Preface

The LabSolutions IR software is one component of the LabSolutions software package and is used with the Shimadzu's Fourier Transform Infrared Spectrophotometer series to control the instrument and perform data analysis.
The operation manual for the LabSolutions IR software comprises four volumes including this manual. This quick guide briefly introduces the LabSolutions IR software from startup through to initial operation.
For more details on usage, refer to the corresponding operation manual.

- Installation and Maintenance Manual — This manual explains software installation, troubleshooting, and environment settings.
- Management Manual — This manual explains how to use the management function and validation software.
- Basic Operation Manual — This manual explains specifically how to perform basic operations using the software.
- Quick Guide — This quick guide briefly introduces software startup through to initial operation.

Quick Guide Notation

NOTE	Emphasizes additional information that is provided to ensure the proper use of this product.
HINT	Indicates information provided to improve product performance.
☞	Indicates the location of related reference information.

NOTICES

- If the user or usage location changes, ensure that this Instruction Manual is always kept together with the product.
- 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.
- All rights are reserved, including those to reproduce this manual or parts thereof in any form without permission in writing from Shimadzu Corporation.
- The contents of the hard disk of the personal computer may be lost as the result of an unforeseen accident. Always create a backup to protect critical data from such accidents.
- 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.
- Original version is approved in English.

Dec. 2012

Contents

Software

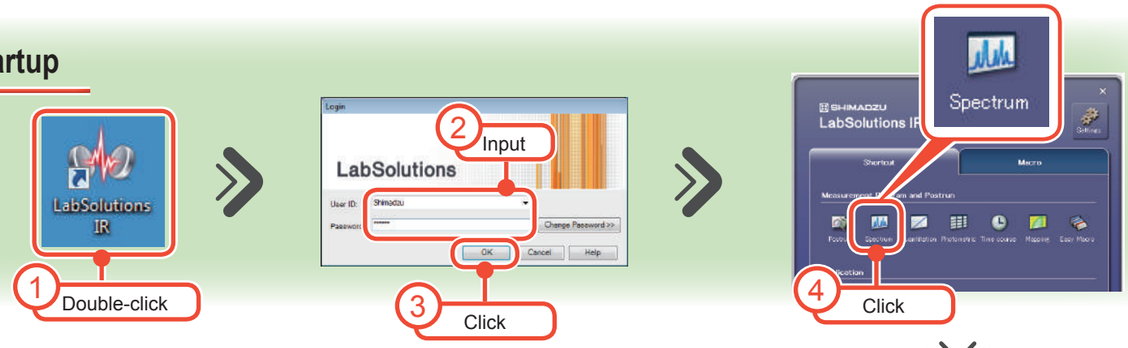
Shimadzu offers the following three software versions in the LabSolutions IR series.
This quick guide uses the file management version of LabSolutions IR to explain operation.

	LabSolutions IR	LabSolutions DB IR	LabSolutions CS IR
Edition	File management edition	Database edition	Client server edition
Data management method	Measured data files are saved and managed in folders on the PC. The existence of data files can be checked using Windows Explorer.	Measured data files are saved and managed in the LabSolutions database. The existence of data files cannot be checked using Windows Explorer.	
Data references	The software references files in folders or drives on the PC.	The software references files in the database.	
Transferring LabSolutions IR data between PCs	Transfer of files	Loading via import (Data can be either copied to a local destination using the data file export function or downloaded from the database manager.)	
LabSolutions database	Unavailable	Available (The database resides on a local PC)	Available (The database resides on a server or local PC)
CLASS-Agent database	Available (Option)	Unavailable (The contents of the CLASS-Agent database can be transferred to the LabSolutions database.)	
User management	Available	Available	
Authorized group management	Available	Available	
Project management	Unavailable	Available	
Standalone / network	Either can be used.	Only the standalone configuration can be used.	Either can be used. (LabSolutions IR data can be viewed using the database manager on a PC set up for viewing purposes. Note that LabSolutions IR must be installed on the PC used for viewing.)
Data backup	Performed on a file-by-file basis using Windows Explorer.	Performed for each database.	
Startup method	LabSolutions IR icon, LabSolutions icon	LabSolutions icon	

Spectrum

This section explains the general spectrum program procedure for samples.

1 Startup



2 Initialization

1. Check that power is supplied to the FTIR.
2. Select [Initialize].

A green rectangle ( ) is displayed in the status monitor.
"Initialization is succeded." is displayed in the log.

3 Set Scan Parameters

1. Click the [Data] tab.
2. Set scan parameters such as the number of scans and resolution.

4 Enter a Filename and Sample Information

1. Enter a filename.
2. Enter the sample information.

5 Perform Background Measurment

1. Set the background sample.
2. Click [BKG Scan].

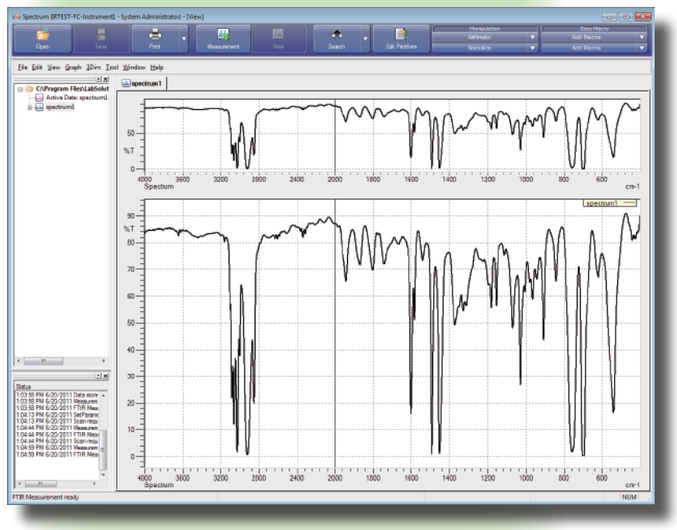
A background spectrum is displayed.

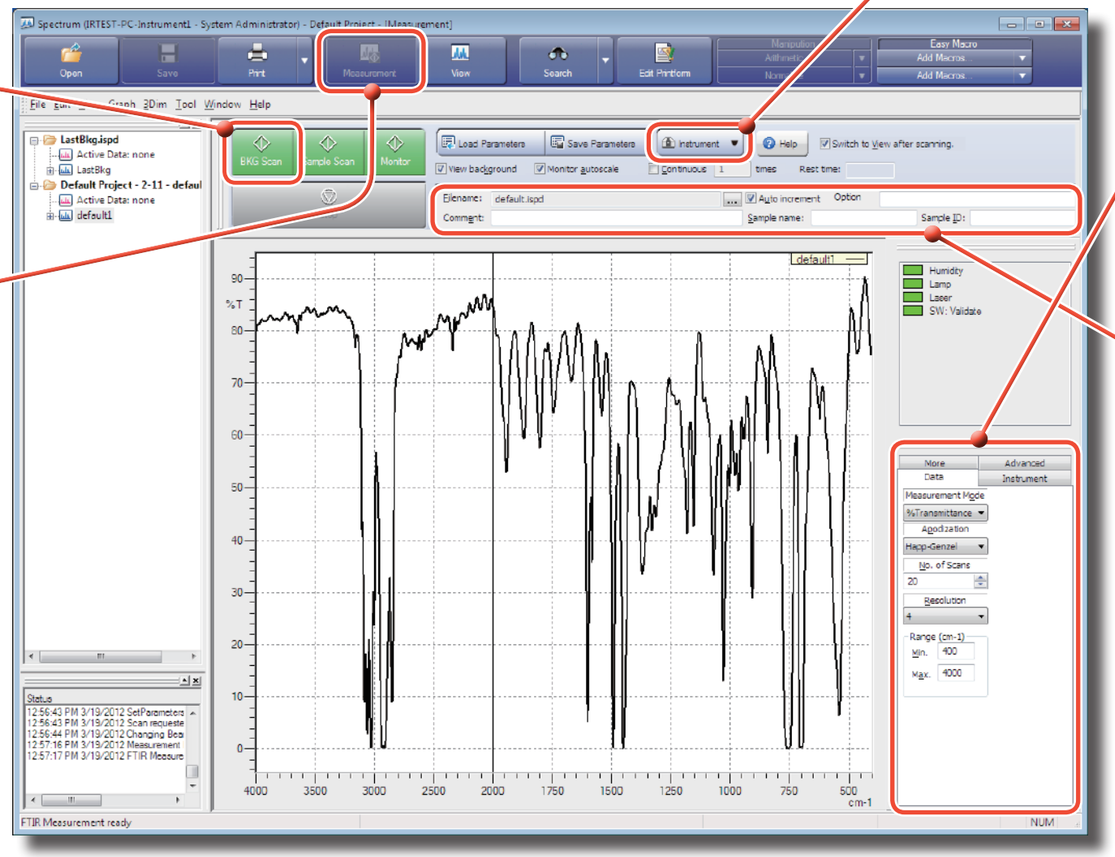
6 Measure the Sample

1. Click [Measurement].
2. Set the sample.
3. Click 

.

A spectrum of the sample is displayed.





7 Postrun

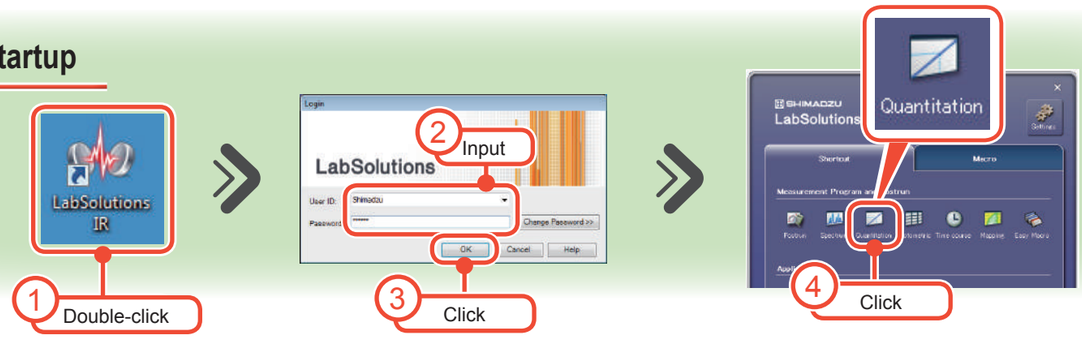
Perform operations including printing, searching, and manipulation with respect to spectra.

☞ See "Postrun/View" on pages 12 to 13

1.Creating a Calibration Curve

This section explains how to create a calibration curve that is required for quantitation of unknown samples.
Calibration curve creation requires a standard sample spectrum measured using spectrum program in absorbance mode to be saved in advance.

1 Startup



If a saved calibration curve already exists, proceed to step 2 in "2. Determining Quantities in Unknown Samples" on page 8

2 Initialization

1. Check that power is supplied to the FTIR.
2. Select [Initialize].

"Initialization is succeded." is displayed in the log.

3 Create a Standard Sample Table

1. Click [Import].

The [Import Spectrum] window is displayed.

2. Select the standard sample spectrum and click [Import].
3. Click [Close] to close the [Import Spectrum] window.
4. Enter the concentration into each row.

4 Set Calibration Curve Parameters

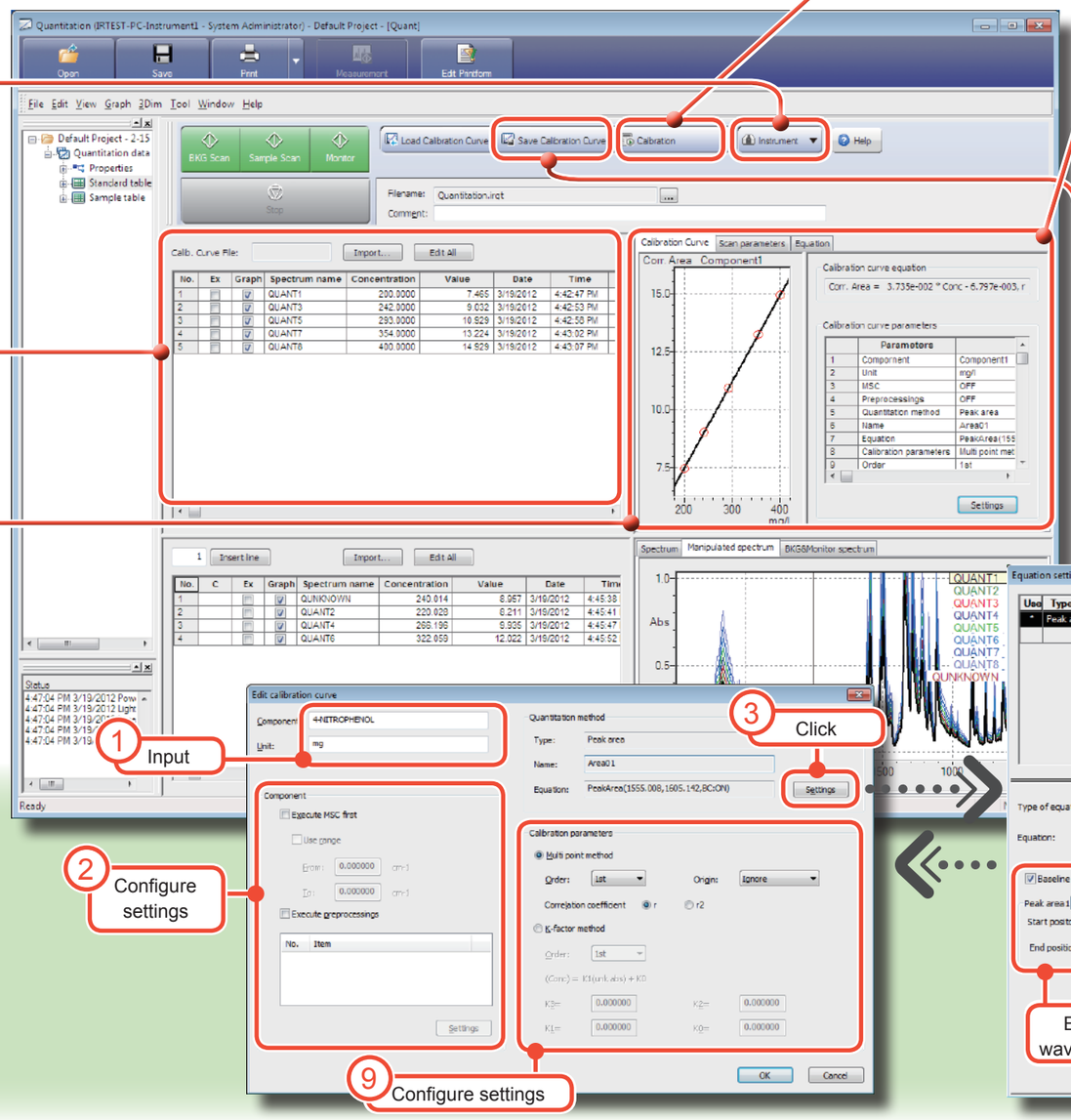
1. Click the [Calibration Curve] tab.
2. Click [Settings].

The [Edit calibration curve] window is displayed.

3. Set the calibration curve parameters.

The input procedure is shown to the right.

4. Click [OK].



5 Create a Calibration Curve

1. Click [Calibration].

A calibration curve is displayed.

6 Set Scan Parameters

1. Click the [Scan parameters] tab.
2. Click [Settings].

The [Instrument Parameters] window is displayed.

3. Set scan parameters such as the number of scans and resolution.
4. Click [OK].

7 Save the Calibration Curve

1. Click [Save Calibration Curve].
2. Enter a filename and click [Save].

Continues from step 3 in "2. Determining Quantities in Unknown Samples" on page 9

2. Determining Quantities in Unknown Samples

This section explains quantitation of unknown samples using calibration curves and how to calculate and assess the measurement results of unknown samples. A calibration curve must be measured and saved in advance.

Proceed from here when continuing from step 7 in "1. Creating a Calibration Curve" on page 7

1 Startup

See "Quantitation 1. Creating a Calibration Curve" on page 6

2 Load a Calibration Curve

1. Click [Load Calibration Curve].
   The [Open] dialog box is displayed.
2. Enter the filename and click [Open].
   The calibration curve is displayed.

3 Prepare the File

1. Click [...].
   file specification dialog box is displayed.
2. Enter the name of the quantitative data file and click [OK].

4 Prepare the Unknown Sample Table

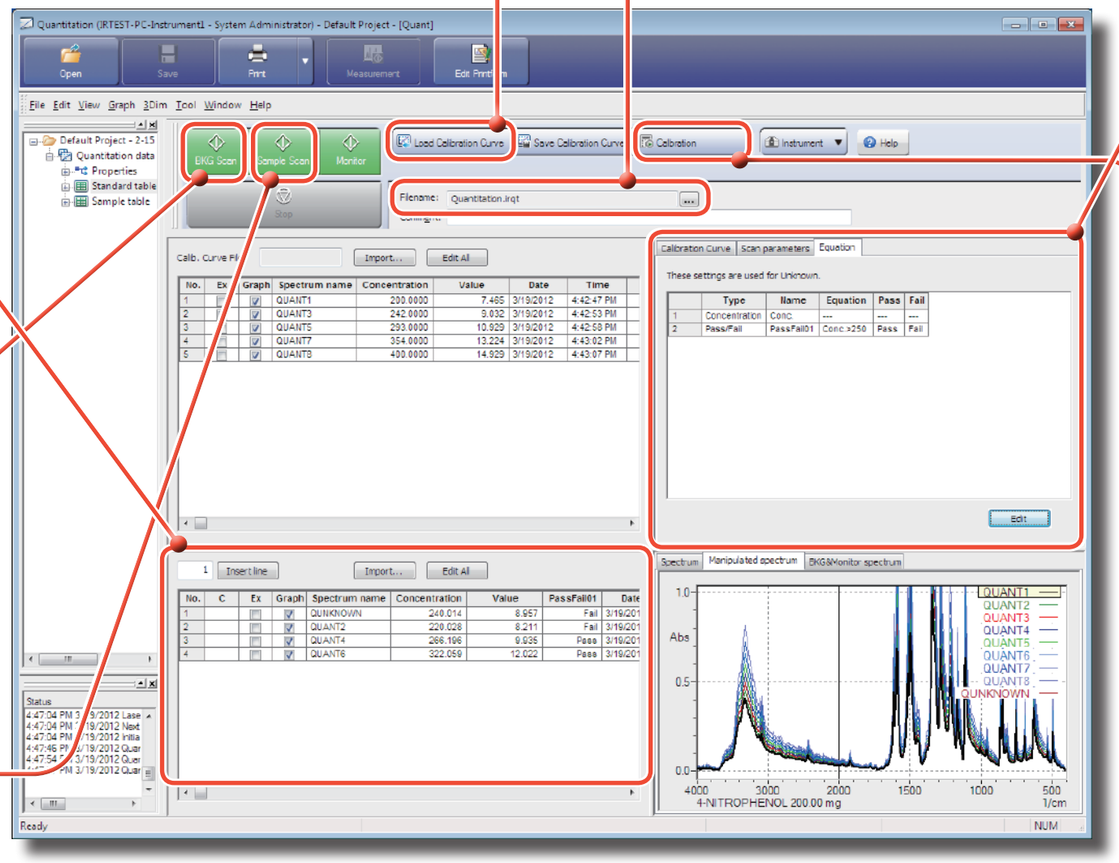
1. Click [Insert Line].
2. Enter the spectrum name (mandatory) and sample information.
   Selecting multiple sample cells and clicking [Edit All] allows collective input in the [batch sample information input] window.

5 Perform Background Measurement

1. Set the background sample.
2. Click [BKG Scan].
   A background spectrum is displayed.

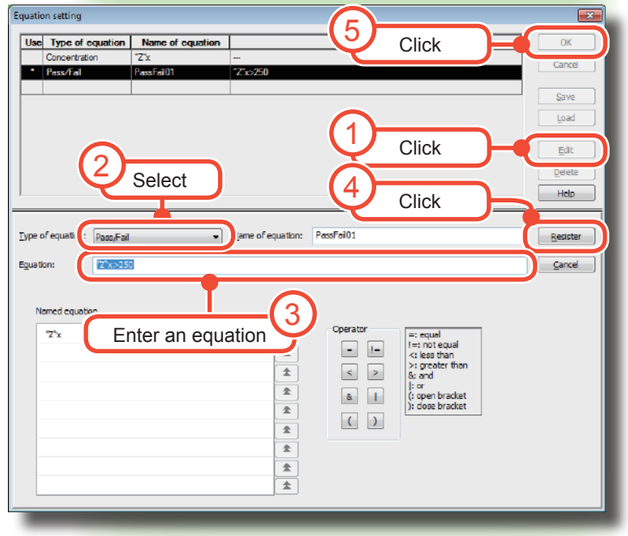
6 Perform Quantitative Measurement of the Unknown Sample

1. Set the unknown sample.
2. Click [Sample Scan].
   A spectrum is displayed.
   When measurement is complete, concentrations are displayed in the unknown sample table.



7 Post-processing

1. Click the [Equation] tab.
2. Click [Edit].
   The [Equation setting] window is displayed.
3. Set an equation.
   The procedure is shown below.



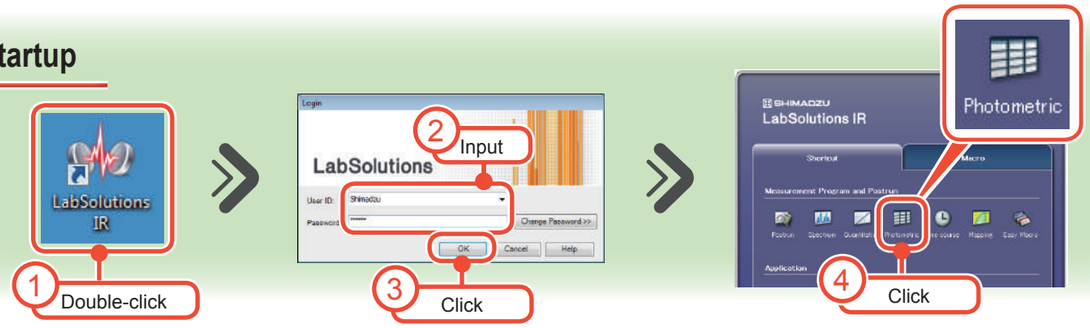
8 Rcalculation

1. Click [Calculation].
   The result is updated to the unknown sample table.

Photometric

This section explains how to scan intensity (such as absorbance and transmittance) as well as peak height and area at specified positions (wave numbers and wavelengths) on a spectrum. A variety of calculations can be performed using the scanned values.

1 Startup



2 Initialization

1. Check that power is supplied to the FTIR.
2. Select [Initialize].

"Initialization is succeeded." is displayed in the log.

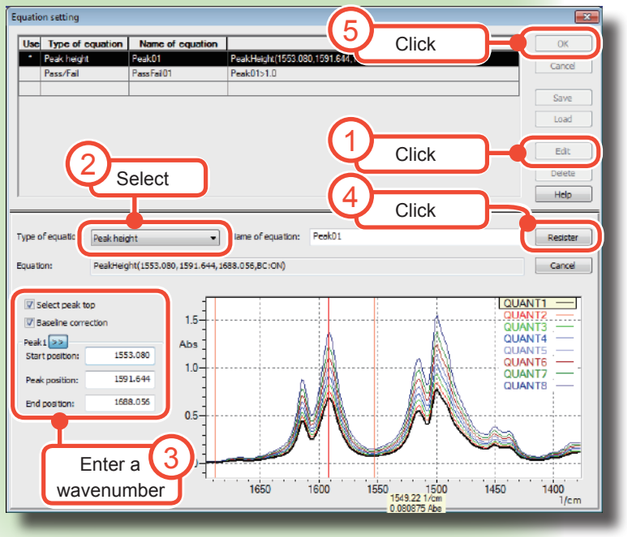
3 Set an Equation

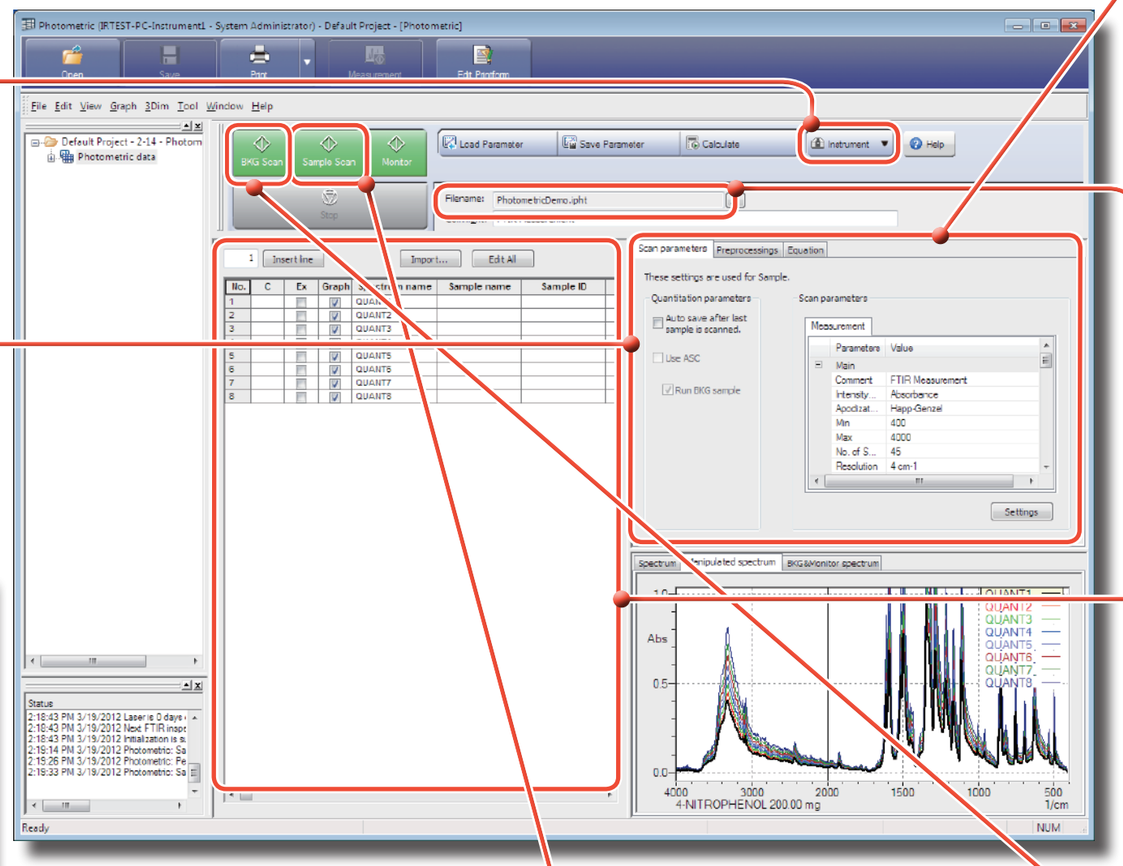
1. Click the [Equation] tab.
2. Click [Edit].

The [Equation setting] window is displayed.

3. Set an equation.

The input procedure is shown below.





4 Set Scan Parameters

1. Click the [Scan parameters] tab.
2. Click [Settings].

The [Instrument Parameters] window is displayed.

3. Set scan parameters such as the number of scans and resolution.
4. Click [OK].

5 Prepare the File

1. Click [...].

A file specification dialog box is displayed.

2. Enter a name for the photometric data file and click [OK].

6 Prepare the Sample Table

1. Click [Insert Line].
2. Enter the spectrum name (mandatory) and sample information.

Selecting multiple sample cells and clicking [Edit All] allows collective input in the [batch sample information input] window.

7 Perform Background Measurement

1. Set the background sample.
2. Click [BKG Scan].

background spectrum is displayed.

8 Measure the Sample

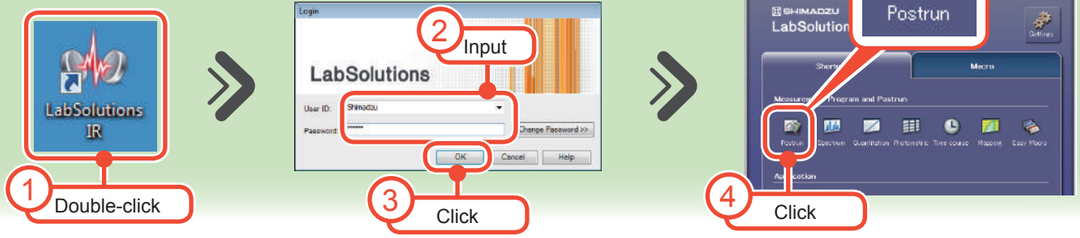
1. Set the sample.
2. Click [Sample Scan].

When measurement is complete, the photometric results are displayed in the sample table.

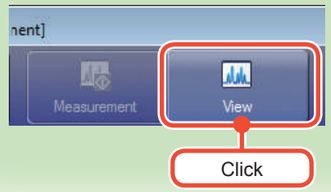
Postrun / View

This section explains the functions for displaying data, peak pick, zooming data on screen,and overlaying data on the vertical axis.

1 Startup



When Performing Postrun from Measurement Programs

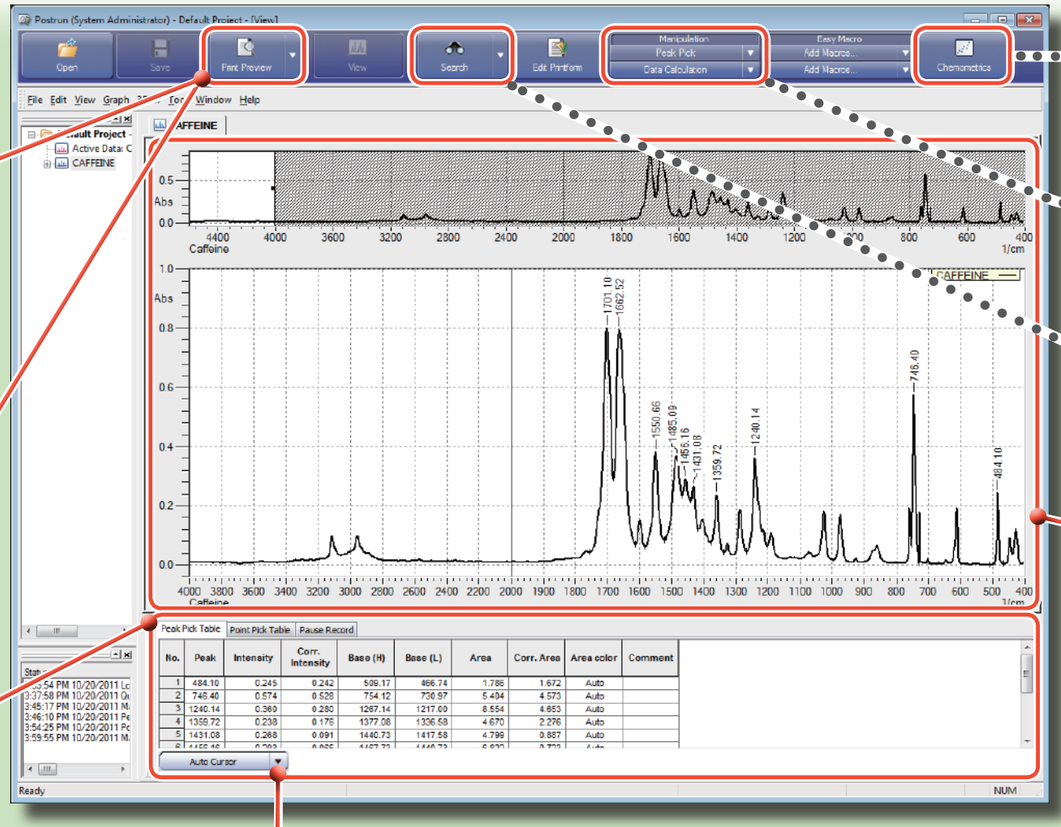


NOTE

- The measurement programs that allow postrun are spectrum program, time course program, and mapping program.
- [Chemometric] and [Edit Library] cannot be selected in the windows of each measurement program.

2 Postrun

Display data for postrun.



Print / Print Preview

Data can be printed using the specified report template.

HINT

- When printing with a report template, click [Print Preference] on the [Tool] menu.
- When printing with a different report template, click [Print with Template] on the [File] menu.

View Print / View Print Preview

Select the information for printing in the [Viewprint Settings] window.

Peak Pick

1. Click the [Peak Pick Table] tab.
2. Click ▼ at the lower left and select [Auto Cursor].
   A red line is displayed in the graph window.
3. Drag and drop the red line onto the loading position.
   Peak point data is displayed in the peak table.
4. Click to confirm.

Point Pick

1. Click the [Point Pick Table] tab.
2. Click ▼ at the lower left and select [Cursor].
   A red line is displayed in the graph window.
3. Drag and drop the red line onto the loading position.
   The coordinate values of the point are displayed in the point pick table.
4. Click to confirm.

Chemometrics

☞ Refer to "Chapter 10 Chemometric Quantitation" in LabSolutions IR INSTRUCTION MANUAL (Basic Operation Guide)

Manipulation

☞ See "Manipulation" on pages 14 and 15

Search / Edit Library

☞ See "Search" on pages 16 and 17
See "Library Creation and Editing" on pages 18 and 19

Zooming Spectrum

1. Drag on the graph window to create a quadrilateral.
2. Click the desired position to magnify.
   The display is magnified.

HINT

- The spectrum can be zoomed in or out automatically by clicking [Autoscale] on the right-click menu.
- Return the spectrum to its original size by clicking [Full view] on the right-click menu.

Joining

1. Click [Join All] on the [Window] menu.
   All currently displayed data is shown in an overlaid state.

Manipulation

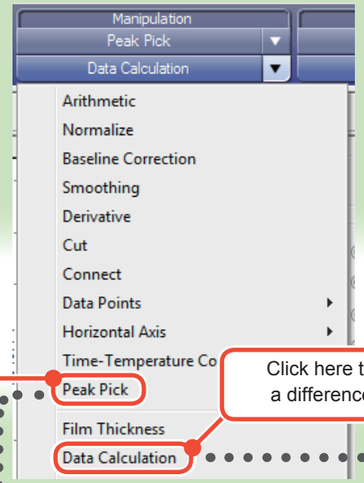
This section explains how to perform manipulation for peak pick and difference spectra.

☞ For details on other manipulation, refer to "Chapter 8 Manipulation" in LabSolutions IR INSTRUCTION MANUAL (Basic Operation Guide).

1 Preparation

1 Display the spectrum required for manipulation in the display window for the relevant measurement program or postrun window.

2 Display the relevant manipulation window.



HINT

The measurement programs that allow manipulation are spectrum program, time course program, and mapping program.

2 Manipulation

Peak Pick

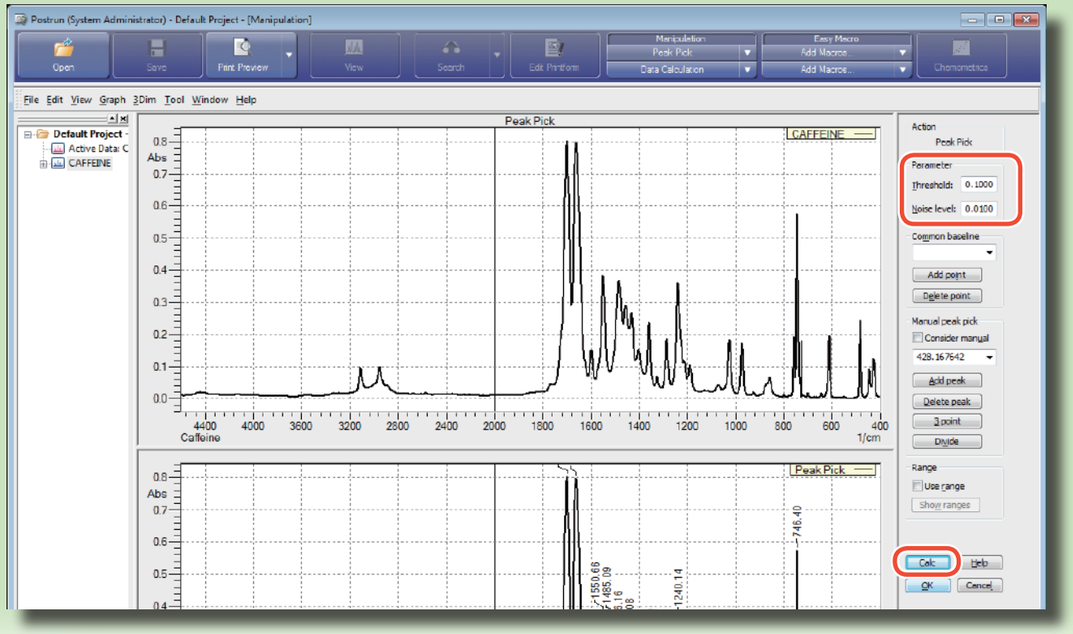
1 Set the peak pick parameters on [Parameter].

2 Click [Calc].

The result of peak pick is displayed.

Click here to detect peaks

Click here to calculate a difference spectrum



Difference Spectrum

1 Select the target spectrum from the tree view.

2 Click [Send to Source] on the right-click menu.

3 Select the reference spectrum from the tree view.

4 Click [Send to Reference] on the right-click menu.

The selected spectra appear overlaid.

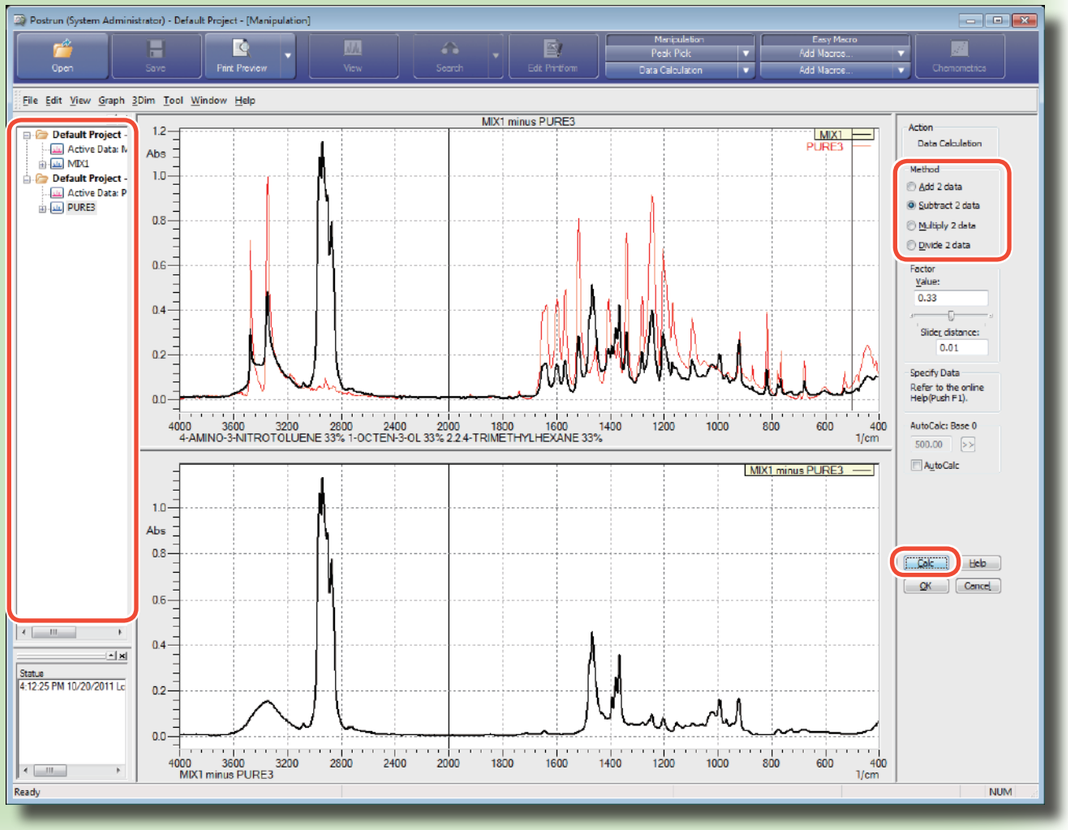
5 Select [Subtract 2 data] under [Method].

6 Click [Calc].

The result of calculation is displayed.

7 Click [OK].

The result of calculation of the spectra is saved.



Search

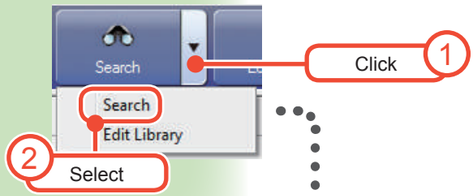
This section explains how to search for the spectrum.

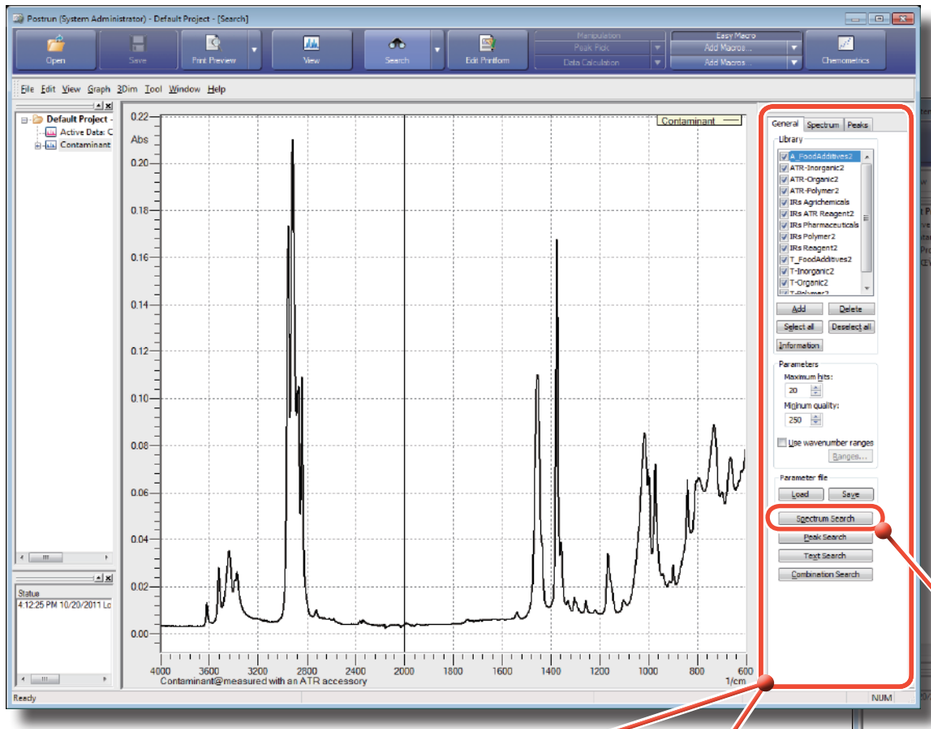
1 Preparation

1 Display the spectrum to be searched in the display window for the relevant measurement program or postrun window.

> **HINT**
> The measurement programs that allow searching are spectrum program, time course program, and mapping program.

2 Display the search window.





2 Select a Library

1 Click the [General] tab and click [Add].

The [Select Libraries] window is displayed.

2 Select a file and click [Open].

The library is added to the list.

3 Select an Algorithm

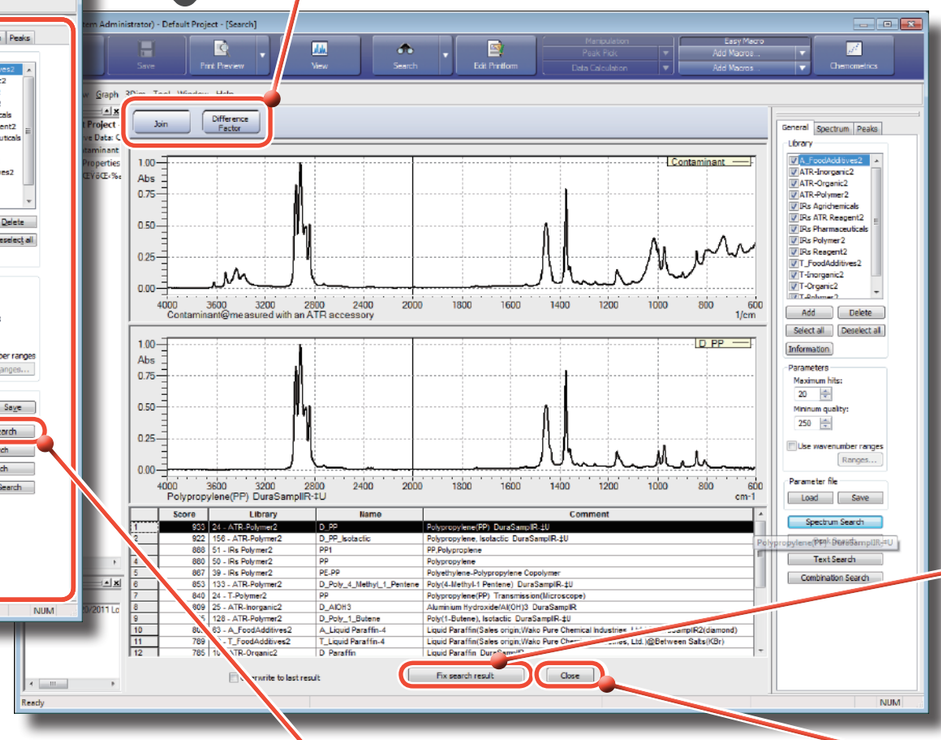
1 Click the [Spectrum] tab.

2 Select [DiffDerive] or [CorrDerive] from the [Algorithm] list.

4 Execute the Search

1 Click [Spectrum Search].

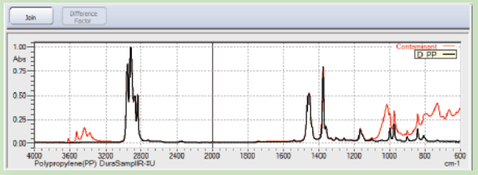
The search results are displayed.



5 Post-Search Processing

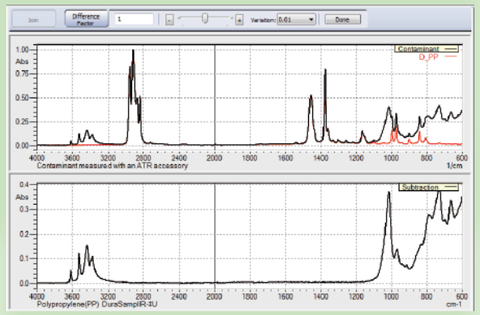
Join

Click [Join] to display the search target spectrum overlaid with the spectrum selected in the hit list.



Subtraction

Click [Difference Factor] to calculate the difference spectrum of the search target spectrum and the spectrum selected in the hit list.



1 Adjust the factor.

2 Click [Done].

The difference spectrum is saved to the spectrum.

> **HINT**
> Return to the original search results display by clicking [Join] or [Difference Factor] again.

6 Saving

1 Click [Fix search result].

The search results are saved.

7 Close

1 Click [Close].

Return to the search window.

2 Click [View].

Search exits.

Library Creation and Editing

This section explains how to insert spectra to a library. This allows searching of spectra inserted in the library.

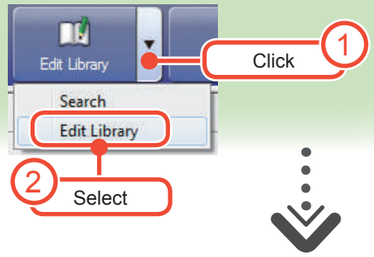
1 Startup

See "Postrun / View" on page 12

2 Preparation

1 Display the spectrum to be inserted to a library.

2 Display the [Edit Library] window.



3 Create a Library

1 Select [New].

The [Create User Library] window is displayed.

2 Enter information for the library and click [OK].

A new edit library window is displayed.

4 Edit the Library

NOTE

Commercial libraries cannot be edited.

Adding a Spectrum

1 Select a spectrum from the tree view.

2 Click [Insert into Library] on the right-click menu.

A message is displayed.

3 Click [Yes].

The selected spectrum is added to the spectrum list.

Deleting a Spectrum

1 Select the spectrum for deletion in the spectrum list.

2 Click [Delete] on the right-click menu.

A message is displayed.

3 Click [Yes].

The selected spectrum is deleted from the spectrum list.

Editing a Spectrum

1 Double-click on the spectrum for editing in the spectrum list.

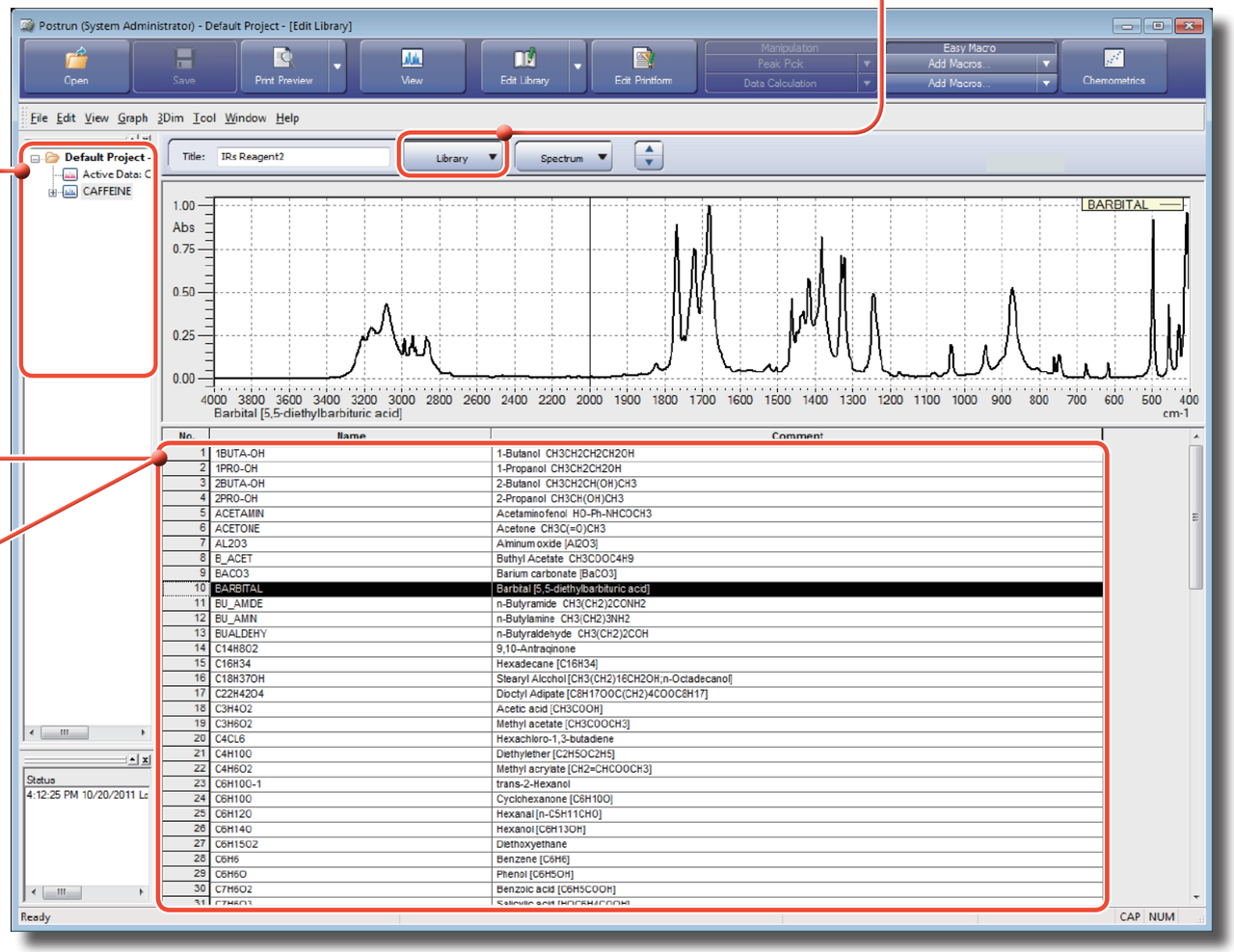
A message is displayed.

2 Click [Yes].

The [Edit Spectrum Information] window is displayed.

3 Click [OK] after editing is complete.

The spectrum is updated in the spectrum list.



No.	Name	Comment
1	1BUTA-OH	1-Butanol CH3CH2CH2CH2OH
2	1PR0-OH	1-Propanol CH3CH2CH2OH
3	2BUTA-OH	2-Butanol CH3CH2CH(OH)CH3
4	2PR0-OH	2-Propanol CH3CH(OH)CH3
5	ACETAMIN	Acetaminofenol HO-Ph-NHCOCH3
6	ACETONE	Acetone CH3C(=O)CH3
7	AL2O3	Aminum oxide [Al2O3]
8	B_ACET	Buthyl Acetate CH3COOC4H9
9	BACO3	Barium carbonate [BaCO3]
10	BARBITAL	Barbital [5,5-diethylbarbituric acid]
11	BU_AMDE	n-Butyramide CH3(CH2)2CONH2
12	BU_AMN	n-Butylamine CH3(CH2)3NH2
13	BUALDEHY	n-Butyraldehyde CH3(CH2)2CCH
14	C14H8O2	9,10-Antraqinone
15	C16H34	Hexadecane [C16H34]
16	C18H37OH	Stearyl Alcohol [CH3(CH2)16CH2OH;n-Octadecanol]
17	C22H42O4	Dioctyl Adipate [C8H17OOC(CH2)4COOC8H17]
18	C3H4O2	Acetic acid [CH3COOH]
19	C3H6O2	Methyl acetate [CH3COOCH3]
20	C4CL6	Hexachloro-1,3-butadiene
21	C4H10O	Diethylether [C2H5OC2H5]
22	C4H6O2	Methyl acryiate [CH2=CHCOOCH3]
23	C6H10O-1	trans-2-Hexanol
24	C6H10O	Cyclohexanone [C6H10O]
25	C6H12O	Hexanal [n-C5H11CHO]
26	C6H14O	Hexanol [C6H13OH]
27	C6H15O2	Diethoxyethane
28	C6H6	Benzene [C6H6]
29	C6H6O	Phenol [C6H5OH]
30	C7H6O2	Benzoic acid [C6H5COOH]

Report Template Creation

This section explains how to arrange LabSolutions IR data and information in order to create a template for printing.

1 Prepare Data

1 Display the data for printing in the relevant measurement program window or postrun window.

2 Display the edit print format window.

2 Select an Item

1 Drag and drop the selected item into the report window.

2 Move the cursor to adjust the size and then click.

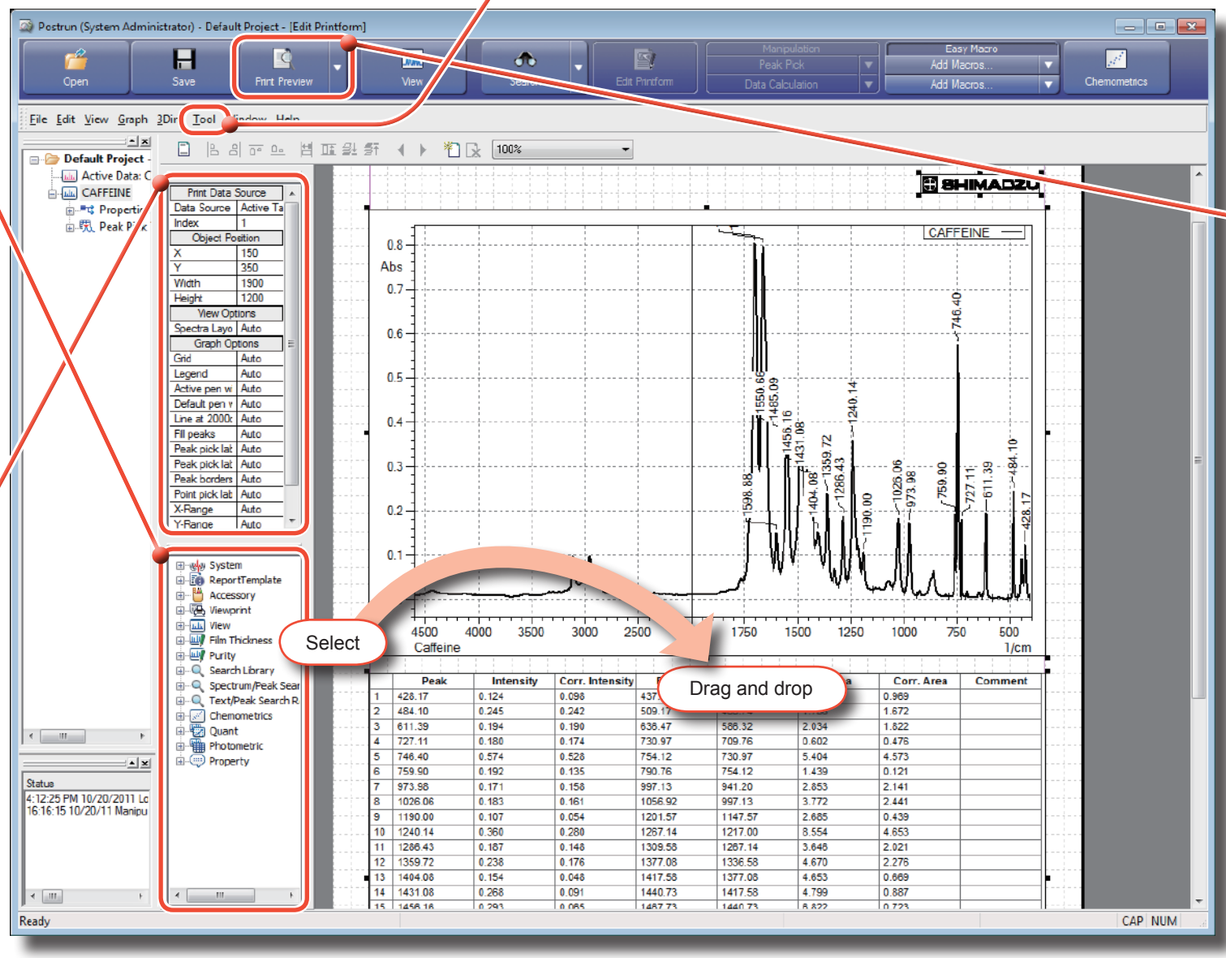
3 Adjust the overall layout.

HINT

- Items in the report layout window can be moved by dragging them.
- Items can be enlarged or reduced by dragging a point on the frame that contains them in the report layout window.

3 Check Properties

Click on an item in the report layout window to display information on the item in the properties window.



4 Registration

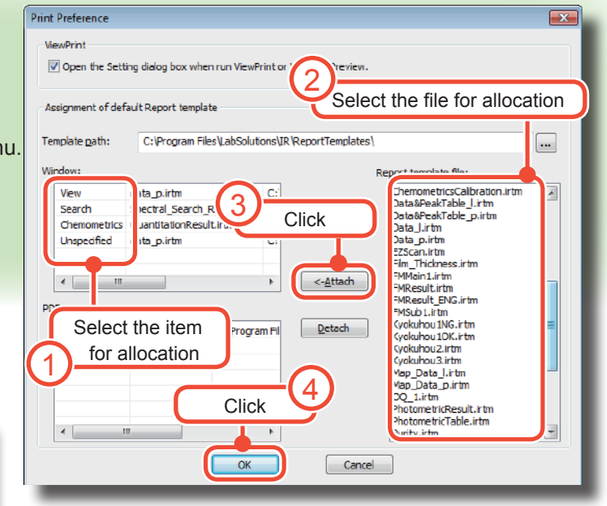
Printing can be made easier by registering created report templates in advance.

1 Click [Print Preferences] on the [Tool] menu.

The [Print Preference] window is displayed.

2 Register the report template.

The registration procedure is shown to the right.



5 Print

1 Select [Print Preview].

The print preview window is displayed.

2 Select [Print] in the print preview window.

The [Print] window is displayed.

3 Set each item and click [OK].

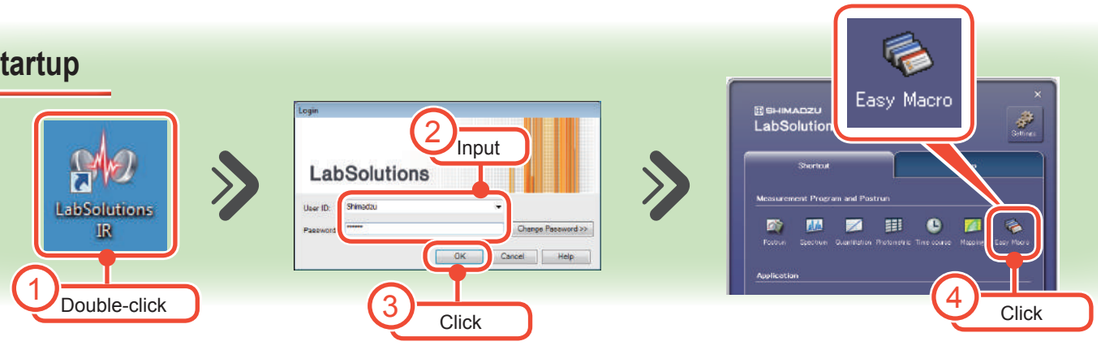
HINT

Select [Print] in the edit print format window when printing without checking the output using print preview.

Easy Macros

This section explains how to arrange a sequence of operations in order beginning with LabSolutions IR startup and register the sequence as a macro program.

1 Startup



2 Select Macro Items

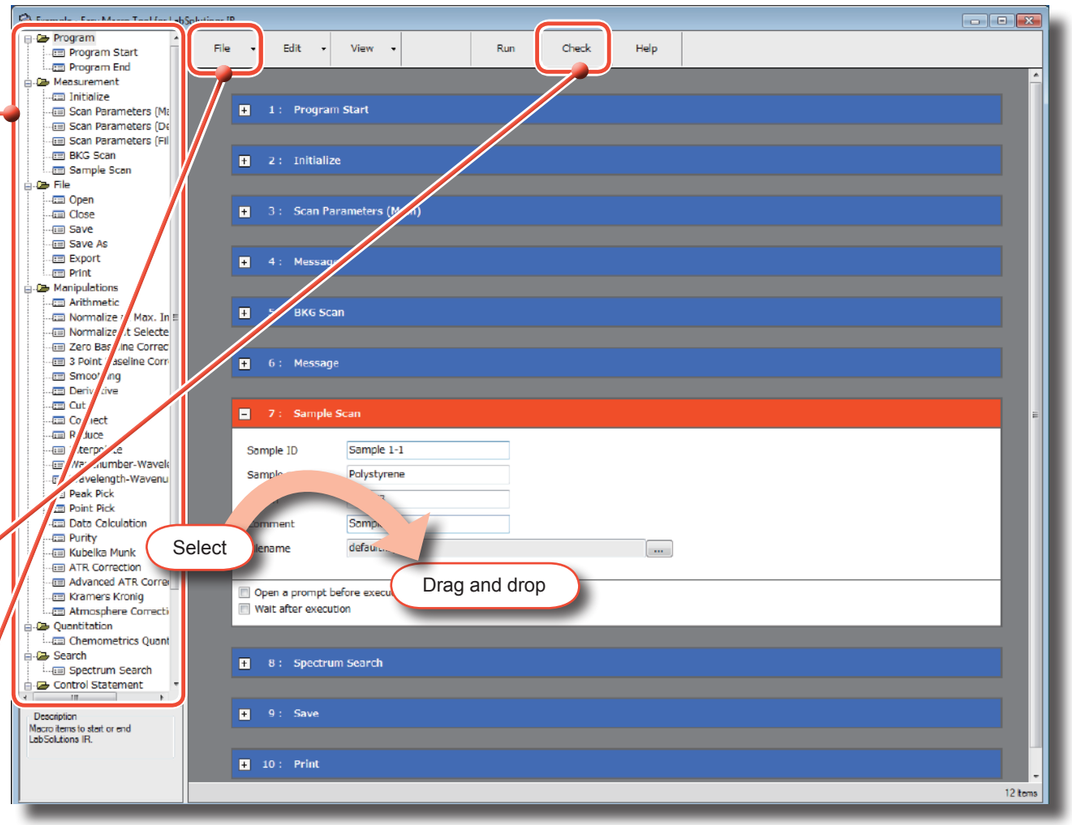
Drag and drop command items into the edit macro sequence window in the order of execution.

NOTE

Always start the sequence with [Program Start] and end the sequence with [Program End].

HINT

is displayed at the insertion position after a second item is added.



3 Macro Sequence Check

1. Click [Check].
   The [Information] window is displayed.
2. Click [OK].

4 Saving

1. Select [Save as].
   The [Save As] dialog box is displayed.
2. Enter a filename and click [Save].

5 Registration

Easy macros can be registered to the following location.

Launcher

1. Click launcher's Settings icon.
   The [Configuration] window is displayed.
2. Click the [Macro] tab and click [Add].
   The [Edit Macro] window is displayed.
3. Enter a title, comment, and filename and click [OK].
   The macro is added to the list.
4. Click [OK].
   The macro is allocated to a launcher button.

Postrun Main Toolbar

1. Start the postrun program.
   See "Postrun / View" on page 12
2. Click under [Easy Macro] and select [Add Macros].
   The [Macro List] window is displayed.
3. Click [Add].
   The [Macro] window is displayed.
4. Enter a macro name and filename and click [OK].
   The macro is added to the macro list.
5. Click [OK].
   The macro is allocated to a registered macro button on the main toolbar.

6 Execution

The following procedure explains execution from the launcher.

1. Click the launcher icon.
   The [Macro Execute] window is displayed.
2. Click [run].