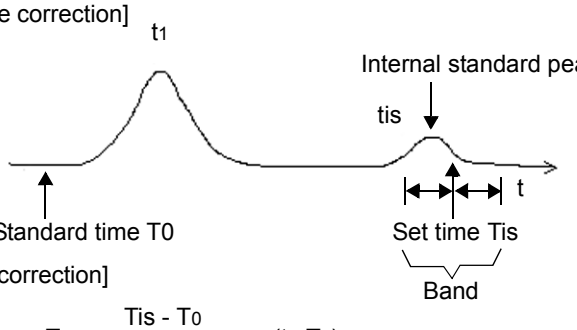
The following time correction can be performed in conversion to the molecular weight distribution:

- Correction using the internal standard method
- Correction using the control sample

## 4.5.4 Time Correction Using the Internal Standard Method

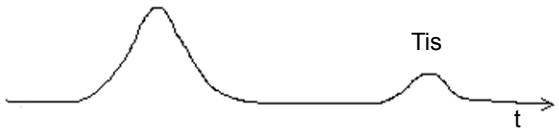
A chromatogram is measured after adding the internal standard sample to the unknown sample that is to be measured. The time axis of the actual chromatogram is corrected using the peak of the internal standard sample of which retention time (Tis) is known. The corrected chromatograms are expanded or reduced along the time axis.

[Before correction]




[After correction]

$$T_0 + \frac{Tis - T_0}{tis - T_0} \times (t_1 - T_0)$$

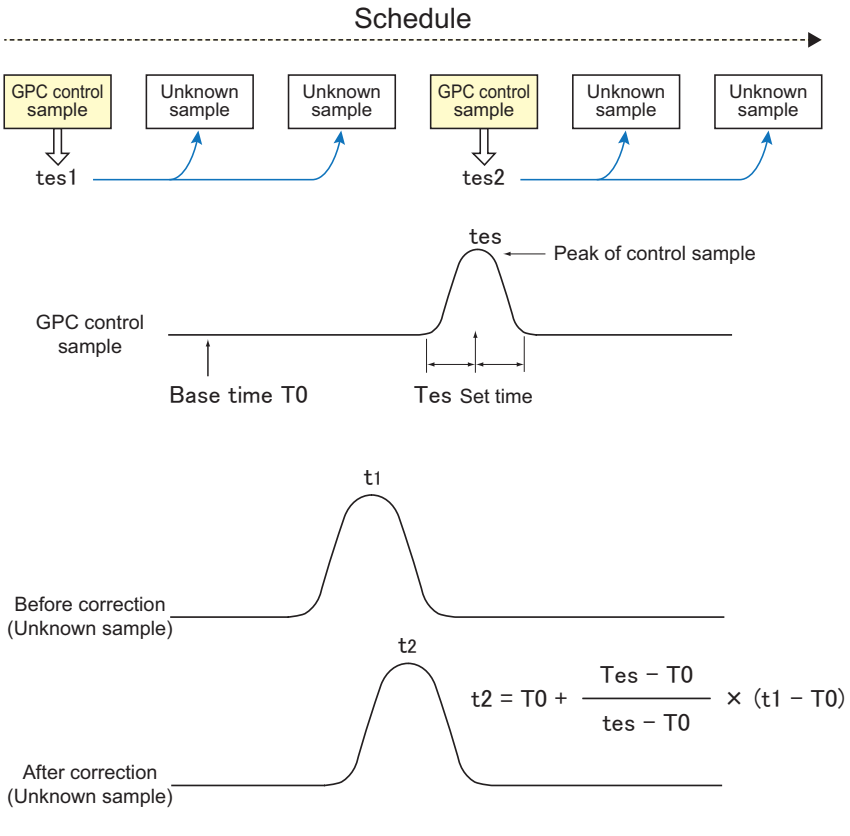



**NOTE**

Time before base time T0 is not corrected.

## 4.5.5 Time Correction Using the Control Sample

In this method, analysis is done using samples at the internal standard peaks as the GPC control samples. As shown in the following figure, GPC control samples are injected among unknown samples in a batch schedule, and the correction values are continually updated.

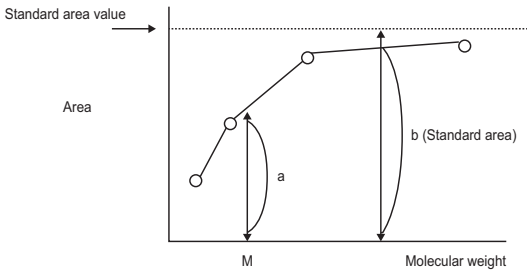



**NOTE**

Time before base time T0 is not corrected.

## 4.5.6 Sensitivity Compensation of RI Detectors

RI detectors have a characteristic that the sensitivity lowers when the molecular weight is low. When the molecular weight distribution of the measuring sample is broad, sensitivity change of the RI detector affect the result.
First, a sample that is a mixture of equal quantity of standard samples that have different molecular weights is analyzed, and the area values for each molecular weight are calculated. The area to be standard is pre-determined, and the relationship between each molecular weight and the area is defined as shown in the following figure.




Molecular weight calculation is performed using a value obtained by multiplying the response amount (the slice value), a molecular weight M, by b/a.

# 5 GPC Data Comparison

In the [GPC Data Comparison] window, the GPC molecular weight calculation results from multiple data files can be displayed in layers as one graphed view, and the statistical calculations are performed. GPC data comparison is performed per detector/channel. When a data file contains multiple calculation results of molecular weight distribution, you can specify a detector/channel and display the data in one graph.

## 5.1 Displaying the [GPC Data Comparison] Window

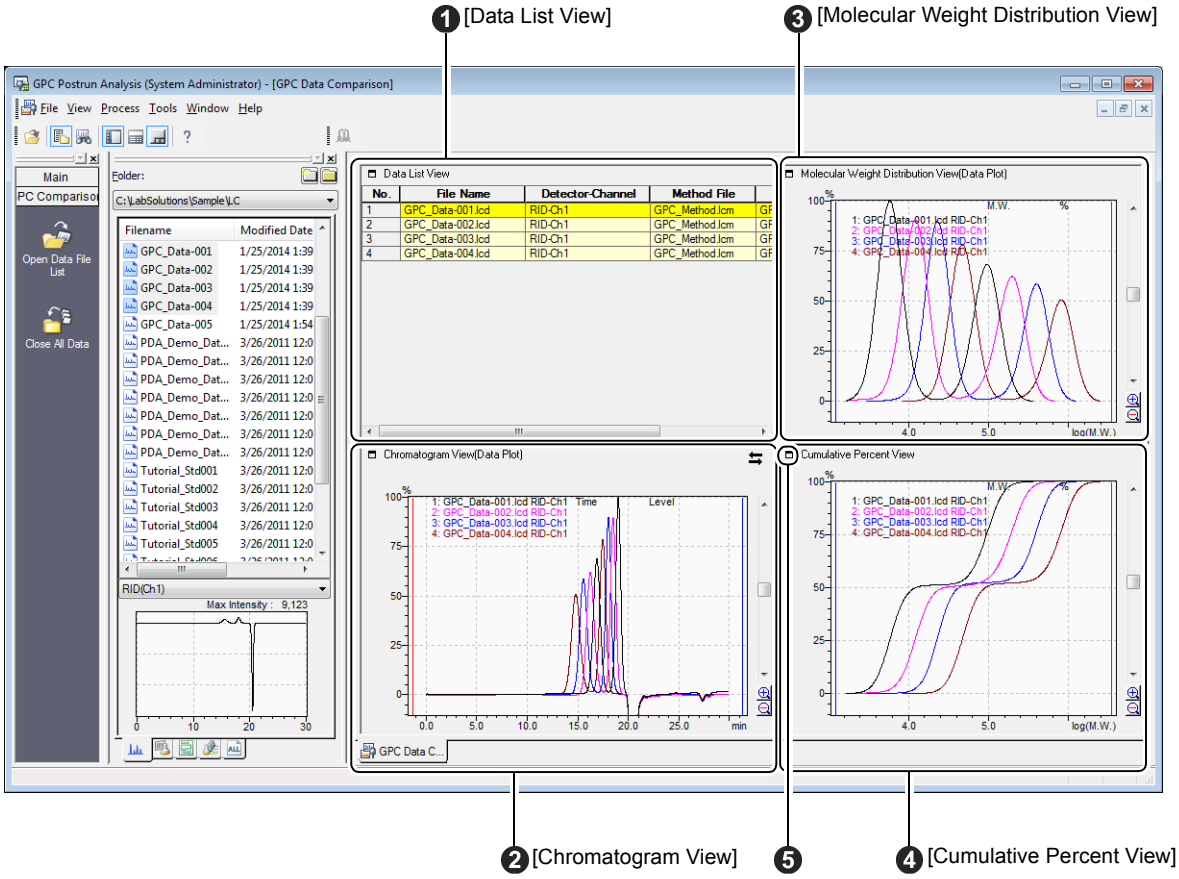
**1** **Click the** 

**(GPC Data Comparison) icon in the [Main] assistant bar of the [GPC Postrun] program.**


The [GPC Data Comparison] window appears.

# 5.2 Using and Viewing the [GPC Data Comparison] Window

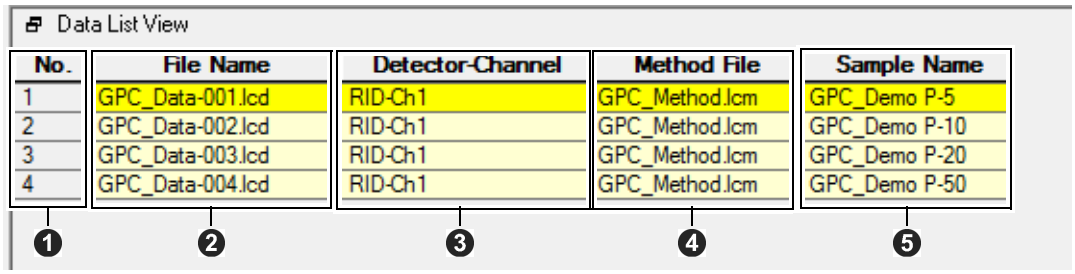
The [GPC Data Comparison] window contains [Data List View], [Chromatogram View], [Molecular Weight Distribution View], and [Cumulative Percent View].




| No. | Description |
|---|---|
| 1 | A data list for the GPC data comparison is displayed. |
| 2 | Chromatograms are displayed in layers. |
| 3 | Differential molecular weight distribution curves are displayed in layers. |
| 4 | Integral molecular weight distribution curves are displayed in layers. |
| 5 | Click this button (change size button) to switch between the full screen and standard displays. |

# 5.3 Data List View

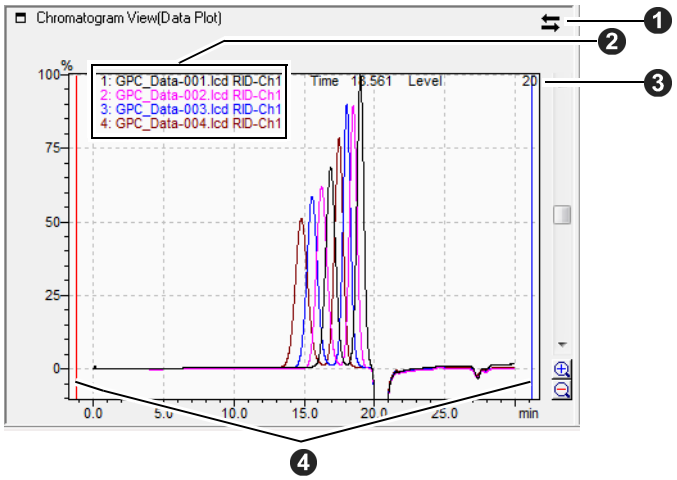
A list of data for the GPC data comparison is displayed in [Data List View].




| No. | Description |
|---|---|
| 1 | Data files are numbered in the order registered. |
| 2 | Data file names are displayed. |
| 3 | Detector/channel names are displayed. |
| 4 | Names of the method files that were used to measure the data are displayed. |
| 5 | Sample names of data files are displayed. |

# 5.4 Chromatogram View

Chromatograms of data registered in [Data List View] are displayed in layers in [Chromatogram View].




| No. | Description |
|---|---|
| 1 | Click to shift the chromatograms in the X axis direction using the mouse. |
| 2 | Displays the data list numbers, data file names, detector names, and channel names in the graph display colors. |
| 3 | The time (or amount of elution) and the intensity (%) at the mouse position when the mouse is located on the graph.<br>(The time and the amount of elution can be switched by the axis configuration of the graph.) |
| 4 | Marker lines. |

**NOTE**

Dragging on the chromatogram to specify the range will zoom in on that range.

## 5.4.1 Display of Marker Lines

Two marker lines are displayed on the left and right of the chromatogram. They can be moved along the X axis by dragging them. This forces the marker lines of the differential molecular weight distribution and the integral molecular weight distribution curves automatically move to the corresponding new positions. Also, by dragging the marker line on the differential or integral molecular weight distribution graphs you can view the corresponding position on the chromatogram.

**NOTE**

When the chromatograms are overlayed using different calibration curves, marker lines are displayed but they are not functional.

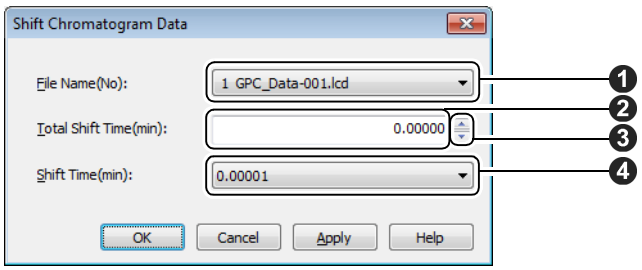
## 5.4.2 Shifting Chromatograms

There are two methods to shift chromatograms in the X axis direction: setting the shift time in the [Shift Chromatogram Data] screen and using the (Move Left/Right) button.
The corresponding differential molecular weight distribution curve graph and integral molecular weight distribution curve graph are shifted accordingly.

### ■ Using the [Shift Chromatogram Data] Screen

**1** **Right-click in the chromatogram view and click [Move Left/Right] from the menu.**

**2** **Configure the settings.**




| No. | Description |
|---|---|
| ❶ | Select a data file name to shift.<br>Numbers and file names registered in the data list are displayed in the combo box. |
| ❷ | Displays the shift time from the initial state. You can also directly enter the shift time.<br>The X axis scale indicates the total shift time (min) or the total shift elution amount (mL). |
| ❸ | The total shift time is increased or decreased from the current position only by the unit specified in [Shift Time]. |
| ❹ | The unit used for increasing and decreasing in ❸ can be selected from among [0.00001], [0.0001], [0.001], [0.01], [0.1] and [1.0]. |

**3** **Click [OK] or [Apply].**

The chromatogram is shifted according to the time specified in the total shift time.

### ■ Using the Move Left/Right Button

**1** **Click the (Move Left/Right).**

It becomes as if the button is held down.

**2** **Drag from the start position to the end position on the chromatogram.**

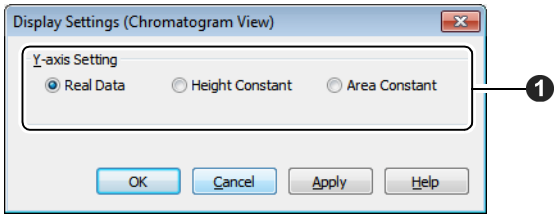
Placing the cursor on the chromatogram will display a vertical line. Drag to specify a range.
The selected data of the chromatogram will be shifted, and the corresponding graph of the differential molecular weight distribution curve and the graph of the integral molecular weight distribution curve will also be shifted.

## 5.4.3 Display Settings of Chromatograms

Display settings for [Chromatogram View] are performed as follows:

**1** **Right-click on the chromatogram and click [Display Settings] from the menu.**

**2** **Configure the settings.**



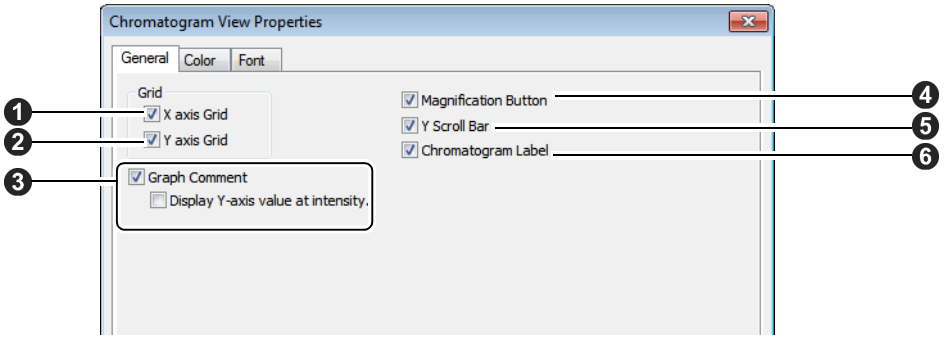

| No. | Description |
|---|---|
| ❶ | Select the display method of the Y axis scale of the chromatogram. |

**3** **Click [OK].**

## 5.4.4 Setting View Properties

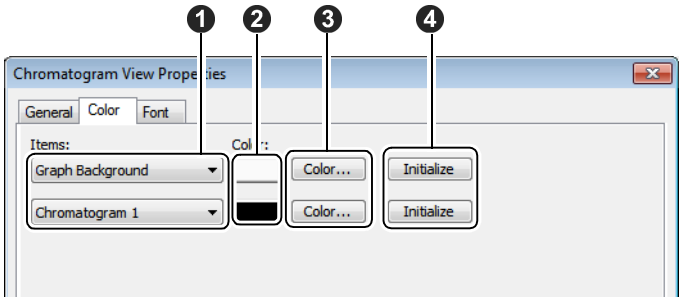
**1** **Right-click on the chromatogram and click [Properties] from the menu.**

**2** **Click the [General] tab and configure the settings.**



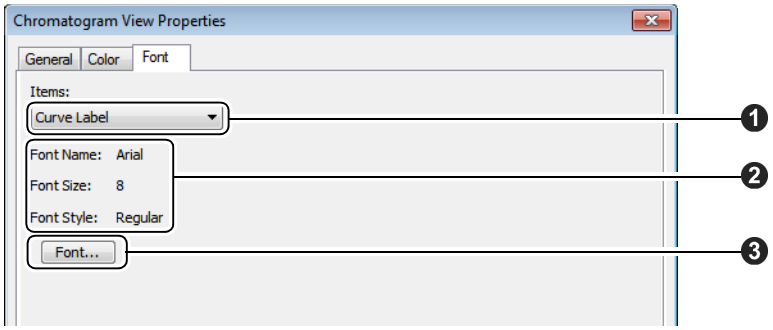

| No. | Description |
|---|---|
| ❶ | Displays or hides the X axis grid. |
| ❷ | Displays or hides the Y axis grid. |
| ❸ | Displays or hides the graph comments.<br>When [Display Y-axis value at intensity.] is checked, the Y-axis coordinate of the mouse will be displayed in the intensity value. |
| ❹ | Displays or hides the magnification buttons (zoom-in and zoom-out). |
| ❺ | Displays or hides the Y axis scroll bar. |
| ❻ | Displays or hides the detector and channel names. |

**3** **Click the [Color] tab and configure the settings.**




| No. | Description |
|---|---|
| ❶ | Allows you to select a display item, such as [Graph Background] or [Graph Frame], for the color setting. |
| ❷ | Displays the color set for the selected display item. |
| ❸ | Sets the color of the selected display item. |
| ❹ | Click this to set the color of the display item. |

## 4 Click the [Font] tab and configure the settings.

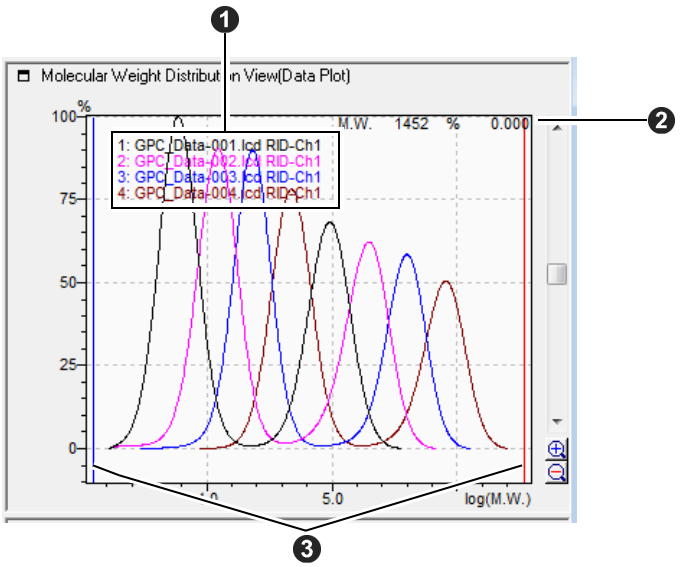



| No. | Description |
|---|---|
| 1 | Allows you to select an item for the font setting. |
| 2 | Displays the selected [Font Name], [Font Size], and [Font Style]. |
| 3 | Displays the [Font] screen. Select a font. |

## 5 Click [OK].

# 5.5 Molecular Weight Distribution View

In [Molecular Weight Distribution View], differential molecular weight distribution curves of data registered in the data file list are displayed in layers.




| No. | Description |
|---|---|
| ❶ | Displays the data list numbers, data file names, detector names, and channel names in the graph display colors. |
| ❷ | Displays the molecular weight (or degree of polymerization) and its percentage at the mouse position if the mouse is located on the graph. |
| ❸ | These are displayed in conjunction with the marker lines of the chromatogram. |

**NOTE**

You can zoom in on an area on the differential molecular weight distribution curve graph by dragging a square to specify the area.

## 5.5.1 Display of Marker Lines

Two marker lines are displayed on the differential molecular weight distribution curve graph. They can be moved along the X axis by dragging them. This forces the marker lines of the chromatogram and the integral molecular weight distribution graph move automatically with them.

## 5.5.2 Display Settings of the Differential Molecular Weight Distribution Curve

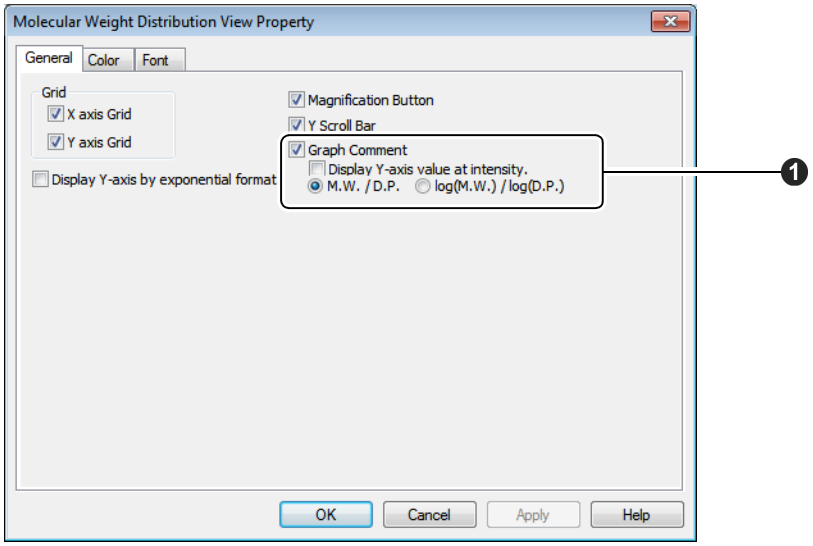
**Reference**

"5.4.3 Display Settings of Chromatograms" on page 73

## 5.5.3 Setting View Properties

**1** **Right-click on the differential molecular weight distribution curve graph, and click [Properties] from the menu.**

**2** **Click the [General] tab and configure the settings.**




| No. | Description |
|---|---|
| ❶ | Displays or hides the graph comments. Select either [M.W./D.P] or [log (M.W.) /log (D.P.)] for the scale display when displaying the molecular weight information (molecular weight or degree of polymerization) in a graph comment. When [Display Y-axis value at intensity.] is checked, the Y-axis coordinate of the mouse will be displayed in the intensity value. |

**3** **Click the [Color] tab and configure the settings.**

**Reference**

For details, see step 3 (P.74) in "5.4.4 Setting View Properties".

**4** **Click the [Font] tab and configure the settings.**

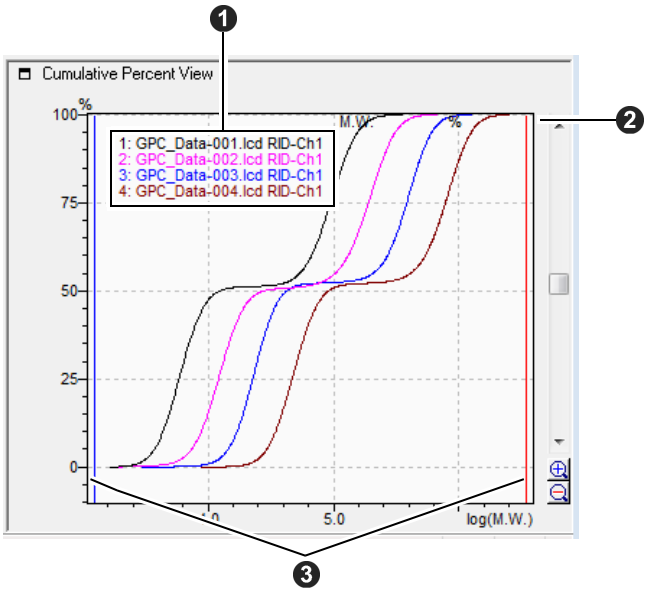
**Reference**

For details, see step 4 (P.74) in "5.4.4 Setting View Properties".

**5** **Click [OK].**

# 5.6 Cumulative Percent View

In [Cumulative Percent View], integral molecular weight distribution curves of data registered in the data file list are displayed in layers.




| No. | Description |
|---|---|
| ❶ | Displays the data list numbers, data file names, detector names, and channel names in the graph display colors. |
| ❷ | Displays the molecular weight (or degree of polymerization) and its percentage at the mouse position if the mouse is located on the graph. |
| ❸ | These are displayed in conjunction with the marker lines of the chromatogram. |

**NOTE**

You can zoom in on an area on the integral molecular weight distribution curve graph by dragging a square to specify the area.

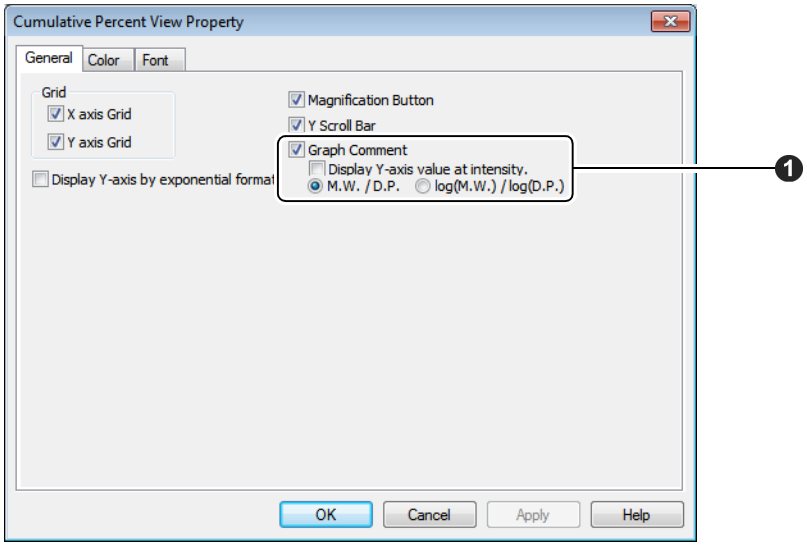
## 5.6.1 Display of Marker Lines

Two marker lines are displayed on the integral molecular weight distribution curve graph. They can be moved along the X axis by dragging them with a mouse while the marker lines of the chromatogram and the differential molecular weight distribution curve graph are moved as well.

## 5.6.2 Setting View Properties

**1** **Right-click on the integral molecular weight distribution curve graph, and click [Properties] from the menu.**

**2** **Click the [General] tab and configure the settings.**




| No. | Description |
|---|---|
| ❶ | Displays or hides the graph comments.<br>Select either [M.W./D.P] or [log (M.W.) /log (D.P.)] for the scale display when displaying the molecular weight information (molecular weight or degree of polymerization) in a graph comment.<br>When [Display Y-axis value at intensity.] is checked, the Y-axis coordinate of the mouse will be displayed in the intensity value. |

**3** **Click the [Color] tab and configure the settings.**

**Reference**

For details, see step 3 (P.74) in "5.4.4 Setting View Properties".

**4** **Click the [Font] tab and configure the settings.**

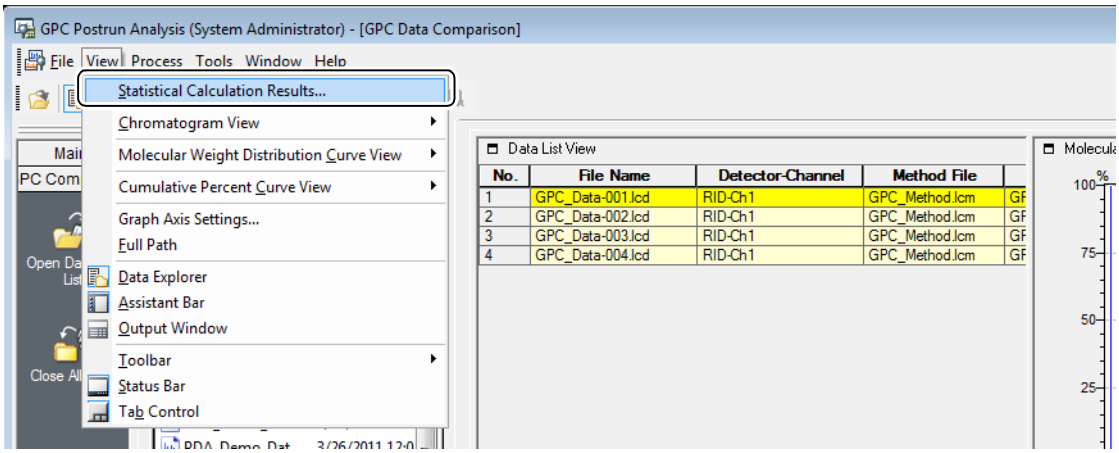
**Reference**

For details, see step 4 (P.74) in "5.4.4 Setting View Properties".

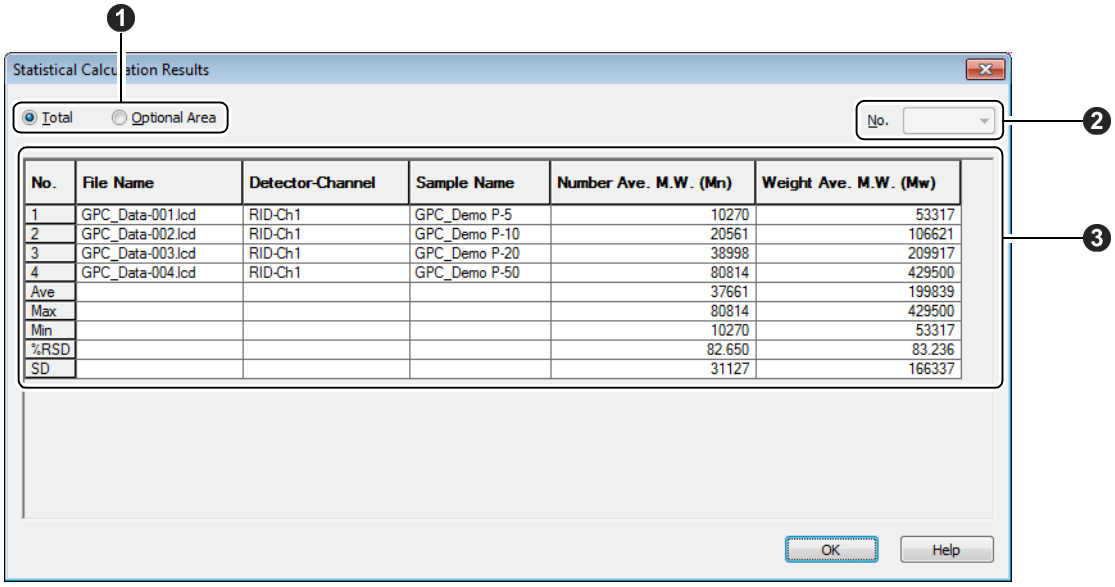
**5** **Click [OK].**

# 5.7 Statistical Calculation Result

**1** **Click [Statistical Calculation Results] from the [View] menu.**




**2** **Configure each setting.**




| No. | Description |
|---|---|
| ❶ | Select either [Total] or [Optional Area] for the display of the statistical results. |
| ❷ | Select the No. to display when [Optional Area] is selected in the type. |
| ❸ | Displays the data list and statistical calculation results. The display items can be specified in [Table Style]. The maximum number of data for the GPC data comparison is 10. |

**3** **Click [OK].**

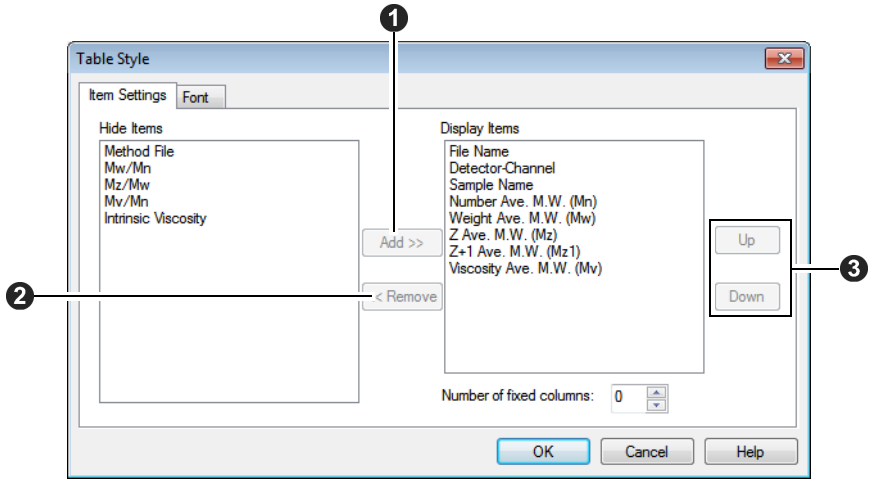
**NOTE**

The display items are set in the [Table Style] screen. When all data cannot be displayed in the data list grid display area, the vertical and horizontal scroll bars are used to scroll the table.

## 5.7.1 Setting the Display Items of the [Statistical Calculation Result] Screen

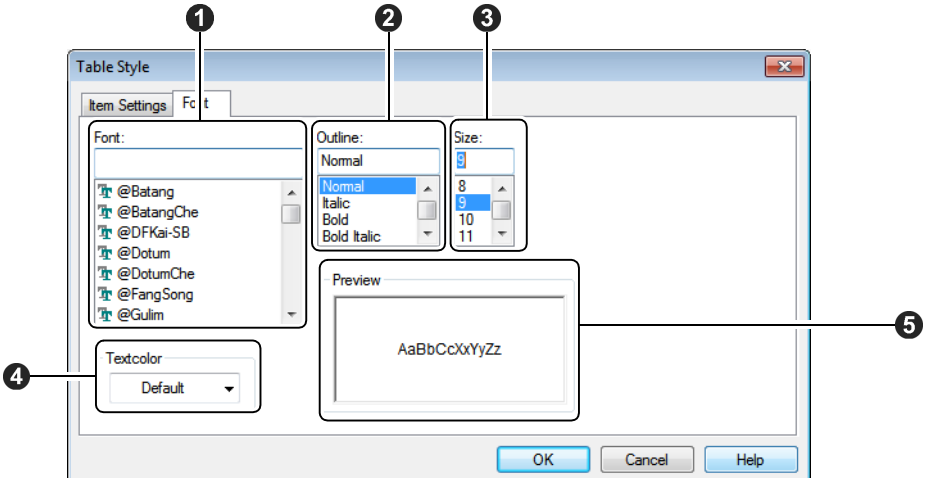
**1** **Right-click on the data table in the [Statistical Calculation Results] screen, and click [Table Style] from the menu.**

**2** **Click the [Item Settings] tab and configure the settings.**




| No. | Description |
|---|---|
| ❶ | Moves items selected in [Hide Items] to [Display Items]. |
| ❷ | Moves items selected in [Display Items] to [Hide Items]. |
| ❸ | Click these to move a selected item in [Display Items] up or down. |

**3** **Click the [Font] tab and configure the settings.**




| No. | Description |
|---|---|
| ❶ | Enter or select a font name. |
| ❷ | Enter or select a font style. |
| ❸ | Enter or select a font size. |
| ❹ | Select a text color. |
| ❺ | Character display sample based on the setting is displayed. |

**4** **Click [OK].**

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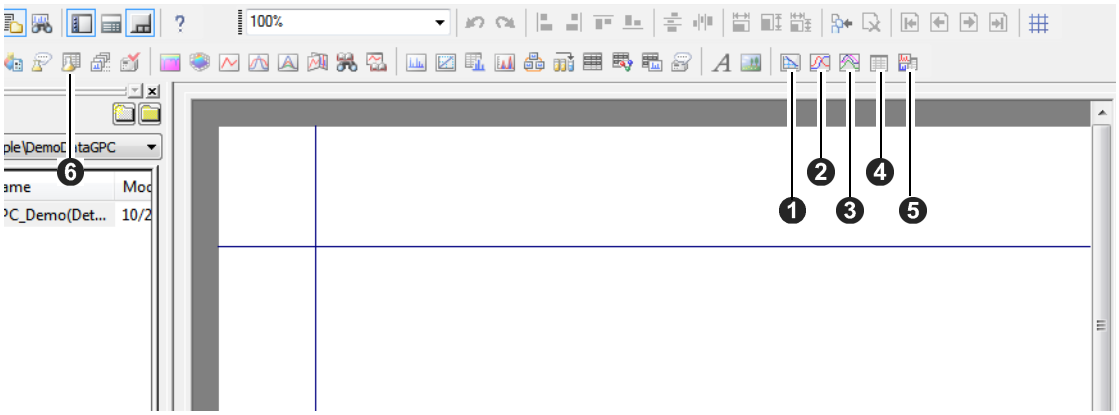
# 6 Report Function

This chapter describes the report function of LabSolutions GPC software.
In addition to the LC Real Time Analysis print items, the following GPC analysis print items are available.

- GPC calibration curve item
  Allows you to print a calibration curve, a calibration curve table, and calibration curve correction parameters.
- GPC graph item
  Allows overlay printing of a chromatograph and a calibration curve, as well as a differential and an integral curves, from a data file.
- GPC overlay item
  Allows overlay printing of the same type of curves from multiple data.
- GPC calculation result item
  Allows printing of slice information, peak information, and average molecular weight information.
- GPC summary item (molecular weight statistic values of multiple data)
  Allows you to print molecular weight statistic values from multiple data.
- Method (GPC parameters)
  Allows printing of GPC method parameters.

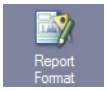
Click any of the following icons to select the items.



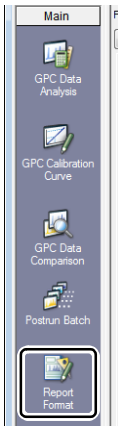

| No. | Icon | Item |
|---|---|---|
| ❶ | | GPC calibration curve |
| ❷ | | GPC graph |
| ❸ | | GPC overlay |
| ❹ | | GPC calculation result |
| ❺ | | GPC summary |
| ❻ | | Method |

# 6.1 Creating Reports

Create a GPC analysis result report as follows:

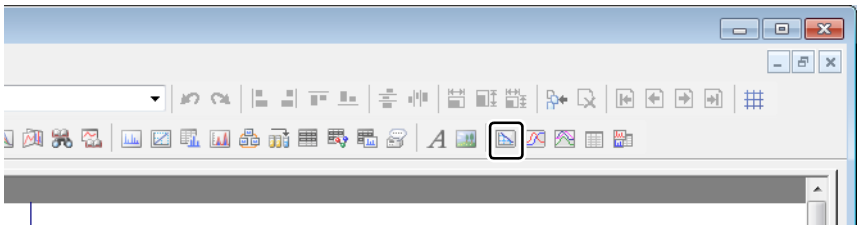
**1** **Click** 

**(Report Format) in the [Main] assistant bar of the [GPC Postrun] program.**



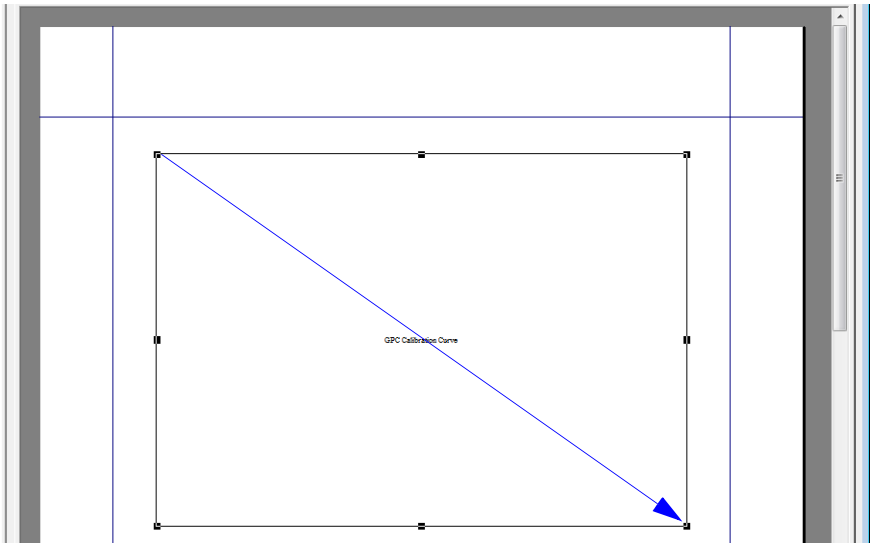

**2** **Click the print item you would like to paste.**

For example, click  (GPC Calibration Curve).



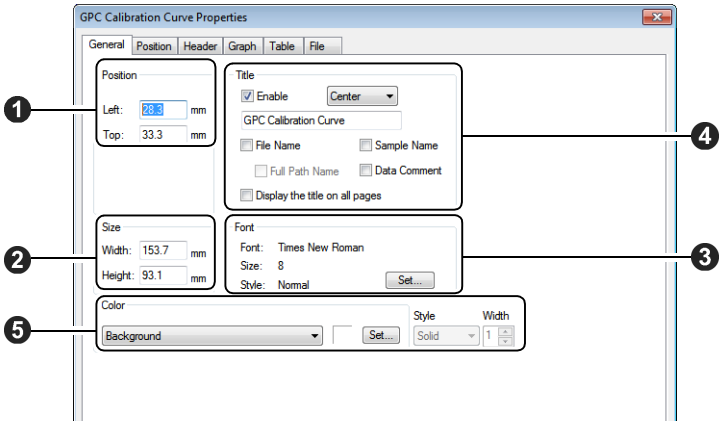
## 3 Select the area where you wish to paste the print item.

On the report creation screen, drag the cursor from the starting point to the ending point of the area where you wish to paste the print item (the calibration curve).



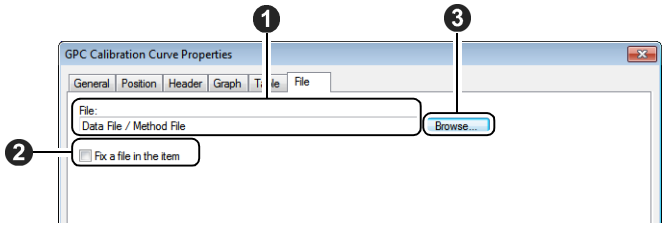
## 4 Specify the print item format.

Set the print position, the size, the font, etc. on the [General] tab.




| No. | Description |
|---|---|
| ❶ | Specify the distance from the upper left corner of the report paper in mm with the [Left] and [Top] print positions. |
| ❷ | Specify the size (in mm) of the print item in [Width] and [Height]. |
| ❸ | Displays the font used for printing. |
| ❹ | Check [Enable] to display the report with a title. |
| ❺ | Select an item to set a color for. |

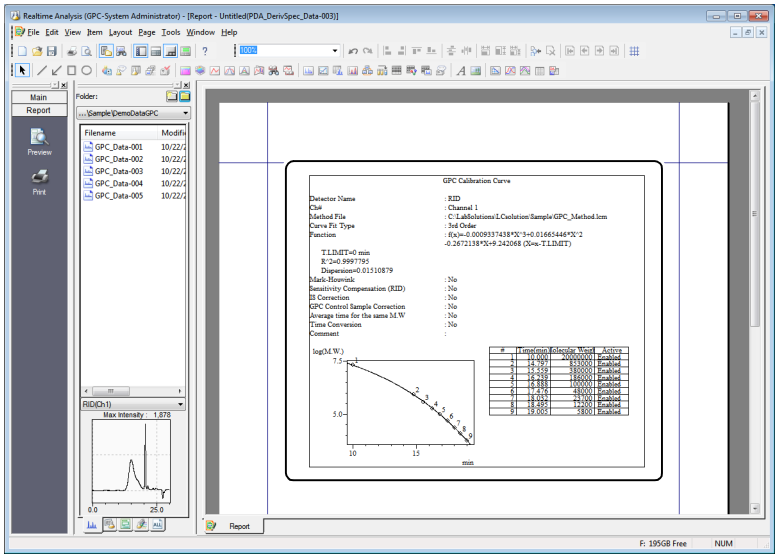
## 5 Click the [File] tab, and specify a file for the print item.



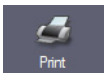

| No. | Description |
|---|---|
| 1 | Specify a file name to print a report. |
| 2 | Check this box to fix the file to print. |
| 3 | Click this to display the file selection screen. |

## 6 Click [OK].

The print item is displayed on the report creation screen.



If you wish to change the position or size of the print item displayed, display the property again and make necessary changes.

Click 

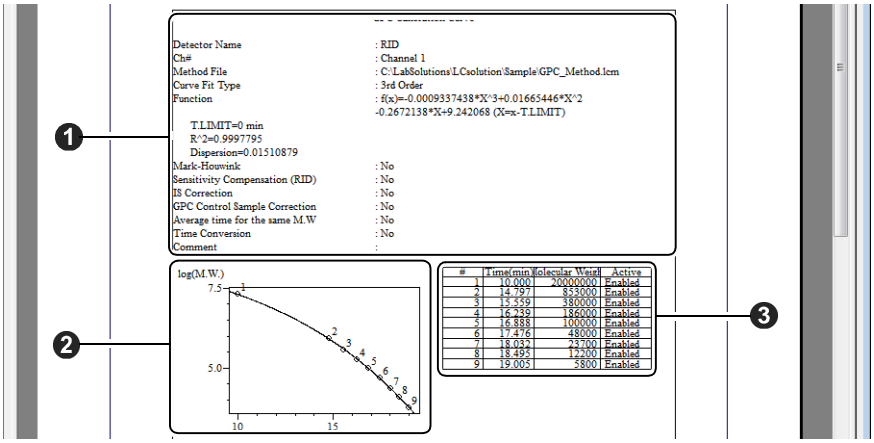
(Print) on the [Report] assistant bar to print the created report.

### NOTE

When you drag and drop a data file from [Data Explorer] to the report creation screen, the actual data is imported and displayed on the report creation screen.

# 6.2 GPC Calibration Curve Item

The calibration curve information used for GPC analysis is laid out on the report as follows:
The header, the calibration curve graph, and the calibration curve table can be configured separately.




| No. | Description |
|---|---|
| ❶ | Header (Calibration curve correction parameters and calibration curve equation information are displayed.) |
| ❷ | Calibration curve graph |
| ❸ | Calibration curve table |

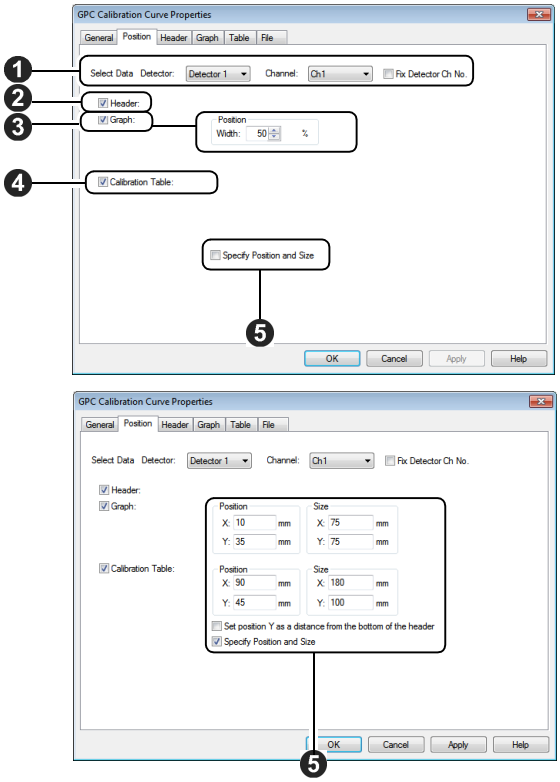
## ■ Setting Position

Positions of the graph and the table in the GPC calibration curve item are set.

**1** **Right-click on an item pasted on the report, and click [Properties] from the menu.**

Double-clicking the item also displays the screen.

**2** **Click the [Position] tab and configure the settings.**

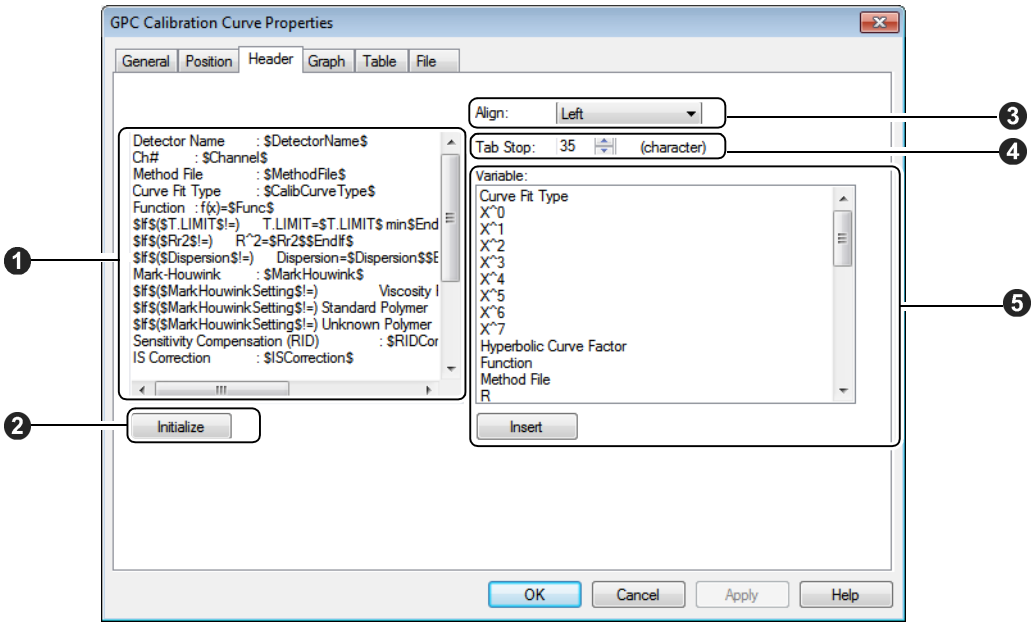



| No. | Description |
|---|---|
| ❶ | Select a detector and a channel to be printed from the combo box.<br>Check [Fix Detector Ch No.] to fix the detector number. |
| ❷ | Check this box to display the header and calibration curve correction parameters. |
| ❸ | Check this box to print the calibration graph. Set the width of the graph optionally. If you make the graph width bigger, the table width becomes smaller. |
| ❹ | Check this box to display the calibration table. |
| ❺ | Check this box to set the position and size of the graph and the table individually. |

## ■ Setting the Header

Set what is to be printed in the header.

### 1 Click the [Header] tab and configure the settings.

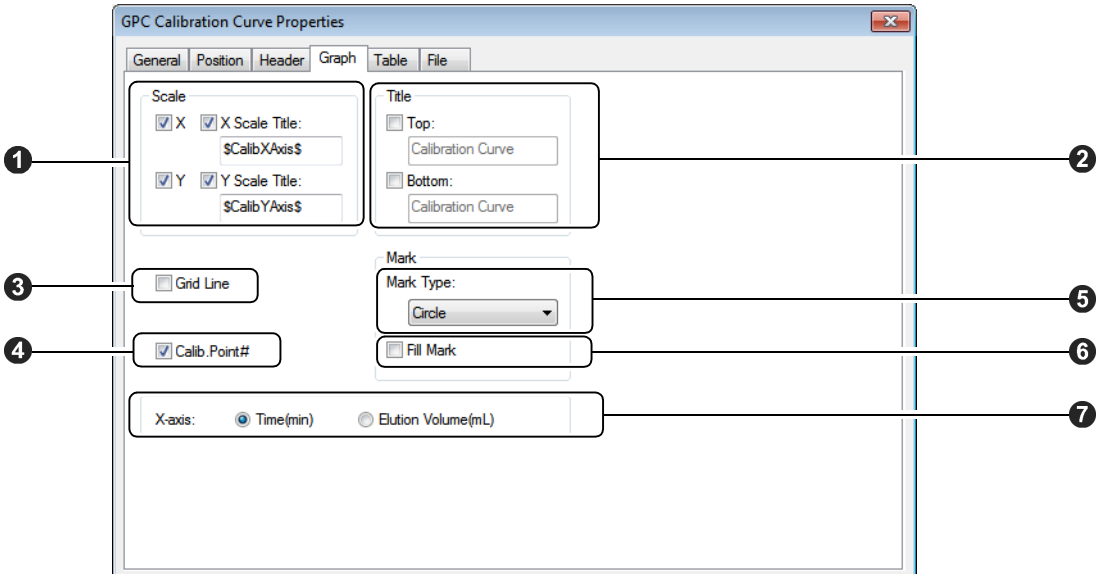



| No. | Description |
|---|---|
| ❶ | Enter and edit letters to be printed. |
| ❷ | Click to restore the text edit area to the initial values. |
| ❸ | Select how you want to align the text in the item frame from the list. |
| ❹ | Specify the number of spaces for a tab stop. Click [▼] or [▲] on the right side or directly enter a desired numeric value. |
| ❺ | Variables can be inserted into the header information. Select them from the variable list. After selecting, click [Insert] to insert the variable at the cursor position in the text edit area. |

## ■ Setting a Graph

Specify how to print out the calibration graph as follows:

**1** **Click the [Graph] tab and configure the settings.**

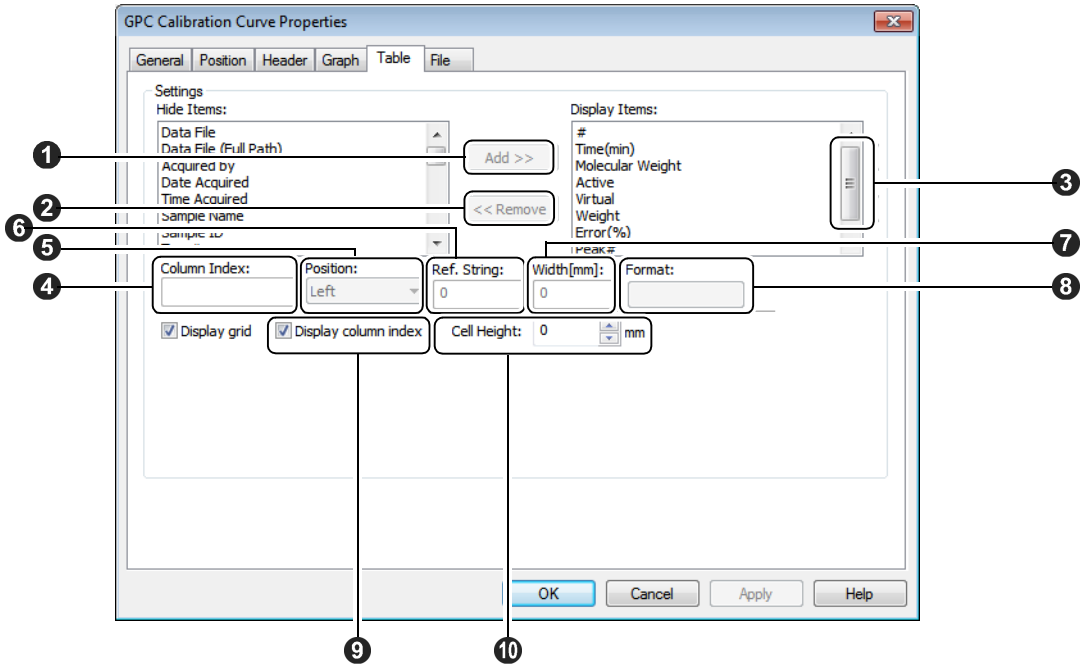



| No. | Description |
|---|---|
| ❶ | Specify the axis types and axis names to be printed on the graph. Check [X] or [Y] to display the graph scale of the axis. $CalibXAxis$ and $CalibYAxis$ can be used as axis names. |
| ❷ | Check these boxes to print a title for each position. |
| ❸ | Check this box to display grid lines. |
| ❹ | Check this box to display a calibration point number on each calibration point. |
| ❺ | Select the mark type of the calibration points. |
| ❻ | Check this box to fill the marks when [Circle] or [Square] is selected in [Mark Type]. |
| ❼ | Select the horizontal axis of the graph. |

## ■ Setting the Table

Set the print format of the calibration table as follows:

**1** **Click the [Table] tab and configure the settings.**



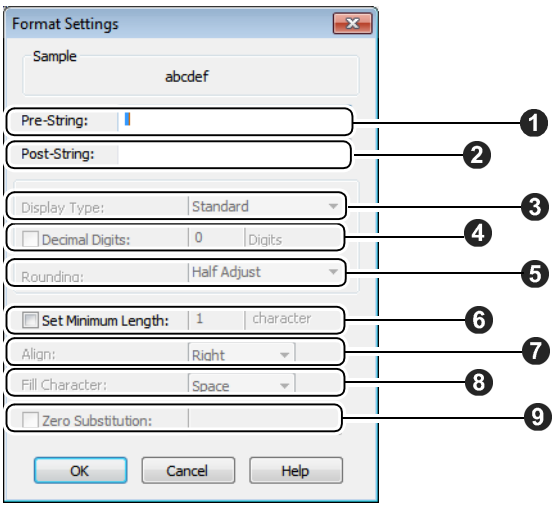

| No. | Description |
|---|---|
| ❶ | Move the item selected in [Hide Items] to [Display Items]. |
| ❷ | Move the item selected in [Display Items] to [Hide Items]. |
| ❸ | Move the item selected in [Display Items] up or down. |
| ❹ | Select a column name to be displayed in the column index row. |
| ❺ | Select the display position for an item from the list. |
| ❻ | Set the number of characters that can be referred to. |
| ❼ | Set the width of the column. |
| ❽ | Click this to display the [Format Settings] screen. (See below) |
| ❾ | Check to display the column index. |
| ❿ | Set the cell height. |

## Setting the format

Set the data format to display in the item frame related to table as follows:
In the properties of the item frame for printing information in a table format, such as in a peak table, click [Format] in the [Format] tab or [Table] tab to display the [Format] screen.

### NOTE

[Format] is enabled when one item of the [Display Items] is selected.




| No. | Description |
|---|---|
| ❶ | Enter characters to be added in the front of data. |
| ❷ | Enter characters to be added in the back of data, such as unit. |
| ❸ | Set the format related to values. |
| ❹ | Check the box to enable the number-of-decimal-digits setting, and enter the number in the text box. |
| ❺ | Select the way to round numbers. |
| ❻ | Check this box to enable the minimum data length setting. Then enter the minimum data length for the data. |
| ❼ | Set the placement within the display range for when the value is less than the minimum data length. |
| ❽ | From the list displayed by clicking [▼] on the right side, select characters to fill in blank digits for the data shorter than the minimum length. |
| ❾ | Set characters to replace the value if it is 0 (zero). |

# 6.3 GPC Graph Item

This item is used to create the print layout for graphs used for GPC analysis.

- Chromatogram
- Calibration curve
- Differential molecular weight curve
- Integral molecular weight curve

These curves in a data file can be output in two graphs.
Combinations which you can overlay are as follows.

- Chromatogram and calibration curve
- Differential curve and integral curve (The horizontal axis is the molecular weight.)

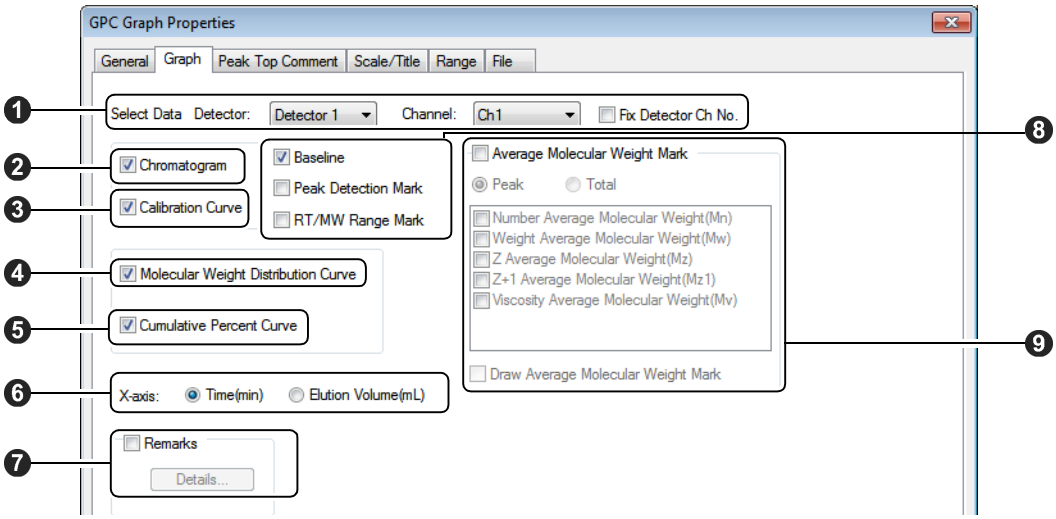
## ■ Setting Graphs to Be Output

Set graphs to be output on report as follows:

**1** **Right-click on an item pasted on the report and click [Properties] from the menu.**

Double-clicking the item also displays the screen.

**2** **Click the [Graph] tab, and configure the settings.**




| No. | Description |
|---|---|
| ❶ | Select a detector and a channel of chromatogram to be output.<br>Check [Fix Detector Ch No.] to fix the detector number. |
| ❷ | Check this box to display the chromatogram. |
| ❸ | Check this box to display the calibration curve. |
| ❹ | Check this box to display the differential curve. |
| ❺ | Check this box to display the integral curve. |
| ❻ | Select the display unit (min. or mL) of the horizontal axis of the graph. |
| ❼ | Check to display annotations. Click [Details] to set the content to be displayed as annotations. |
| ❽ | Check these boxes to display the baseline or peak detection marks on the chromatogram.<br>Check [RT/MW Range Mark] to display marks for the RT/MW range segment. |
| ❾ | Check to display the average molecular weight on the graph. The calculation method for the average molecular weight can be selected from either the detection peak unit or from the entire chromatogram.<br>Check [Draw Average Molecular Weight Mark] to draw a mark noting the average molecular weight. |

# 6.4 GPC Overlay Item

This item is used to overlay graphs of the channel to which the GPC calculation is specified to be done from multiple data files. This is used when you wish to compare chromatograms or differential curves.

**NOTE**

- Different types of curves, such as differential curves and integral curves, cannot be overlayed on a graph.
- Reports with GPC overlay items can be output from the [Report Generator] window.

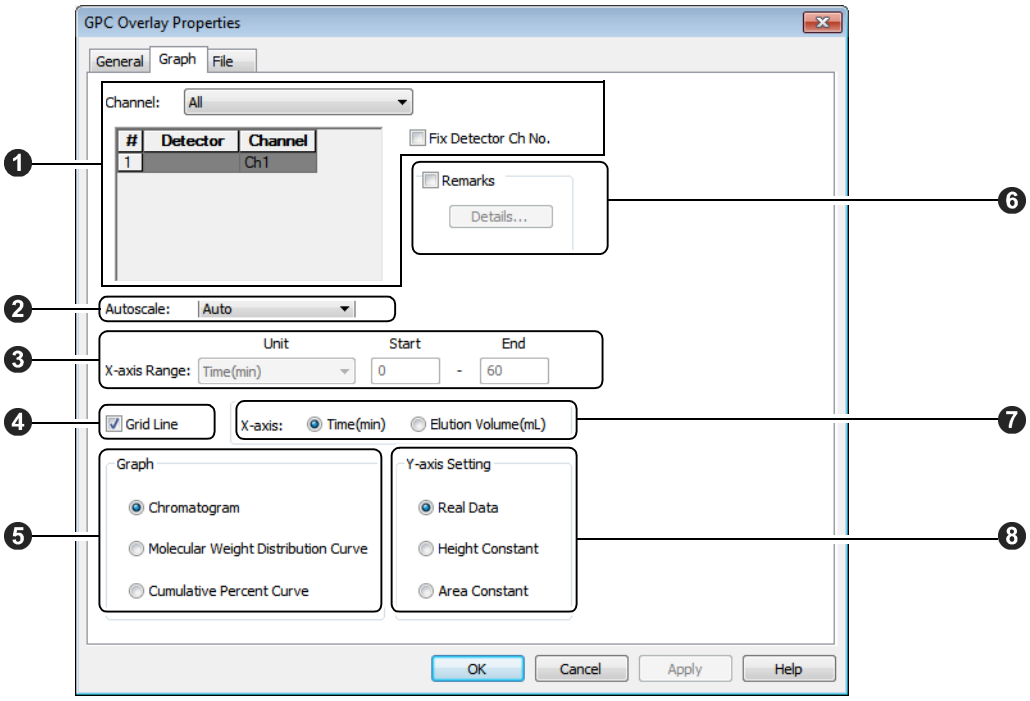
## ■ Setting Graphs to Be Output

Select the type of curves to be overlayed, and specify the output channels.

**1** **Right-click on an item pasted on the report and click [Properties] from the menu.**

Double-clicking the item also displays the screen.

**2** **Click the [Graph] tab in the [GPC Overlay Properties] screen, and configure the settings.**




| No. | Description |
|---|---|
| ❶ | Specify channels to print report.<br>Check [Fix Detector Ch No.] to fix the detector number. |
| ❷ | Select the way to set x-axis display range, automatically or manually. |
| ❸ | Specify the graph output range in time, molecular weight, or log(molecular weight). |
| ❹ | Check this box to display grid lines in the graph. |
| ❺ | Select one from chromatogram, molecular weight distribution curve, and cumulative percent curve. |
| ❻ | Check to display annotations. Click [Details] to set the content to be displayed as annotations. |
| ❼ | Select the horizontal axis of the graph. |
| ❽ | Select the way to display the graph. This selection is disabled for a cumulative percent curve. |

# 6.5 GPC Summary Item

This item is used to perform statistical calculations with molecular weight calculation results from multiple data and to calculate and output the statistics (average, %RSD, maximum value, minimum value, and standard deviation) to report.
You can select whether to perform statistical calculations by chromatogram or RT/MW range.
Statistical calculations are performed for the following molecular weight calculation results.

- Number average molecular weight (Mn)
- Weight average molecular weight (Mw)
- Z average molecular weight (Mz)
- Z+1 average molecular weight (Mz1)
- Viscosity average molecular weight (Mv)
- Mw/Mn
- Mv/Mn
- Mz/Mw
- Intrinsic viscosity

## Printing by chromatogram

Statistical calculation is performed with the total molecular weight of the channel in which "GPC Calculation" is enabled at the selected channel, and statistic values are output in the following print image.

GPC Summary

Chromatogram Det.A Ch1

| Title | Mn | Mw | Mz | Mz1 | Mv | Mw/Mn | Mv/Mn |
|---|---|---|---|---|---|---|---|
| Demo_Data-001.lcd | 540003 | 649782 | 785064 | 922862 | 0 | 1.20329 | 1.20819 |
| Demo_Data-002.lcd | 528411 | 648459 | 780364 | 902890 | 0 | 1.22719 | 1.20341 |
| Average | 534207.73 | 649121.38 | 782714.22 | 912876.38 | 0.00 | 1.22 | 1.21 |
| %RSD | 1.53 | 0.14 | 0.42 | 1.55 | 0.00 | 1.39 | 0.28 |
| Maximum | 540003.71 | 649782.93 | 785064.35 | 922862.18 | 0.00 | 1.23 | 1.21 |
| Minimum | 528411.76 | 648459.83 | 780364.09 | 902890.59 | 0.00 | 1.20 | 1.20 |
| SD | 8196.75 | 935.57 | 3323.59 | 14122.04 | 0.00 | 0.02 | 0.00 |

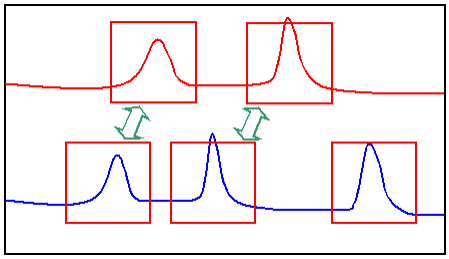
Adding data files increases number of these rows.

You can configure which statistical calculation values should be included in the table.

## Printing by RT/MW range

Various types of average molecular weight are displayed by RT/MW range of the channel in which GPC calculation is enabled, and the statistic values are output. Since you can set multiple RT/MW ranges for a channel, statistical calculations are performed in the ascending order of the retention time of each channel.

- RT/MW range mapping image



The time range of RT/MW range set by data differs, but statistical calculations are performed by RT/MW range where the retention time is short, and the results are output.
Output image

GPC Summary

RT/MW Range1 Det.A Ch1

| Title | Mn | Mw | Mz | Mz1 | Mv | Mw/Mn | Mv/Mn |
|---|---|---|---|---|---|---|---|
| Demo_Data-001.lcd | 1193565 | 1198146 | 1203054 | 1208309 | 0 | 1.00384 | 1.00410 |
| Demo_Data-002.lcd | 1177332 | 1178125 | 1178949 | 1179817 | 0 | 1.00067 | 1.00070 |
| Average | 1185448.97 | 1188135.85 | 1191002.19 | 1194063.78 | 0.00 | 1.00 | 1.00 |
| %RSD | 0.97 | 1.19 | 1.43 | 1.69 | 0.00 | 0.22 | 0.24 |
| Maximum | 1193565.88 | 1198146.59 | 1203054.74 | 1208309.90 | 0.00 | 1.00 | 1.00 |
| Minimum | 1177332.06 | 1178125.11 | 1178949.64 | 1179817.67 | 0.00 | 1.00 | 1.00 |
| SD | 11479.04 | 14157.32 | 17044.88 | 20147.05 | 0.00 | 0.00 | 0.00 |

RT/MW Range2 Det.A Ch1

| Title | Mn | Mw | Mz | Mz1 | Mv | Mw/Mn | Mv/Mn |
|---|---|---|---|---|---|---|---|
| Demo_Data-001.lcd | 828772 | 830381 | 832046 | 833765 | 0 | 1.00194 | 1.00201 |
| Demo_Data-002.lcd | 818922 | 820140 | 821426 | 822783 | 0 | 1.00149 | 1.00157 |
| Average | 823847.66 | 825260.93 | 826736.70 | 828274.26 | 0.00 | 1.00 | 1.00 |
| %RSD | 0.85 | 0.88 | 0.91 | 0.94 | 0.00 | 0.03 | 0.03 |
| Maximum | 828772.94 | 830381.49 | 832046.54 | 833765.41 | 0.00 | 1.00 | 1.00 |
| Minimum | 818922.37 | 820140.38 | 821426.86 | 822783.12 | 0.00 | 1.00 | 1.00 |
| SD | 6965.40 | 7241.56 | 7509.25 | 7765.65 | 0.00 | 0.00 | 0.00 |

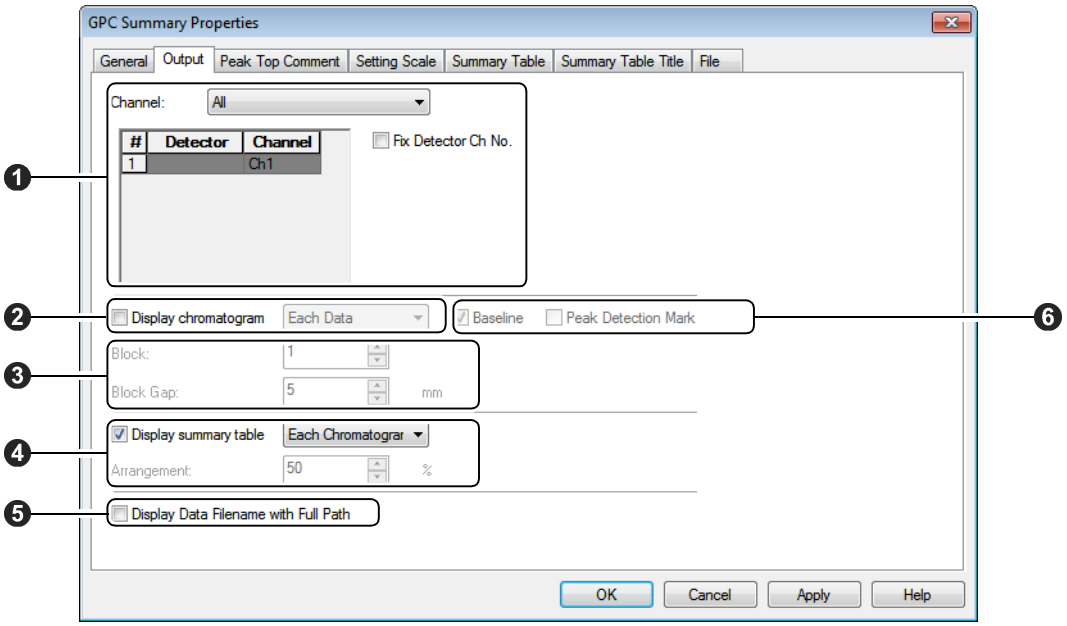
## ■ Setting Summary Output

Select the statistical values for the output and whether the output is by chromatogram or by RT/MW range.

**1** **Right-click on an item pasted on the report and click [Properties] from the menu.**

Double-clicking the item will also display the [Properties].

**2** **Click the [Output] tab, and configure the settings.**

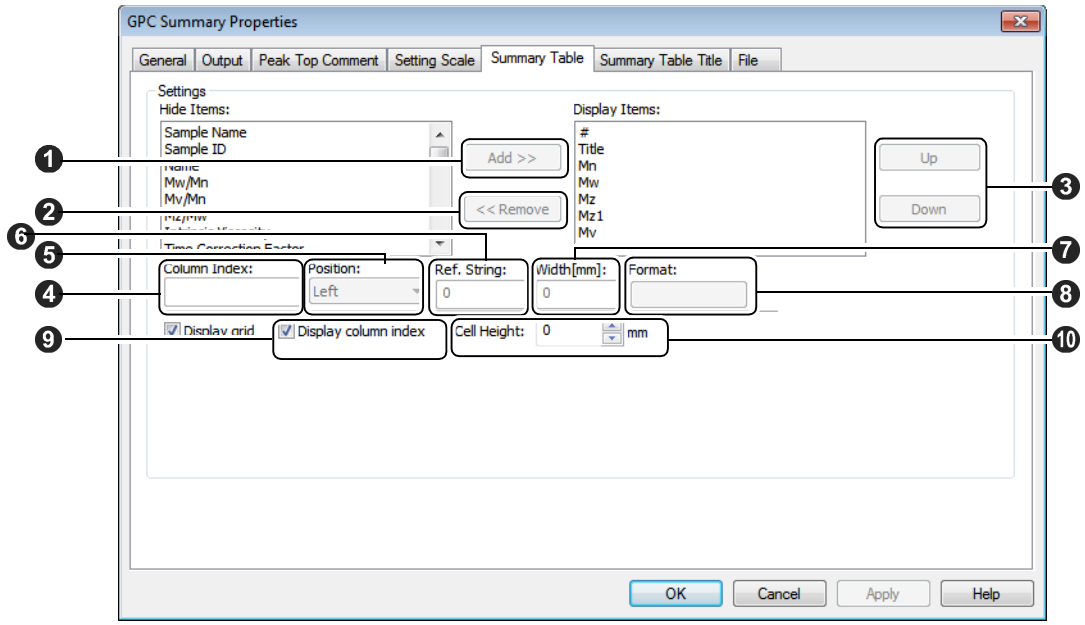



| No. | Description |
|---|---|
| ❶ | Specify the channel to be output. Check [Fix Detector Ch No.] to fix the detector number. |
| ❷ | Check this box to display the chromatogram.<br>Set the chromatogram to be output by [Each Data], [Each Detector], or [Each Channel]. |
| ❸ | Set the lateral arrangements of the chromatogram. You can also set the width between the blocks. |
| ❹ | Check to display the summary table. Specify the output unit as either [Each Chromatogram] or [Each RT/MW]. You can also specify the display ratio of the chromatogram and the table. |
| ❺ | Check this box to display data file names in the title column with their paths. |
| ❻ | Check [Baseline] to connect peak baselines with a line.<br>Check [Peak Detection Mark] to display peak detection marks. |

## ■ Setting Summary Table (Column Setting)

Set column configuration of the summary calculation result table as follows:

**1** **Click the [Summary Table] tab, and configure the settings.**

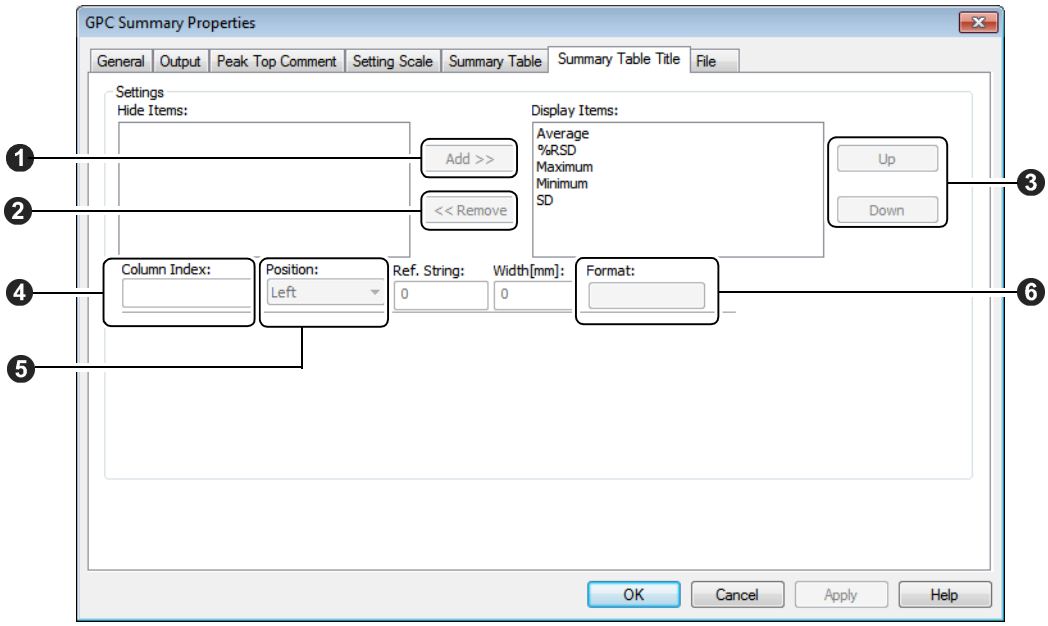



| No. | Description |
|---|---|
| ❶ | Move the item selected in [Hide Items] to [Display Items]. |
| ❷ | Move the item selected in [Display Items] to [Hide Items]. |
| ❸ | Move the item selected in [Display Items] up or down. |
| ❹ | Select a column name to be displayed in the column index row. |
| ❺ | Select the display position for an item from the list. |
| ❻ | Set the number of characters that can be referred to. |
| ❼ | Set the width of the column. |
| ❽ | Click to display the [Format] screen. |
| ❾ | Check this box to display the column index. |
| ❿ | Set the cell height. |

## ■ Setting Summary Table (Setting Title)

Set row configuration of the summary calculation result table as follows:

**1 Click the [Summary Table Title] tab, and configure the settings.**

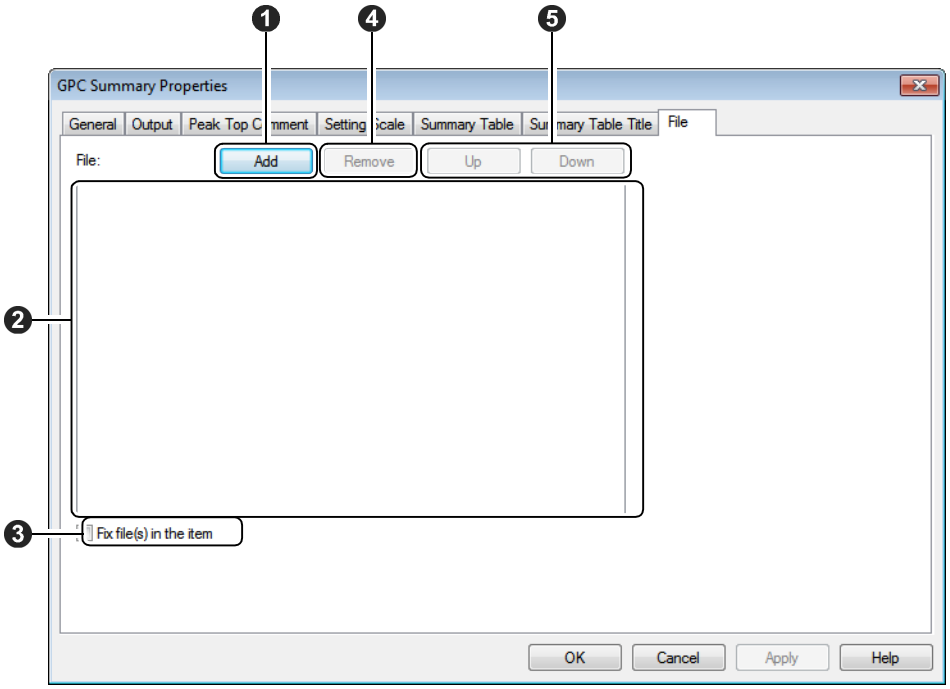



| No. | Description |
|---|---|
| ❶ | Move the item selected in [Hide Items] to [Display Items]. |
| ❷ | Move the item selected in [Display Items] to [Hide Items]. |
| ❸ | Move the item selected in [Display Items] up or down. |
| ❹ | Set the title to be displayed in the row index column (leftmost column). |
| ❺ | Select the display position for an item from the list. (Position setting is available only for %RSD.) |
| ❻ | Click to show the [Format] screen. (Format setting is available only for %RSD.) |

## ■ Setting Files

Set the list of data files to create a summary.

### 1 Click the [File] tab, and configure the settings.




| No. | Description |
|---|---|
| ❶ | Click to display the [Open File] screen. Select the data files. |
| ❷ | Displays a data file list. |
| ❸ | Check this box for a fixed file name to print. |
| ❹ | Click this to remove the file selected in the data file list from the calculation target, and delete it from the list. |
| ❺ | Click the [Up] or [Down] to change the order of files in the data file list. |

# 6.6 Method Item

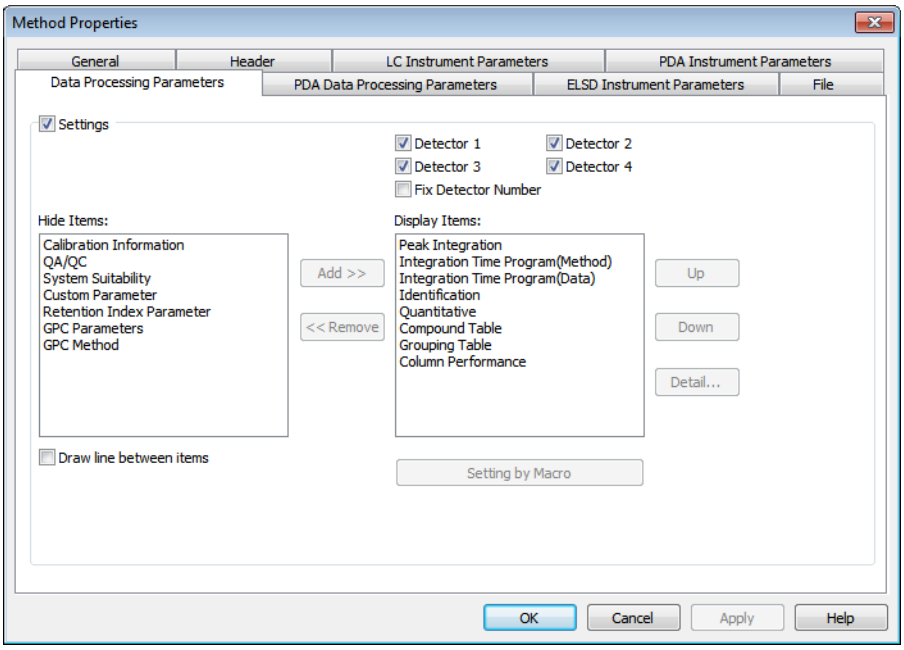
Method parameters of the GPC analysis can be output from the conventional method report items. Following parameters that are necessary for GPC analysis are output.

- Title
- Element name
- Q factor
- Alpha value
- K value
- Flow setting
- Flow value
- Molecular weight distribution
- Molecular weight per degree of polymerization
- Channel number
- Filtration limit time
- Time correction method
- Time correction parameters
- Delay time correction
- Sensitivity Compensation of RI Detectors
- RT/MW range setting

## ■ GPC Parameters

**1** **Right-click on an item pasted on the report and click [Properties] from the menu.**

**2** **Click the [Data Processing Parameters] tab and configure the settings.**



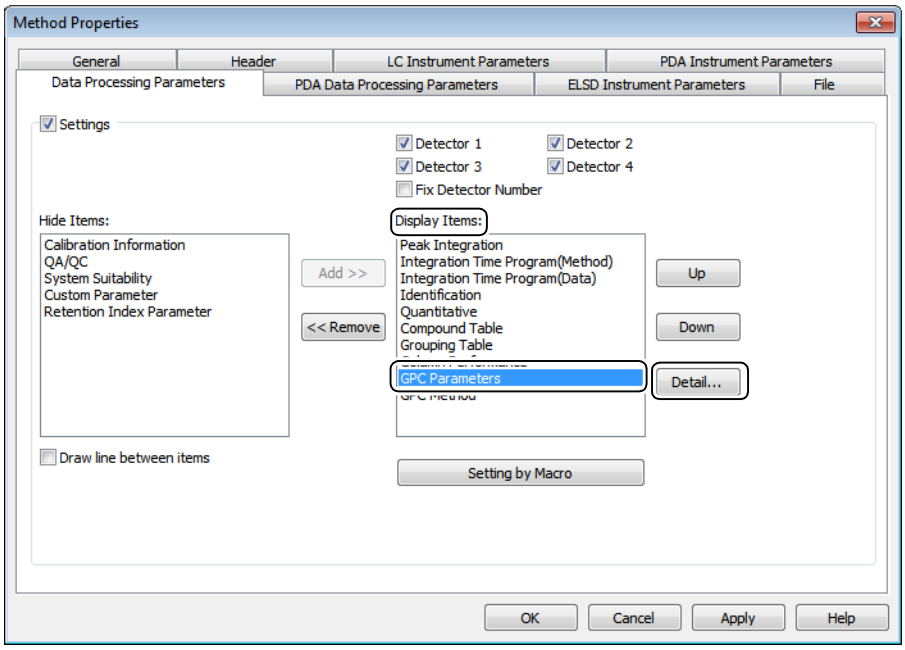

**NOTE**

The GPC items are [GPC Parameters] and [GPC Method].

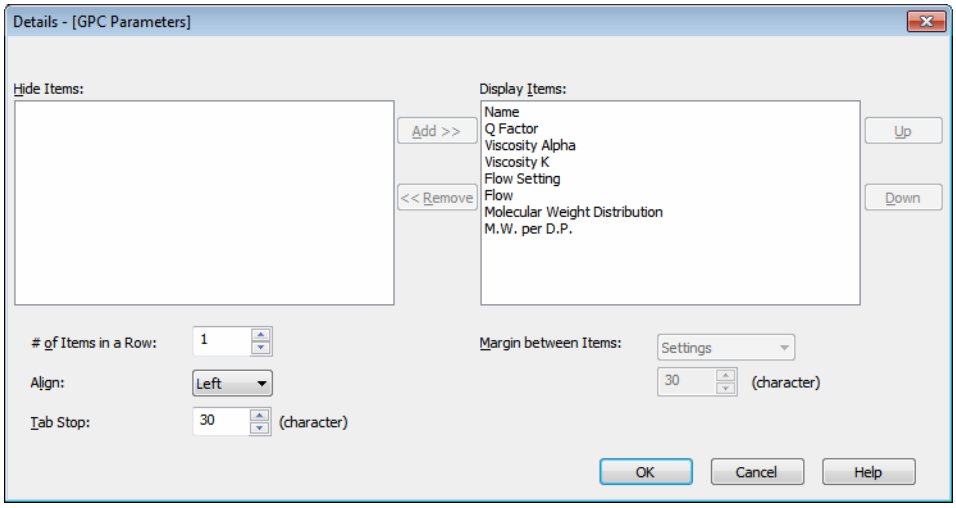
## ■ Setting [Details of GPC Parameters]

Set the output items for method information set as GPC parameters.

### 1 Select [GPC Parameters] from the [Display Items], and click [Detail].




### 2 Configure the settings.




**NOTE**

All items are [Display Items] by default.
Move items that should not be output to [Hide Items] and click [OK].

## ■ Setting [Details of GPC Methods]

Set the output items for method information for each channel set as the GPC method.

**Reference**

See "■ Setting [Details of GPC Parameters]" for operation of the [Detail] screen of the GPC methods.

# 6.7 GPC Calculation Result

Slice information, peak information, and various average molecular weight information are output as the GPC calculation result. The calculation result can be output by peak or RT/MW range.

GPC Results

Peak#:1 (RID Channel 1)

[Slice Information]

| Slice# | Time(min) | ıtion Volume(m | olecular Weigl | Height | Area | Sub Total | % |
|---|---|---|---|---|---|---|---|
| 1 | 12.138 | 12.138 | 6062679 | 0 | 0 | 291334 | 100.0000 |
| 2 | 12.971 | 12.971 | 3470651 | 42 | 21 | 290006 | 99.5439 |
| 3 | 13.804 | 13.804 | 1865625 | 299 | 149 | 275842 | 94.6822 |
| 4 | 14.638 | 14.638 | 934679 | 779 | 390 | 220669 | 75.7443 |
| 5 | 15.471 | 15.471 | 433194 | 757 | 379 | 138719 | 47.6150 |
| 6 | 16.304 | 16.304 | 184350 | 444 | 222 | 78900 | 27.0824 |
| 7 | 17.138 | 17.138 | 71499 | 294 | 147 | 42898 | 14.7245 |
| 8 | 17.971 | 17.971 | 25085 | 203 | 102 | 17766 | 6.0980 |
| 9 | 18.804 | 18.804 | 7902 | 78 | 39 | 3705 | 1.2718 |
| 10 | 19.638 | 19.638 | 2218 | 8 | 4 | 107 | 0.0367 |

[Peak Information]

| Title | Time(min) | ıtion Volume(m | olecular Weigl | Height |
|---|---|---|---|---|
| Start | 12.133 | 12.133 | 6078726 | 9 |
| Top | 14.974 | 14.974 | 692160 | 848 |
| End | 19.917 | 19.917 | 1411 | 50 |

Area : 145667
Area% : 100.000
Resolution(GPC) : 0.621
GPC Calibration Slope : -0.3965208

[Average Molecular Weight]

| | |
|---|---|
| Number Average Molecular Weight(Mn) | 96308 |
| Weight Average Molecular Weight(Mw) | 646690 |
| Z Average Molecular Weight(Mz) | 1292398 |
| Z+1 Average Molecular Weight(Mz1) | 1893795 |
| Viscosity Average Molecular Weight(Mv) | 0 |
| Mw/Mn | 6.71480 |
| Mv/Mn | 0.00000 |
| Mz/Mw | 1.99848 |
| Intrinsic Viscosity | 1.00000 |
| % | 100.0000 |

RID Channel 1

[Average Molecular Weight(Total)]

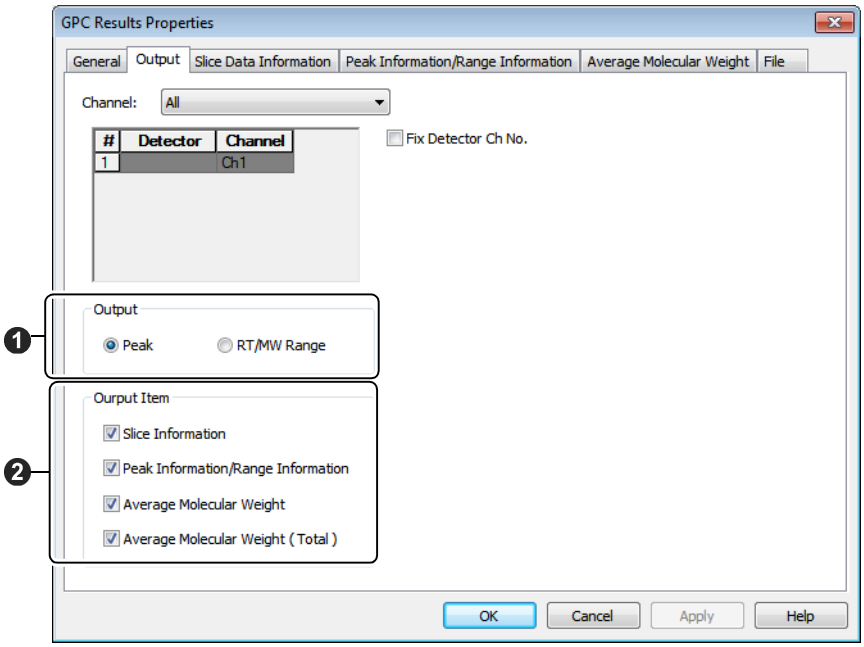
| | |
|---|---|
| Number Average Molecular Weight(Mn) | 96308 |
| Weight Average Molecular Weight(Mw) | 646690 |
| Z Average Molecular Weight(Mz) | 1292398 |
| Z+1 Average Molecular Weight(Mz1) | 1893795 |
| Viscosity Average Molecular Weight(Mv) | 0 |
| Mw/Mn | 6.71480 |
| Mv/Mn | 0.00000 |
| Mz/Mw | 1.99848 |
| Intrinsic Viscosity | 1.00000 |
| % | 100.0000 |

## ■ Output Setting

Select whether the GPC calculation result is output by peak or by RT/MW range. You can also select calculation result items of slice information, peak information or average molecular weight.

**1** **Right-click on an item pasted on the report and click [Properties] from the menu.**

**2** **Click the [Output] tab, and configure the settings.**



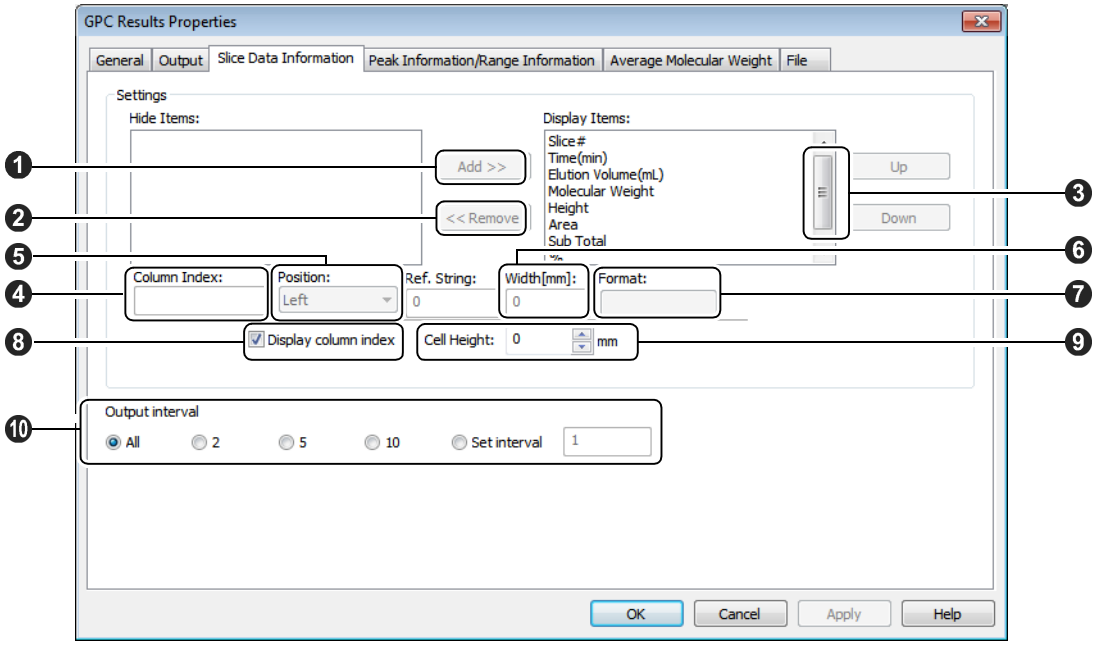

| No. | Description |
|---|---|
| ❶ | Select whether the calculation result is printed by peak or by RT/MW range. |
| ❷ | Select items to display as calculation result. Uncheck all to display only titles such as peak number or RT/MW range number. |

## ■ Slice Information

Set the display format of the slice information as follows: You can set the display format by grid.

### 1 Click the [Slice Data Information] tab, and configure the settings.

The [Slice Data Information] screen appears.

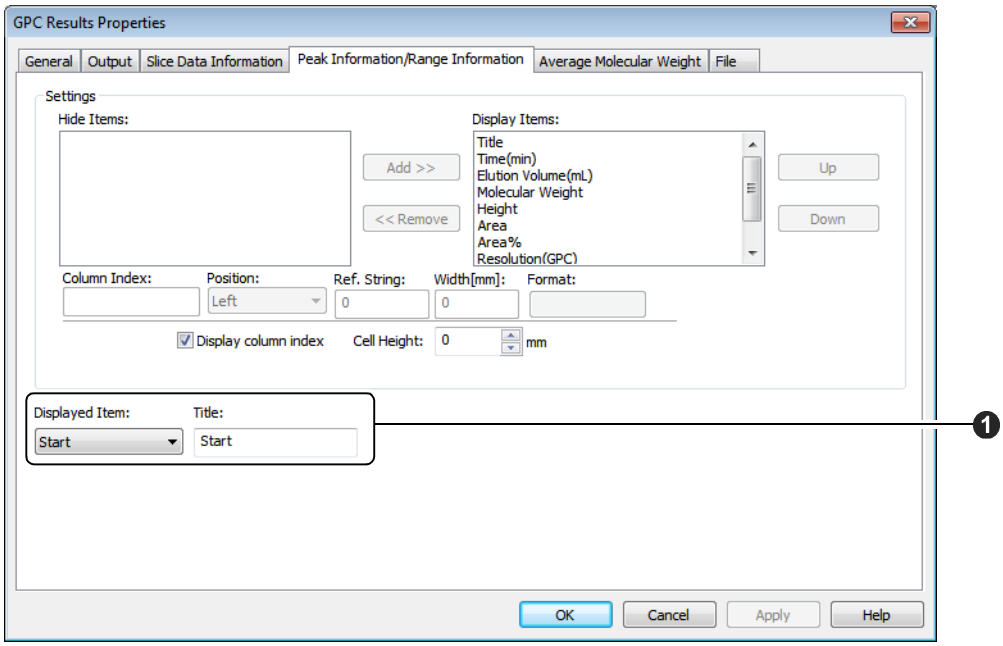



| No. | Description |
|---|---|
| ❶ | Move the item selected in [Hide Items] to [Display Items]. |
| ❷ | Move the item selected in [Display Items] to [Hide Items]. |
| ❸ | Move the item selected in [Display Items] up or down. |
| ❹ | Select a column name to be displayed in the column index row. |
| ❺ | Select the display position for an item from the list. |
| ❻ | Set the width of the column. |
| ❼ | Click to display the [Format] screen. |
| ❽ | Check this box to display the column index. |
| ❾ | Set the cell height. |
| ❿ | You can select whether to display all of the slice information or to skip a certain number of slices. |

## ■ Peak Information

Set each title of the peak information data.

**1** **Click the [Peak Information/Range Information] tab, and configure the results.**

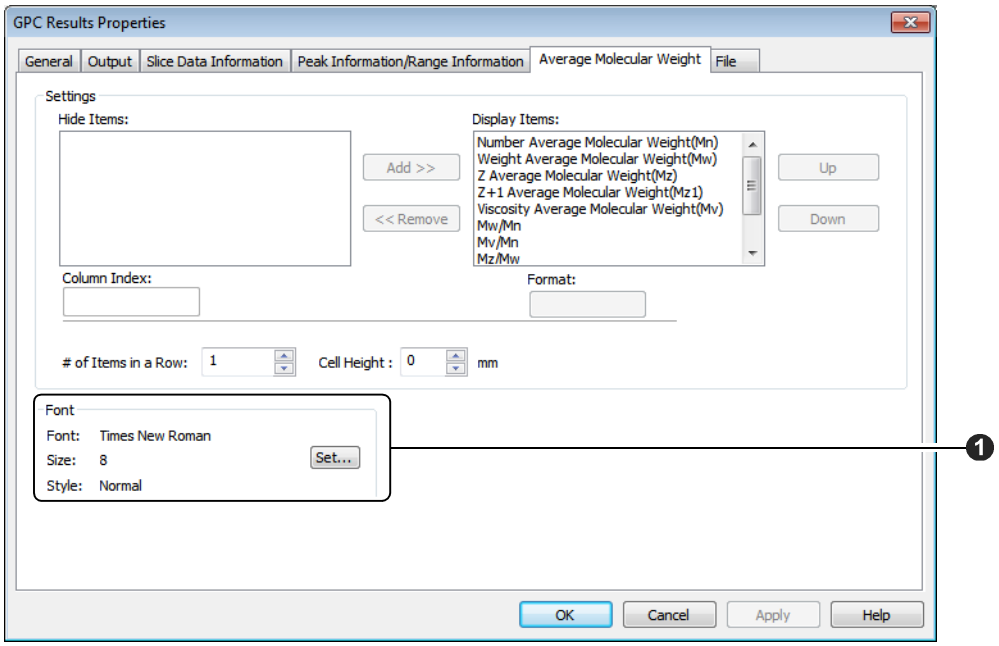



| No. | Description |
|---|---|
| ❶ | You can select title items of the peak information and change the titles.<br>Start: Peak start time, Top: Peak top time, End: Peak end time |

## ■ Average Molecular Weight

Set the print output format of the average molecular weight result.

**1** **Click the [Average Molecular Weight] tab, and configure the settings.**




| No. | Description |
|---|---|
| ❶ | You can select fonts of the molecular weight result to be output. You can emphasize the molecular weight result by selecting fonts. |

# 7 GPC File Converter

The GPC file converter provides the following functions:

- Importing of method files created by CLASS-LC10/CLASS-VP GPC software
- Creation of files by merging a LabSolutions method file and a CLASS-LC10/CLASS-VP GPC method file

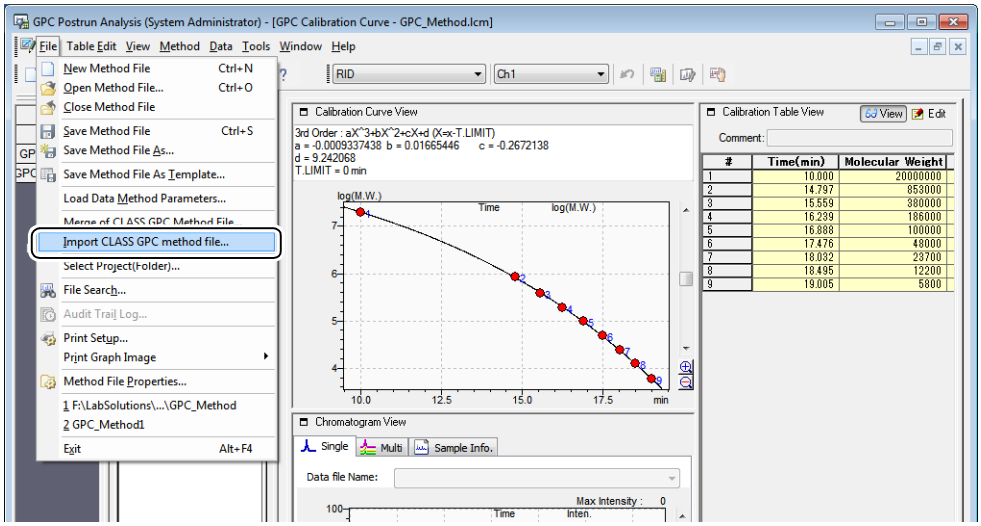
The conversion items in a file are as follows:

- User who created the file, date created, comment
- GPC parameters (such as GPC parameters, correction parameters, RT/MW range table)
- Calibration curve information

## 7.1 Importing a Method File

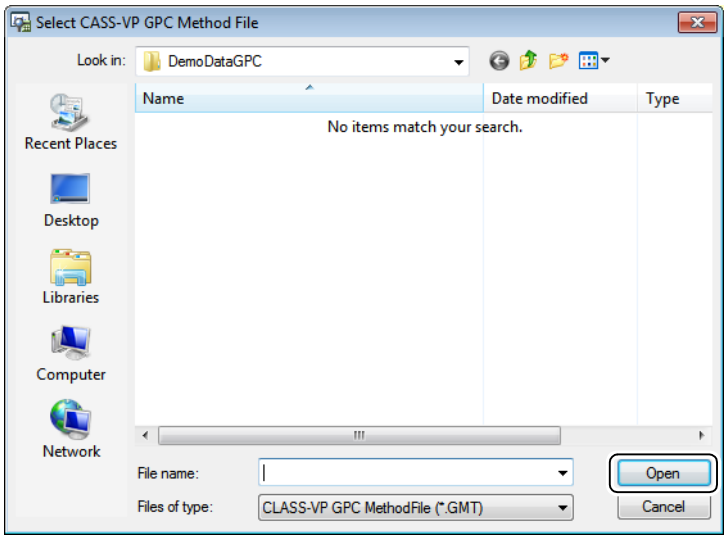
Import the information of a CLASS-LC10/CLASS-VP GPC method file by opening it.
Information of a CLASS-LC10/CLASS-VP method file is imported to the current detector channel.

**1** **Click [Import CLASS GPC Method File] from the [File] menu in the [GPC Calibration Curve] window.**



**2** **Select a CLASS GPC method file and click [Open].**

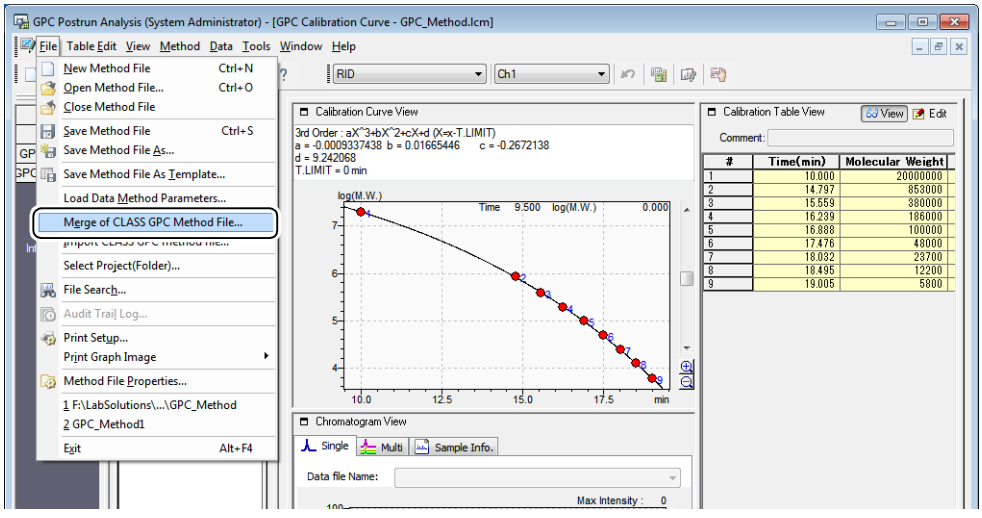
A CLASS-LC10/CLASS-VP GPC method file is opened.



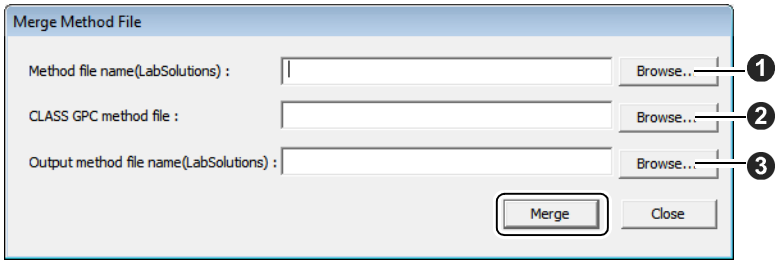

# 7.2 Merging GPC Method Files

Create a new LabSolutions method file by merging an existing LabSolutions method file and a CLASS-LC10/CLASS-VP GPC method file.
Information of a CLASS GPC method file is deployed to all the channels of detectors in a LabSolutions method file.

**1** **Click [Merge of CLASS GPC Method File] from the [File] menu of the [GPC Calibration Curve] window.**



## 2 Specify file to be merged and click [Merge].




| No. | Description |
|---|---|
| ❶ | Select or input [Method file(LabSolutions)]. |
| ❷ | Select or input [CLASS GPC method file]. |
| ❸ | Select or input [Output method file name(LabSolutions)]. |

**NOTE**

- When you select or input the name of an existing file in ❸, the file is overwritten.
- If there are multiple files you wish to merge, repeat the above.

## 3 Click [Close].

If the audit trail setting is enabled with a method file, a CLASS-LC10/CLASS-VP GPC method file cannot be merged with it.

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# 8 Appendix

This chapter details help for problems with software operation, the method for checking the content of online manuals, and information on LabSolutions GPC specifications.

## 8.1 When Having Problems with the Operation

This software provides the help menu and online manuals. Use these for any uncertainties in operation and the terms on the screen.

### 8.1.1 Using Help

To check the help for this software, open the help using one of the following methods.

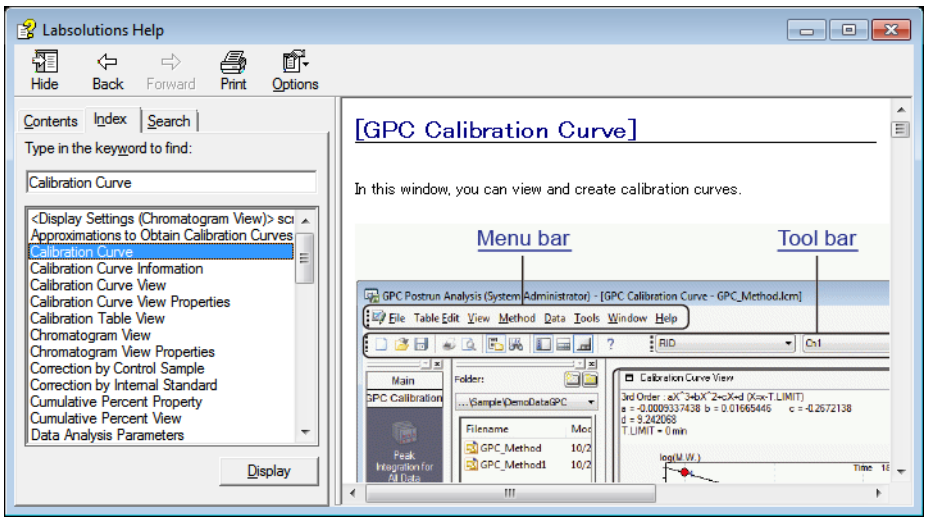
| Operation Type | Operation Method |
|---|---|
| [Help] | Click [Help] on the screen.<br>Display the help for the open window. |
| ? (Contents) | Click ? (Contents) in the toolbar. |
| [Help] menu | Click [Contents] from the [Help] menu. |
| [F1] key | Press the [F1] key on the keyboard.<br>To verify the content of the open screen, press the [F1] key to display the help that corresponds to the open screen. |

#### ■ Searching by Keyword

For unfamiliar terms and parameters, enter a keyword and search. A list of topics matching the keyword will be displayed. You can view the help that matches the term or parameter from the topic.

**1** **Open the help.**

**2** **Click the [Index] tab, and perform a search.**



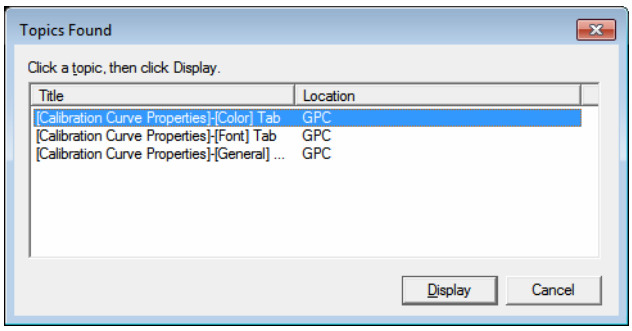
1 Enter a keyword to search, and press the [Enter] key on the keyboard.
Topics that match the keyword will be displayed in alphabetical order.

2 Click a topic.

3 Click [Display].
The content of the selected topic will be displayed.

**NOTE**

- When there are multiple topics for a specific keyword, the [Topics Found] screen is opened. Select the specific keyword from the list of titles on the screen, and click [Display].



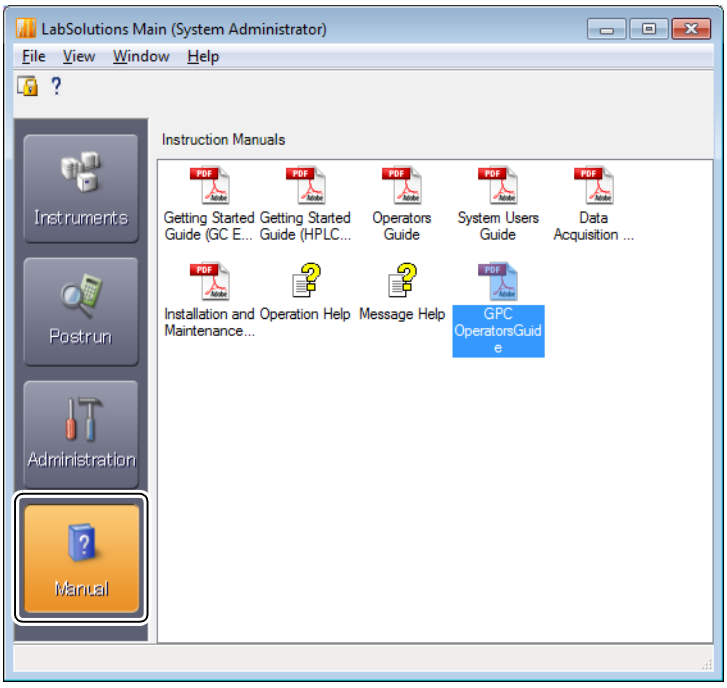

- The [Search] tab of the help allows full-text searching of help content for terms registered in the help.

## 8.1.2 Using Online Manuals

The contents of the 'Operation Manual' and 'Administration Manual' of the LabSolutions Instruction Manual can be viewed on the screen.

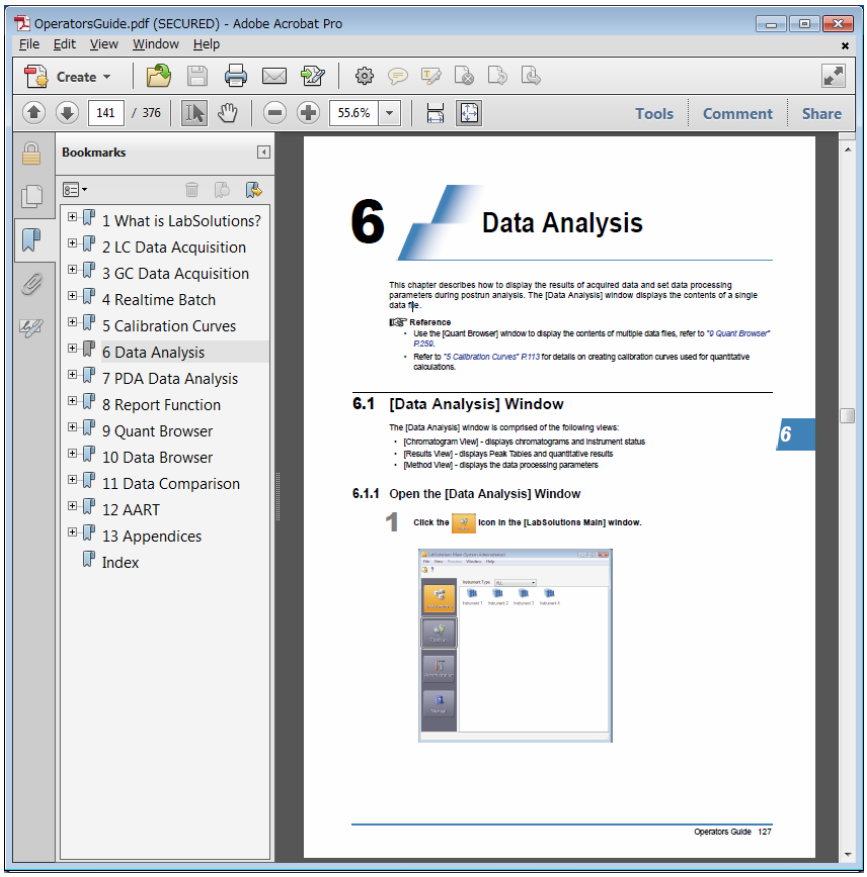
**1 Click  (Manual) on the [LabSolutions Main] window.**





**2** **Click the icon of the instruction manual to be viewed.**

"Adobe Reader" is started, and the instruction manual is opened.




| No. | Description |
|---|---|
| ❶ | Click the hierarchically structured bookmarks (table of contents) to display the desired page. |
| ❷ | Search for terms used in the manual. |
| ❸ | Click the references or the terms in blue to jump to the page of the related item. |

**NOTE**

- The "Operation Manual" online manual can be opened by clicking [Online Manual] from the [Help] menu.
- Adobe Reader is started for opening the online manual.
- Visit the Adobe web site for more information about Adobe Reader.

# 8.2 Specifications of LabSolutions GPC

## ■ Control Device

- Up to 4 systems can be controlled by one PC, and PDA detectors can be connected to 2 of these systems at maximum.
- GPC analysis and ordinary analysis can be performed simultaneously on one PC.
- Data from a GPC or LC device from other manufacturers can be processed by installing an A/D board on the system controller (CBM-20A, SCL-10Avp).

**NOTE**

Number of controllable systems and the type of controllable devices depend on the LabSolutions license.

## ■ Peak Integration

- Peak integration by peak integration parameters, time programs and manipulations can be performed.
- Number of slices: Up to 5000 (by channel. Up to 4 channels can be used in a PDA detector.

## ■ Data Analysis

| | |
|---|---|
| Calibration curve approximate equations | Straight line by the least square method, third order equation, third order equation + hyperbolic curve, fifth order equation, fifth order equation + hyperbolic curve, seventh order equation, seventh order equation + hyperbolic curve, and point-to-point |
| Number of data in calibration curve | Up to 64 |
| Calibration curve correction | Conversion using the Q factor or Mark-Houwink equation. |
| Time correction | Time correction using the internal standard peak or the control sample. |
| GPC calculation | Number average molecular weight (Mn), weight average molecular weight (Mw), Z average molecular weight (Mz), Z+1 average molecular weight (Mz1), viscosity average molecular weight (Mv), intrinsic viscosity, and polydispersity (such as Mw/Mn) calculations for the entire elution curve, for each peak, and for each specified range. |
| Others | Correction of the RID sensitivity. |

## ■ Data Comparison

- Number of data files that can be compared: Up to 10
- Chromatograms, the differential molecular weight distribution curve, and the integral molecular weight distribution curve can be overlayed.
- Parallel displacement of chromatograms in the direction of time axis, recalculation of the molecular weight distribution by the correction time after parallel displacement, and displaying the molecular weight distribution curve are possible.
- Statistical calculation results (average, maximum, minimum, %RSD, standard deviation) of the number average molecular weight (Mn), the weight average molecular weight (Mw), the Z average molecular weight (Mz), the Z+1 average molecular weight (Mz1), the viscosity average molecular weight (Mv), the intrinsic viscosity, and the polydispersity (such as Mw/Mn) for the entire elution curve or any specified range can be displayed.

## ■ Report

- Reports can be created using flexible formats by selecting the report items (such as chromatogram, calibration curve, GPC graph, GPC overlay, and GPC calculation result).
- The output of summary reports and statistical calculation results (average, maximum, minimum, %RSD, standard deviation) using the GPC summary items is possible.
- Multiple page layout is supported.
- Reports can be previewed.

## ■ File Conversion

- GPC method files of CLASS-LC10/CLASS-VP GPC software can be imported.
- GPC calculation results can be output into an ASCII file.
- LCsolution GPC data files and method files can be read as they are. However, files created with LabSolutions GPC cannot be read by LCsolution GPC.