ADVANTEST

ADVANTEST CORPORATION

TAS7x00 Series Terahertz Spectroscopy & Imaging System System Software Operation Manual (Quantitative Analysis Option)

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Applicable System

TAS7500

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Revision History

Rev.	Date	Notes
01	Apr 16/12	
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Preface

Purpose of This Manual

This manual describes how to install the quantitative analysis option used with the System Software, how to register the license, and how to operate the quantitative analysis option, as well as its functions.

Related Manuals

TAS7500 Series Terahertz Spectroscopy & Imaging System Instruction Manual

This manual describes the procedures required to perform measurement and analysis operations including handling notes for safe use, after the system is installed.

TAS7x00 Series Terahertz Spectroscopy & Imaging System System Software Operation Manual

This manual describes how to operate the system software for spectroscopic measurements/analyses and imaging measurements/analyses using the TAS7x00 Series Terahertz Spectroscopy & Imaging System.

1. Overview

The quantitative analysis option creates a quantification model from multiple spectra and provides a function that estimates the quantity of a component from the spectra measured by using the model.

2. The Unscrambler® X

The Unscrambler® X is a multivariate analysis tool of CAMO Software, Inc.

The Unscrambler® X is required in order to execute quantitative analyses using this option.

The Unscrambler® X is used to create a quantification model file.

➔ For more information on quantification model files, refer to 7. 2 "Quantification Model File" on page 7-2.

Users of this option need to have knowledge of spectrum multivariate analysis and The Unscrambler® X.

The operating procedures for The Unscrambler® X described in this manual are the minimum procedures for creating a quantification model file that can be used for this option.

➔ For more information, refer to the manuals for The Unscrambler® X.

The version of quantification model files supported by this option is 10.1 and 10.2.

The operating procedures for The Unscrambler® X described in this manual are based on version 10.1. Note that the procedures may be different if a different version is used.

3. Installation and Uninstall

This chapter describes how to install and uninstall the quantitative analysis option.

3. 1 Installation

The procedure for installing the quantitative analysis option is as follows:

1) Put the quantitative analysis option installation CD in the disk tray.
2) Use Explorer to display the folders on the CD-ROM.
3) Right click InstallTAS7x00Quantification.bat and click **[Run as administrator (A) ...]**.
4) The User Account Control dialog box opens. Click the **[OK]** button to start installation.
   - Quantification execution library (OLUPX)
     The quantification execution library is installed. Various dialog boxes appear sequentially. Press the **[Next >]** button in each dialog box with the default settings to proceed with the installation. Press the **[Finish]** button to complete the installation.
     During installation, the operator is asked to enter the Activation Key on the Personal Information input screen. Enter the Activation Key sent by Advantest on this screen.
5) When **[Press any key to continue...]** is displayed on the command prompt screen, press the [Enter] key to exit.

The installation of the quantitative analysis option is now complete.

After installation, register the license to enable its functions.

➔ For more information on how to register the license, refer to 4. 1 "Registering Licenses" on page 4-1.

3. 2 Uninstall

The procedure for uninstalling the quantitative analysis option is as follows:

1) Select **[Start]** → **[All Programs]** → **[TAS7x00]** → **[Uninstall TAS7x00 Quantification]** and click it with the right mouse button, and then click **[Run as administrator (A) ...]**.
2) The User Account Control dialog box opens. Click the **[OK]** button to start uninstall.
3) This will uninstall the quantification execution library (OLUPX). Click the **[OK]** button to start uninstall. Press the **[OK]** button to complete the uninstall.
4) When **[Press any key to continue...]** is displayed on the command prompt screen, press the [Enter] key to exit.

The uninstall of the quantitative analysis option is now complete.

After uninstall, be sure to delete the license.

➔ For more information on how to delete the license, refer to 4. 2 "Deleting Licenses" on page 4-3.

4. License Management

This chapter describes the license management of the functions for this option. By registering the license, the functions for this option become enabled.

This option can be registered on one computer per license.
To register a license, a password sheet is required.
Password sheets include online and offline versions.
Each product number is as follows:

- Online version: PYSI75-02M
- Offline version: PYSA75-02M

The following descriptions use the online version as an example.

4. 1 Registering Licenses

The procedure for registering a license is as follows:

1) Prepare the password sheet sent by Advantest.

Figure 4-1 Sample Password Sheet (CpuFixed)

```
             L i c e n s e P a s s w o r d S h e e t
                                          Date of issue: 2012/02/17
Serial#:  C050012
# Product Number              -> PYSI75-02M
# License Type                -> CpuFixed
# Expiration Client License   -> 000
# Password                    -> AA9DCC963F0B685A9FDF710091C164E9A
# Expiration Date             -> 2017/03/22
# Number of License           -> 1

#***** license *****
CpuFixed 000 AA9DCC963F0B685A9FDF710091C164E9A 00000edcba98 PYSI75-02M
2017/03/22 1 00000edcba98     ←  Enter this one line.
```

2) Select **[Start]** → **[All Programs]** → **[Accessories]** → **[Command Prompt]** and click it with the right mouse button, and then click **[Run as administrator (A) ...]**.

3) The User Account Control dialog box opens. Click the **[OK]** button.

4) To register a license, enter the command using the line that begins with "CpuFixed 000 ..." (shown in Figure 4-1) as an argument.
The following shows an example execution:

Figure 4-2 Example Execution of License Registration

```
C:\>%PLMS_ROOT%\bin\License_Add  CpuFixed 000 AA9DCC963F0B685A9FDF710091C164E9A0
00000edcba98 PYSI75-02M 2017/03/22 1 00000edcba98↵
License Added

C:\>
```

4. 2 Deleting Licenses

The procedure for deleting a license is as follows:

1) Prepare the password sheet used in 4. 1 "Registering Licenses" on page 4-1.

2) Select **[Start]** → **[All Programs]** → **[Accessories]** → **[Command Prompt]** and click it with the right mouse button, and then click **[Run as administrator (A) ...]**.

3) The User Account Control dialog box opens. Click the **[OK]** button.

4) Entering the license deletion command displays a list of registered licenses. Enter the label number that includes a line beginning with "CpuFixed 000 ..." in the password sheet and enter [y] to delete the license.
The following shows an example execution.

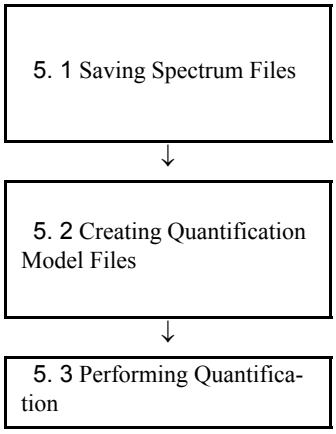
Figure 4-3 Example Execution of License Deletion

```
C:\>%PLMS_ROOT%\bin\License_Rem↵
(1):CpuFixed 000 AA9DCC963F0B685A9FDF710091C164E9A00000edcba98 PYSI75-02M 2017/0
3/22 1 00000edcba98
Input the label Number for the product that you want to delete. [1] or Quit[Q]:1↵
(1):CpuFixed 000 AA9DCC963F0B685A9FDF710091C164E9A00000edcba98 PYSI75-02M 2017/0
3/22 1 00000edcba98
Will be Deleted. [Y/N]:y↵
License Removed

C:\>
```

5. Operating Procedures

This chapter describes the operating procedures for quantitative analysis. The procedures are as follows:



Save multiple spectra that were measured with the System Software to a file. This file is called a spectrum file.

➔ For more information on spectrum files, refer to 7. 1 "Spectrum File" on page 7-1.

Use The Unscrambler® X to load the spectrum file, create a quantification model, and save it to a file. This file is called a quantification model file.

➔ For more information on quantification model files, refer to 7. 2 "Quantification Model File" on page 7-2.

Use the System Software to load the quantification model file, apply the model to the measured spectra, and quantify the desired component.

If the quantification model file already exists, the procedures described in 5. 1 "Saving Spectrum Files" on page 5-1 and 5. 2 "Creating Quantification Model Files" on page 5-4 are not needed.

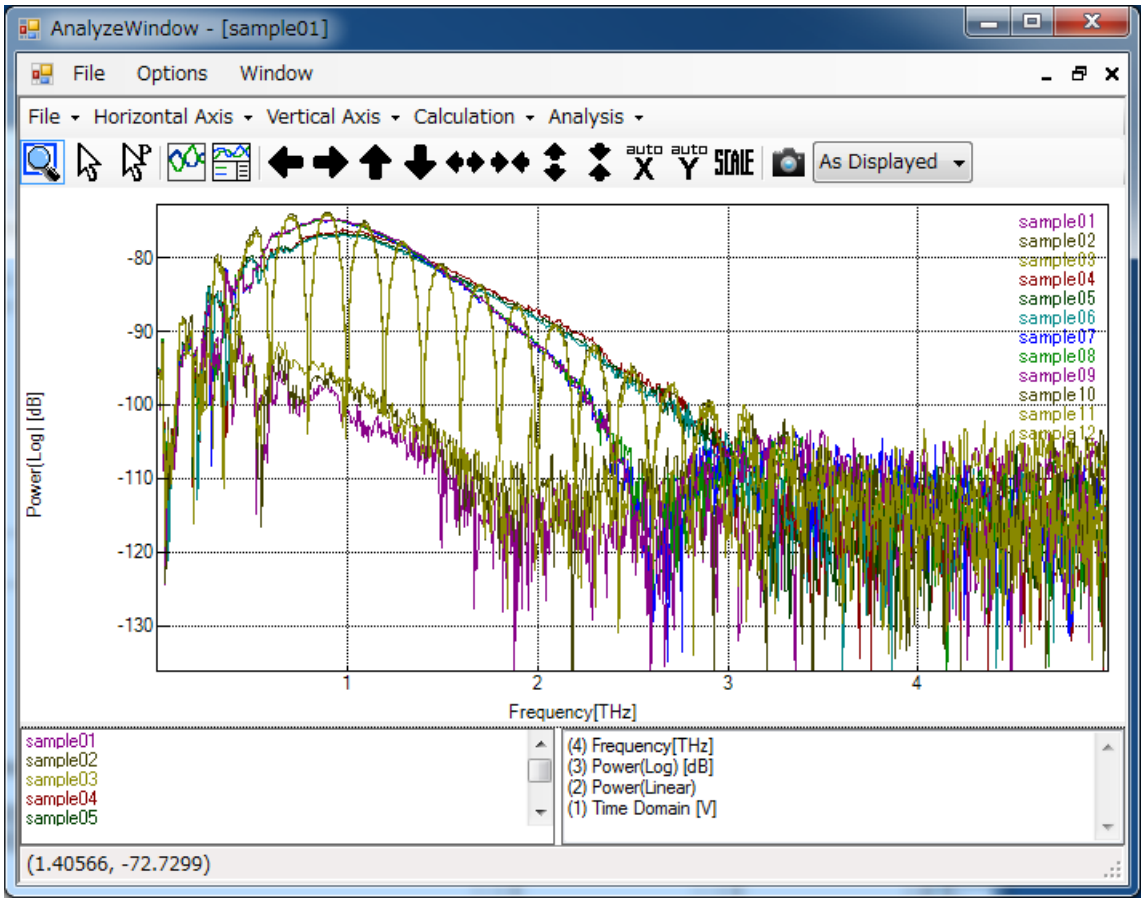
The following subsections describe the details of the preceding steps.

5. 1 Saving Spectrum Files

1) Display multiple spectra, which are sources for creating quantification models, in the Analyze window
   Either execute a measurement to transfer the spectra to the Analyze window or load the spectrum measurement data file.

2) Overlay the displayed spectra in a graph window
   To copy the waveform to another graph window, select the spectra to copy and press [Ctrl+C], and then select a graph window on which the copied waveform is to be overlaid and press [Ctrl+V].

Figure 5-1 Graph Window Displaying Multiple Spectra



Important

Unless the following conditions agree, the waveform cannot be overlaid.

Type of vertical axis

Type of horizontal axis

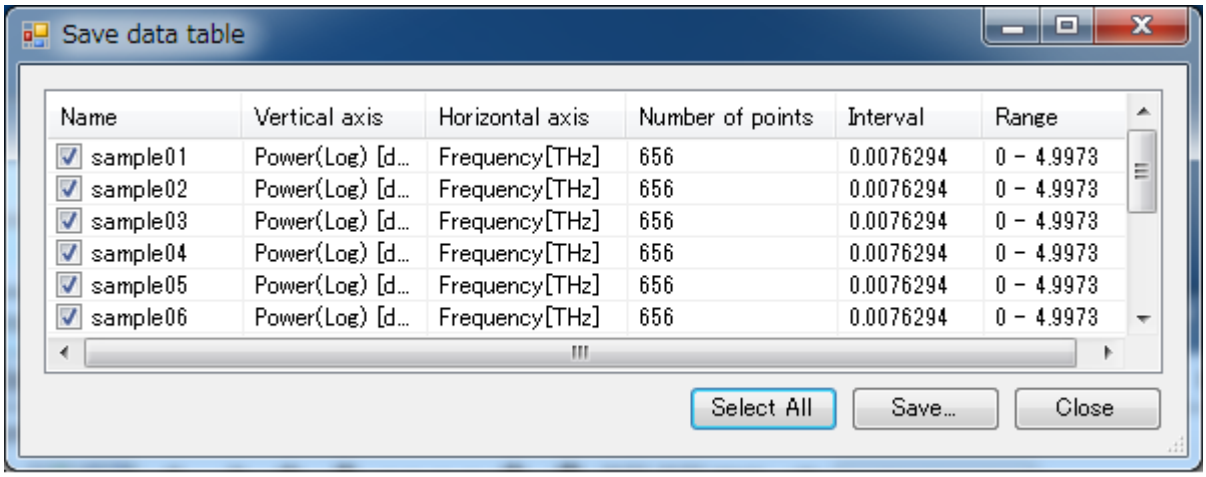
Number of data items to display

Tip

When loading a spectrum measurement data file from ***[File]*** *→* ***[Load PointData...]*** *in the Analyze window, by selecting more than one file and loading them together, all of the spectra are overlaid and displayed in one graph window, saving you the trouble of having to overlay them later.*

3) Click **[File]** → **[Save data table...]** in the graph window. The Save data table dialog box opens.

Figure 5-2 Save data table Dialog Box



The names and information of all the spectra in the graph window are displayed in the dialog box.
Select the names of the spectra to save. To select a name, check the checkboxes under Name.
Click the **[Save...]** button and enter a file name to save the file.
Here, the file is saved with the name "SpectraTable.csv" as an example.

Important

If any of the following conditions does not agree, multiple spectra cannot be selected.

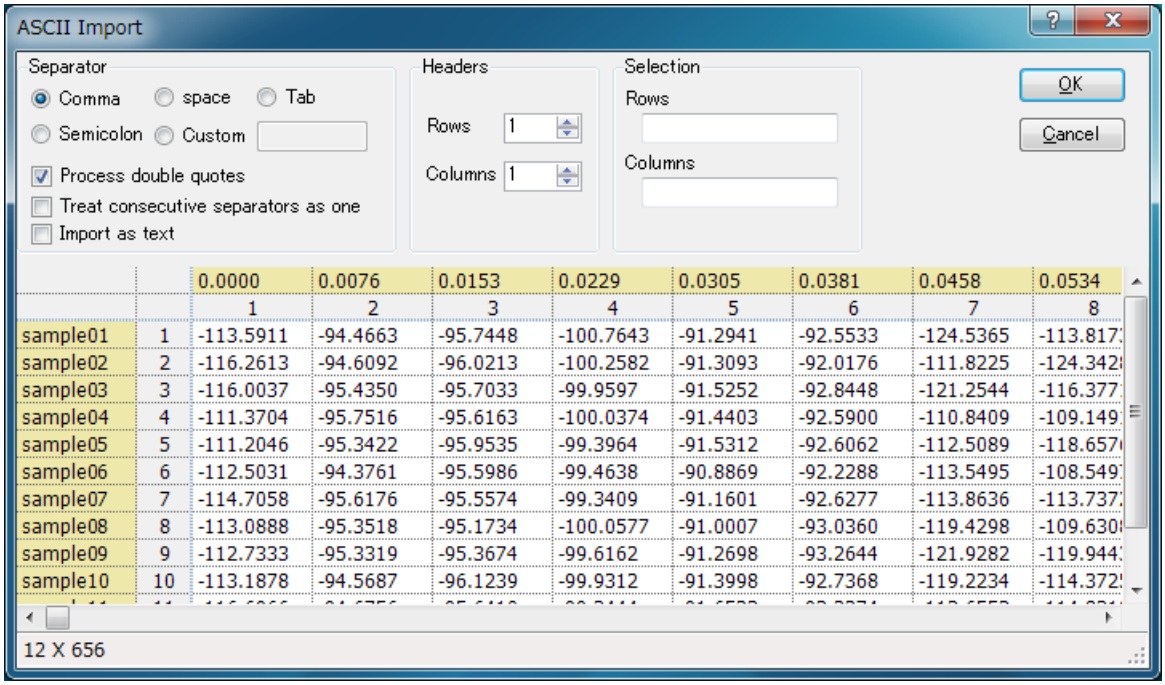
Type of vertical axis
Type of horizontal axis
Number of data items to display
Data interval
Data range

5. 2 Creating Quantification Model Files

1) Start The Unscrambler® X
Execute **[Start]** → **[All Programs]** → **[The Unscrambler® X 10.1 (64-bit)]** → **[The Unscrambler® X 10.1 (64-bit)]**.

2) Load the spectrum file
Click **[File]** → **[Import Data]** → **[ASCII...]**. In the file load dialog box, specify the spectrum file (SpectraTable.csv) that was created in the previous section. The ASCII Import dialog box opens. Click the **[OK]** button.

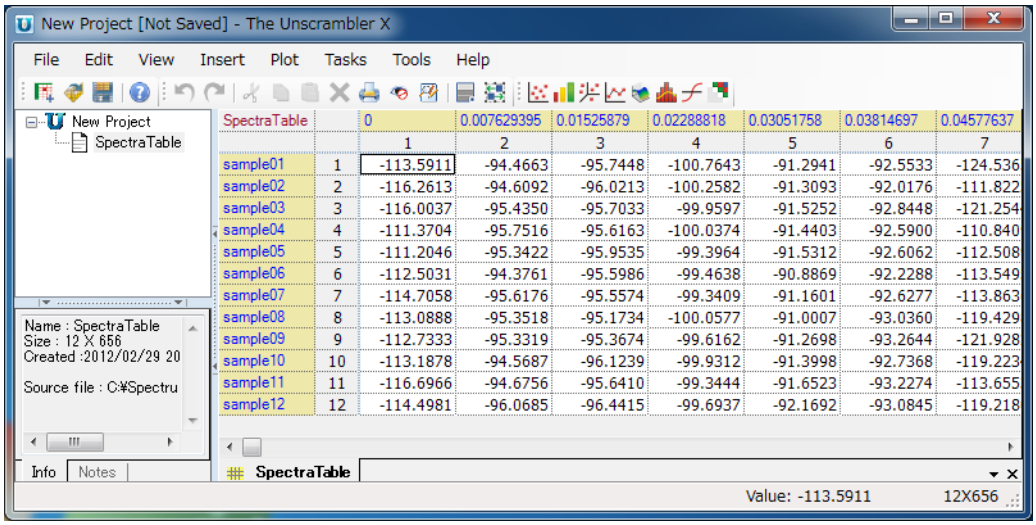
Figure 5-3 ASCII Import Dialog Box



		0.0000	0.0076	0.0153	0.0229	0.0305	0.0381	0.0458	0.0534
		1	2	3	4	5	6	7	8
sample01	1	-113.5911	-94.4663	-95.7448	-100.7643	-91.2941	-92.5533	-124.5365	-113.817
sample02	2	-116.2613	-94.6092	-96.0213	-100.2582	-91.3093	-92.0176	-111.8225	-124.342
sample03	3	-116.0037	-95.4350	-95.7033	-99.9597	-91.5252	-92.8448	-121.2544	-116.377
sample04	4	-111.3704	-95.7516	-95.6163	-100.0374	-91.4403	-92.5900	-110.8409	-109.149
sample05	5	-111.2046	-95.3422	-95.9535	-99.3964	-91.5312	-92.6062	-112.5089	-118.657
sample06	6	-112.5031	-94.3761	-95.5986	-99.4638	-90.8869	-92.2288	-113.5495	-108.549
sample07	7	-114.7058	-95.6176	-95.5574	-99.3409	-91.1601	-92.6277	-113.8636	-113.737
sample08	8	-113.0888	-95.3518	-95.1734	-100.0577	-91.0007	-93.0360	-119.4298	-109.630
sample09	9	-112.7333	-95.3319	-95.3674	-99.6162	-91.2698	-93.2644	-121.9282	-119.944
sample10	10	-113.1878	-94.5687	-96.1239	-99.9312	-91.3998	-92.7368	-119.2234	-114.372

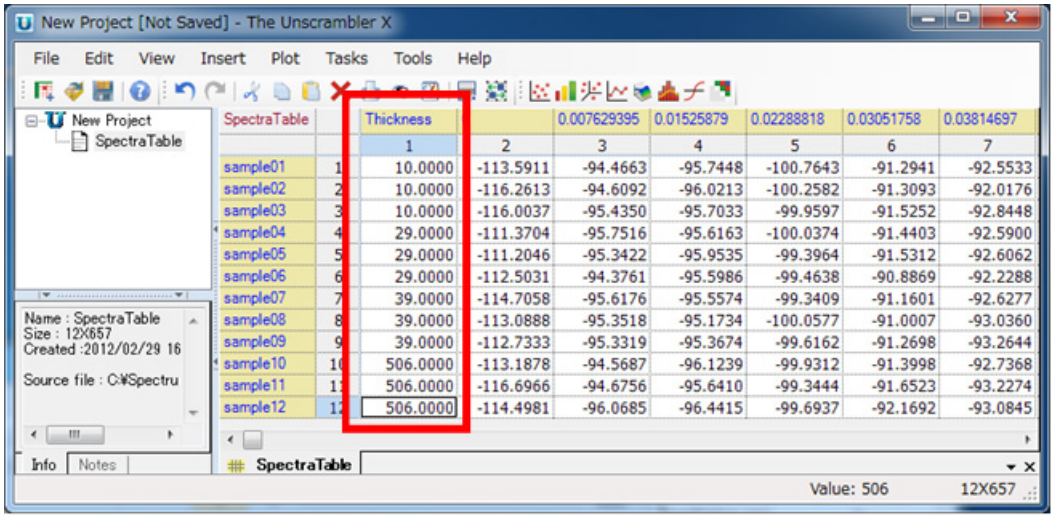
3) The table of spectra that have been loaded in the main window is displayed.

Figure 5-4 Main Window in which Spectrum File Has Been Loaded



4) Use the mouse to select the column of number 1, and then right click the mouse on the column and execute **[Insert]** → **[Row(s)/Column(s)...]**.
In the Insert Columns dialog box, enter 1 in Number of new columns and click the **[OK]** button.
Enter the component name in the column title and component values in the columns corresponding to each spectrum.
Here, Thickness is entered as the component name as an example.

Figure 5-5 Main Window in which Thickness Has Been Added

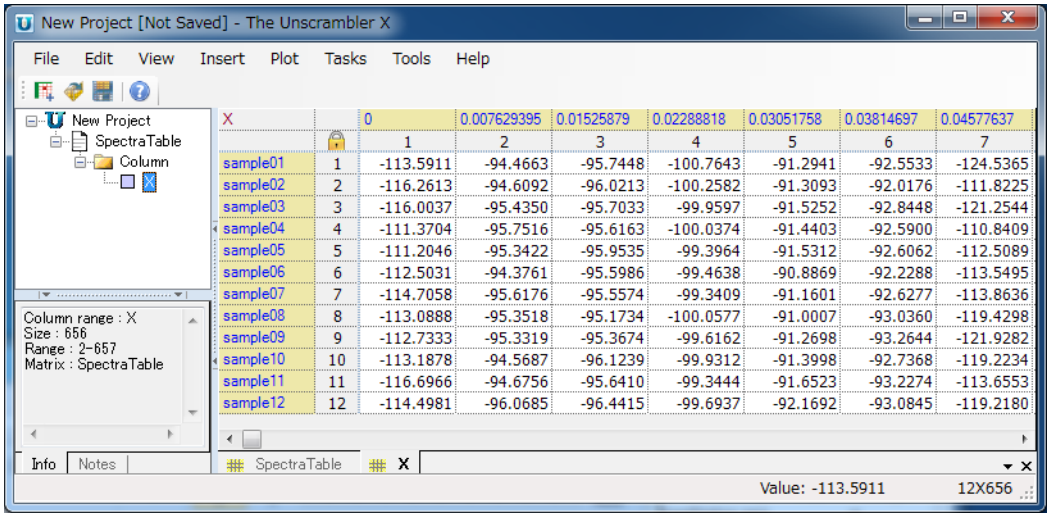


* To perform a quantitative analysis on more than one component, add as many columns as the number of components to be added.

5) Create an input variable table (X)

Select all columns other than Thickness, and then right click the mouse and execute **[Create Column Range]**.
Columnset is added to the tree. Select Columnset, and then right click the mouse and select **[Rename]** to change the name to X.

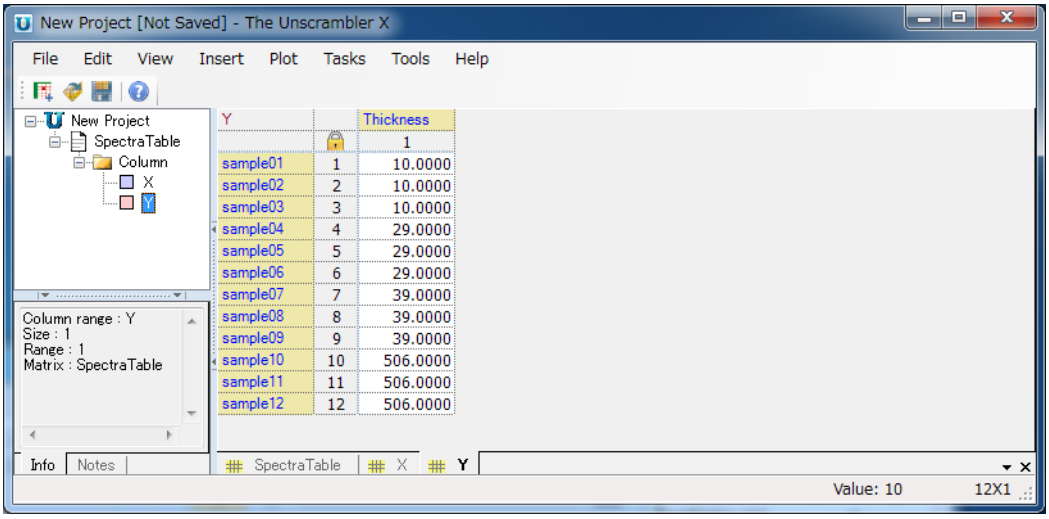
Figure 5-6 Input Variable Table



X		0	0.007629395	0.01525879	0.02288818	0.03051758	0.03814697	0.04577637
		1	2	3	4	5	6	7
sample01	1	-113.5911	-94.4663	-95.7448	-100.7643	-91.2941	-92.5533	-124.5365
sample02	2	-116.2613	-94.6092	-96.0213	-100.2582	-91.3093	-92.0176	-111.8225
sample03	3	-116.0037	-95.4350	-95.7033	-99.9597	-91.5252	-92.8448	-121.2544
sample04	4	-111.3704	-95.7516	-95.6163	-100.0374	-91.4403	-92.5900	-110.8409
sample05	5	-111.2046	-95.3422	-95.9535	-99.3964	-91.5312	-92.6062	-112.5089
sample06	6	-112.5031	-94.3761	-95.5986	-99.4638	-90.8869	-92.2288	-113.5495
sample07	7	-114.7058	-95.6176	-95.5574	-99.3409	-91.1601	-92.6277	-113.8636
sample08	8	-113.0888	-95.3518	-95.1734	-100.0577	-91.0007	-93.0360	-119.4298
sample09	9	-112.7333	-95.3319	-95.3674	-99.6162	-91.2698	-93.2644	-121.9282
sample10	10	-113.1878	-94.5687	-96.1239	-99.9312	-91.3998	-92.7368	-119.2234
sample11	11	-116.6966	-94.6756	-95.6410	-99.3444	-91.6523	-93.2274	-113.6553
sample12	12	-114.4981	-96.0685	-96.4415	-99.6937	-92.1692	-93.0845	-119.2180

6) Create an output variable table (Y)
Select the Thickness column, and then right click the mouse and execute **[Create Column Range]**.
Columnset is added to the tree. Select Columnset, and then right click the mouse and select **[Rename]** to change the name to Y.

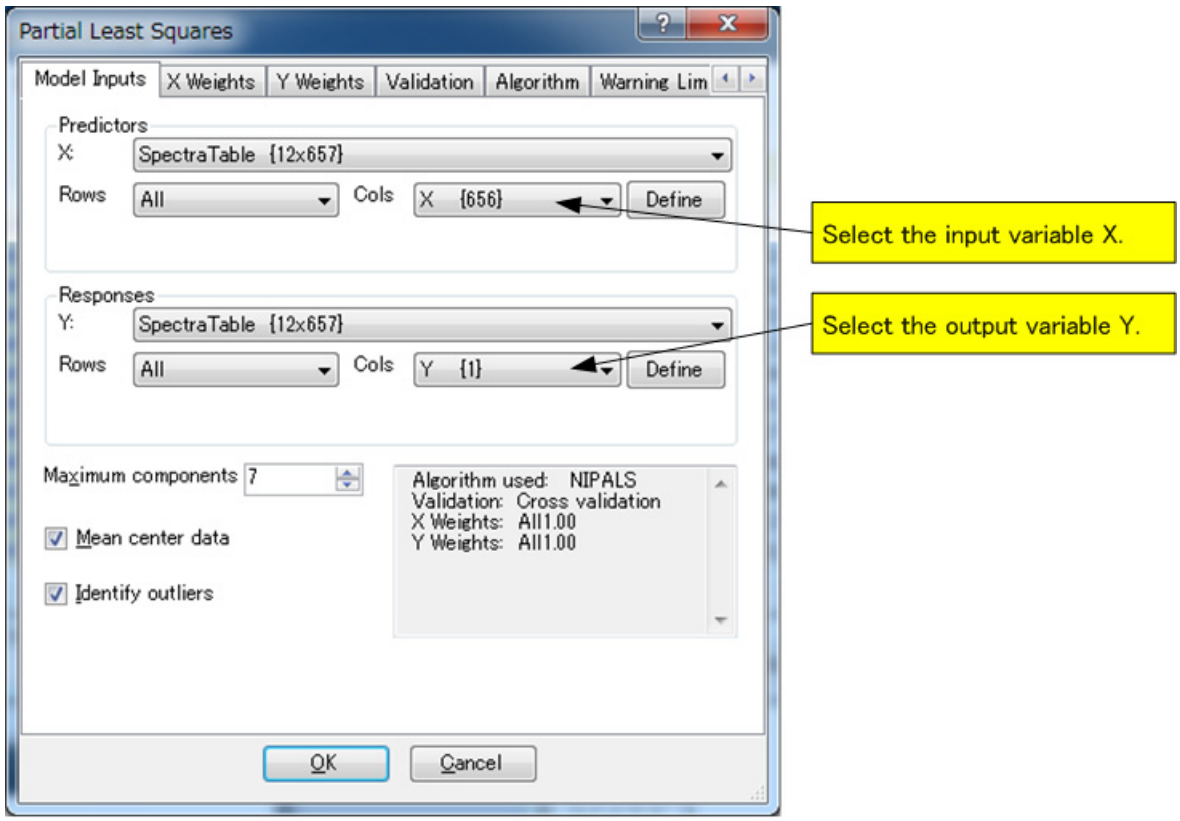
Figure 5-7 Output Variable Table



Y		Thickness
		1
sample01	1	10.0000
sample02	2	10.0000
sample03	3	10.0000
sample04	4	29.0000
sample05	5	29.0000
sample06	6	29.0000
sample07	7	39.0000
sample08	8	39.0000
sample09	9	39.0000
sample10	10	506.0000
sample11	11	506.0000
sample12	12	506.0000

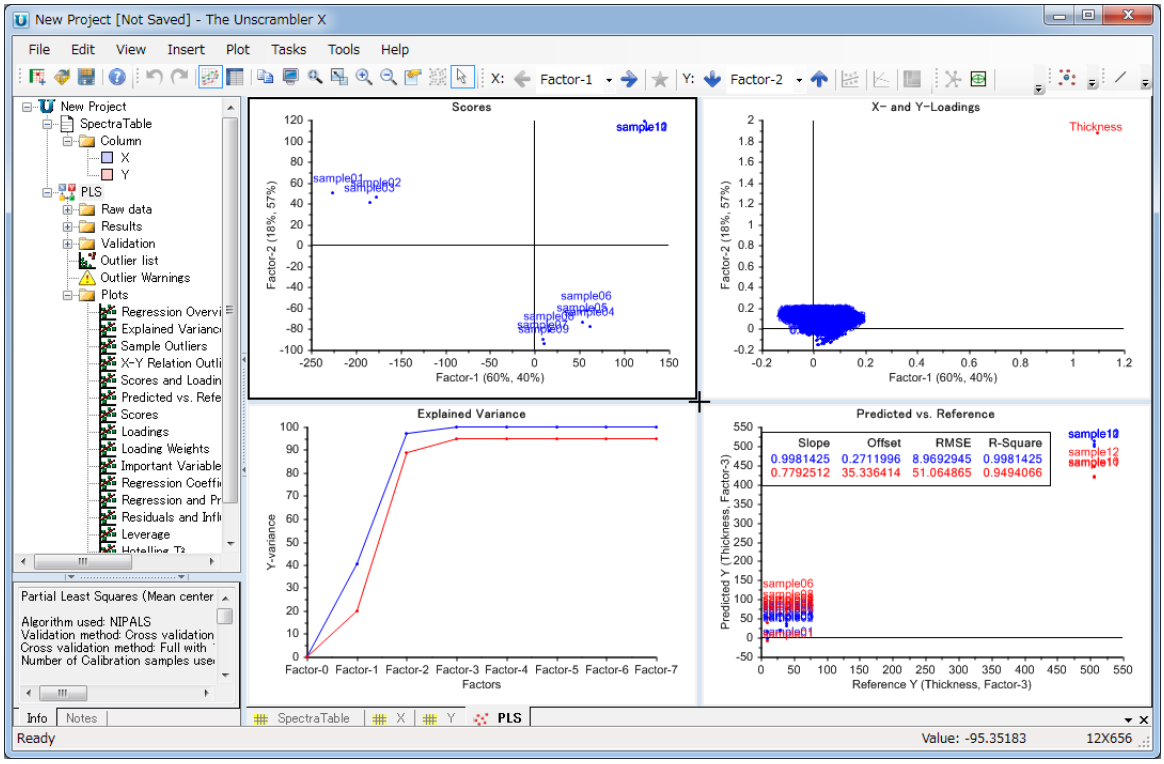
7) Execute partial least squares regression (PLSR)
Execute **[Tasks]** → **[Analyze]** → **[Partial Least Squares Regression ...]**. The Partial Least Squares dialog box opens.

Figure 5-8 Partial Least Squares Dialog Box



Click the **[OK]** button. The View Plots dialog box opens. Click the **[OK]** button to display the PLSR results.

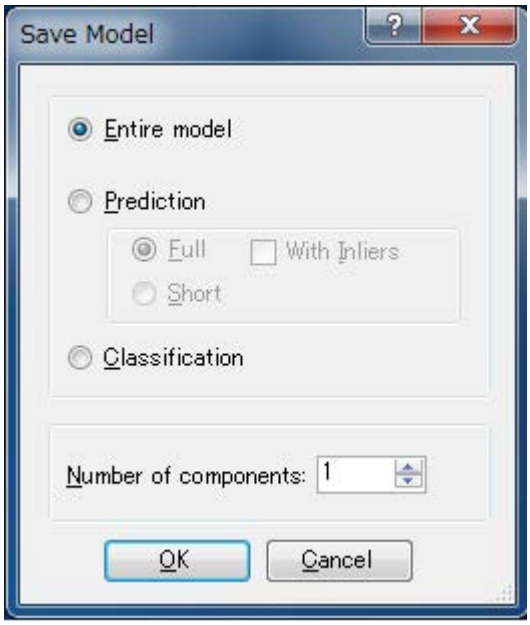
Figure 5-9 PLSR Results



8) Save the model to a file

Select PLS on the tree, and then right click the mouse and execute **[Save Model]**. The Save Model dialog box opens.

Figure 5-10 Save Model Dialog Box



Leave the Entire model radio button on and click the **[OK]** button.
Enter a file name and save the file. Here, PLS.unsb is used as the file name.
The unsb file which was saved here is the quantification model file.

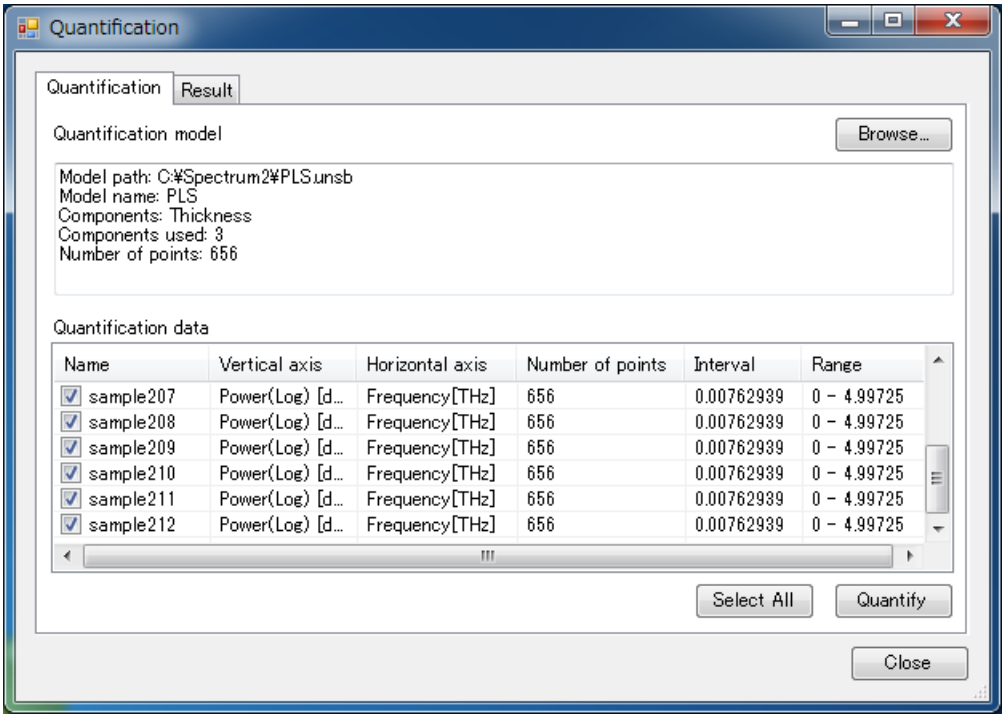
This completes the description of the operations of The Unscrambler® X.

5. 3 Performing Quantification

1) Display spectra for which to perform quantification in the Analyze window
Either execute a measurement to transfer the spectra to the Analyze window or load the spectrum measurement data file.

2) Click **[Analysis]** → **[Quantification]** in the graph window. The Quantification dialog box opens.

Figure 5-11 Quantification Tab in Quantification Dialog Box



3) Select the Quantification tab.

4) Now load a quantification model file. Click the **[Browse...]** button and select PLS.unsb which was created in the previous section.

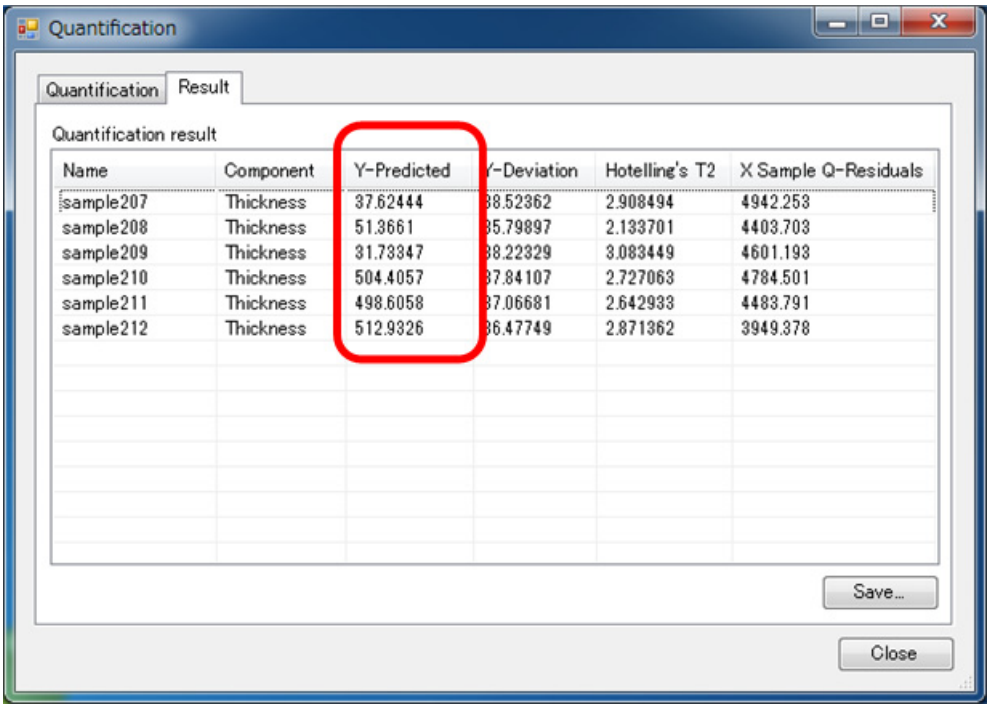
5) A list of spectrum names is displayed in Quantification data. Check the Name checkboxes of the spectra to be quantified and click the **[Quantify]** button.

Important

Selected spectra must have the same vertical axis as those that were used to create the quantification model. Note that correct quantitative values may not be obtained if their vertical axes are different.

6) The Result tab is displayed if quantification has been successfully completed.
The quantification results are displayed in Quantification result. The results of all the spectra that were selected in Quantification data are displayed. The quantitative values for each component shown in Component are displayed in the Y-Predicted columns.
Quantification results can be saved to a text file by pressing the **[Save...]** button.

Figure 5-12 Result Tab of Quantification Dialog Box



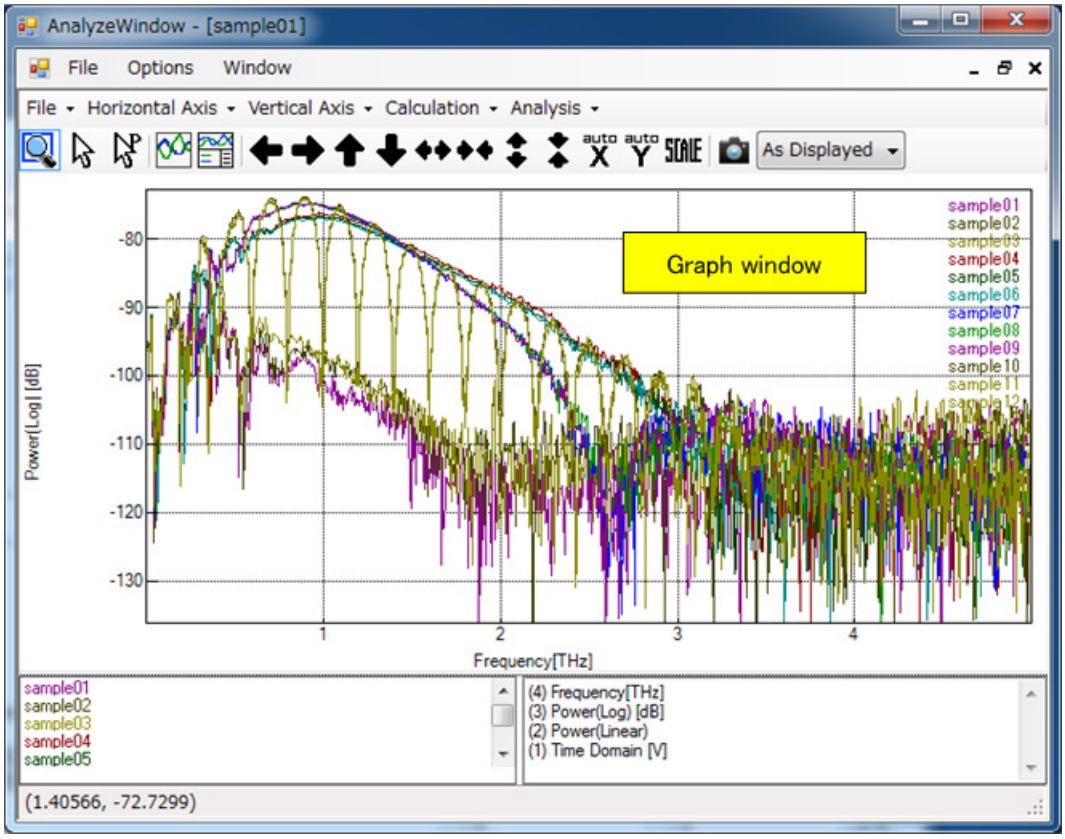
6. Menu Details

This chapter describes the menus used to execute a quantitative analysis.

6. 1 Graph Window of Analyze Window

Quantitative analyses are executed by using menus in the graph window of the Analyze window.

Figure 6-1 Graph Window of Analyze Window



◆ [File] → [Save data table...]

This command saves multiple spectra used to create a quantification model to a file.

Clicking this command opens the Save data table dialog box.

➔ For more information on the dialog box, refer to 6. 2 "Save data table Dialog Box" on page 6-3.

◆ [Analysis] → [Quantification]

This command executes quantification. Clicking this command opens the Quantification dialog box.

➔ For more information on this dialog box, refer to 6. 3 "Quantification Dialog Box" on page 6-4.

◆ Right click the mouse → [Properties...]

This command allows users to reference quantification results of the selected spectra. Clicking this command opens the Properties dialog box.

➔ For more information on the dialog box, refer to 6. 4 "Properties Dialog Box" on page 6-6.

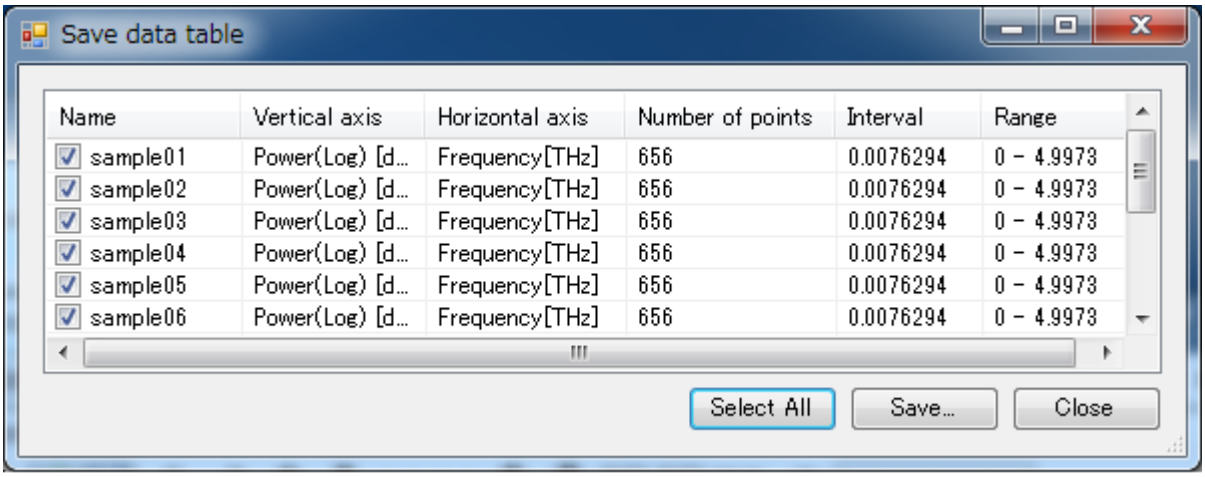
6. 2 Save data table Dialog Box

This dialog box is used to create a spectrum file.

➔ For more information on spectrum files, refer to 7. 1 "Spectrum File" on page 7-1.

This dialog box is opened from **[File]** → **[Save data table...]** in 6. 1 "Graph Window of Analyze Window" on page 6-1.

Figure 6-2 Save data table Dialog Box



Name	Spectrum name
Vertical axis	Vertical axis for the spectrum
Horizontal axis	Horizontal axis for the spectrum
Number of points	Number of data items to display for the spectrum
Interval	Data interval for the spectrum
Range	Data range for the spectrum
[Select All] button	Selects all spectra.
[Save...] button	Saves spectra to a file. Clicking this button opens the File Save dialog box.
[Close] button	Closes the dialog box.

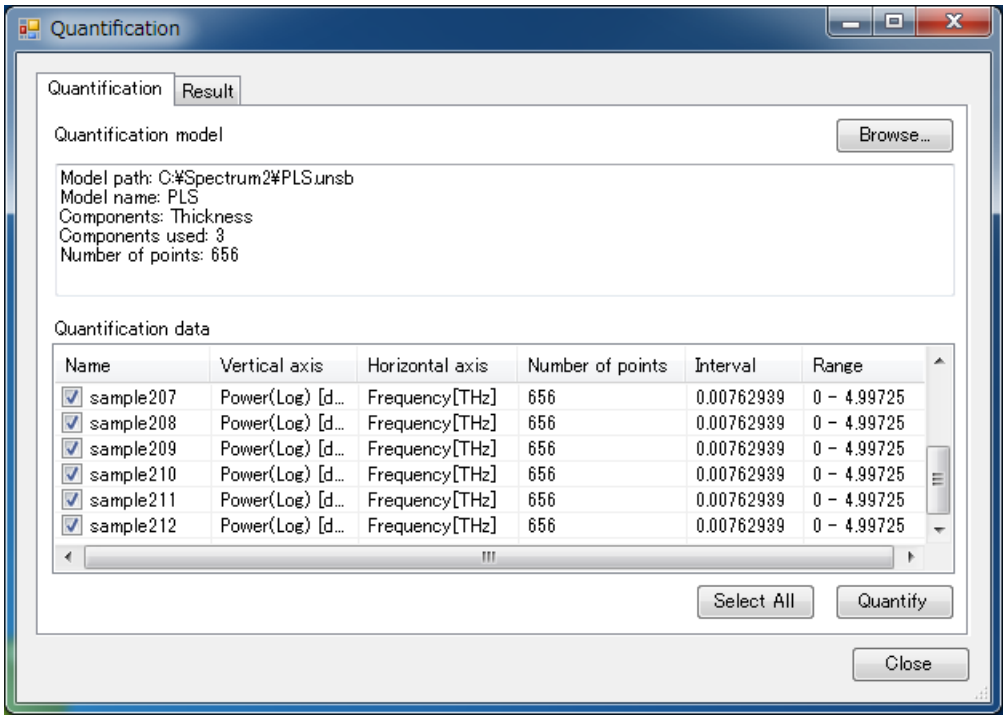
6. 3 Quantification Dialog Box

This dialog box performs quantification using a quantification model file. Quantification results can be saved to a text file.

➔ For more information on quantification model files, refer to 7. 2 "Quantification Model File" on page 7-2.

This dialog box is opened from **[Analysis]** → **[Quantification]** in 6. 1 "Graph Window of Analyze Window" on page 6-1.

Figure 6-3 Quantification Dialog Box



◆ Quantification tab

[Browse...] button	Loads a quantification model file.
Quantification model	Displays quantification model information.
Model path	Name of the path of the loaded quantification model file
Model name	Model name selected in the quantification model file
Components	Names of components that were specified when the model was created
Components used	Number of components that were specified when the model was created
Number of points	Number of data items to display for the spectrum that were used when the model was created
Quantification data	Displays spectra information. Spectra to be quantified are selected by checking the checkboxes.
Name	Spectrum name
Vertical axis	Vertical axis for the spectrum
Horizontal axis	Horizontal axis for the spectrum
Number of points	Number of data items to display for the spectrum
Interval	Data interval for the spectrum
Range	Data range for the spectrum
[Select All] button	Checks the checkboxes of the spectra that have already been selected. If not any spectra has been selected, spectra which satisfy the same conditions of the first spectrum are searched for from the remaining spectra, and their checkboxes are checked.
[Quantify] button	Quantifies the selected spectra and displays the results in Quantification result of the Result tab.

◆ Result tab

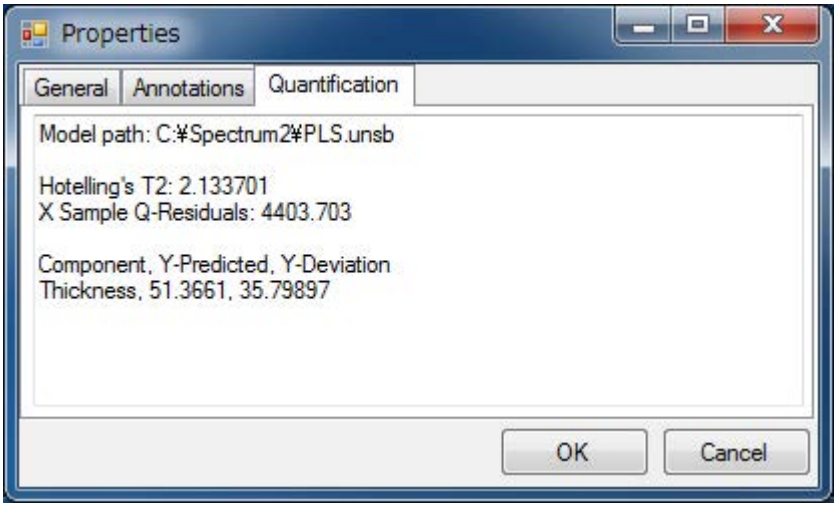
Quantification result	Displays quantification results.
Name	Name of the quantified spectrum
Component	Name of the quantified component
Y-Predicted	Quantitative value
Y-Deviation	Deviation
Hotelling's T2	T2 statistic (an index that indicates the validity of a quantification model)
X Sample Q-Residuals	Residual (an index that indicates the validity of a quantification model)
[Save] button	Saves the quantification results shown in Quantification result to a text file.
[Close] button	Closes the dialog box.

6. 4 Properties Dialog Box

Quantification results of spectra can be referenced by using the Quantification tab in this dialog box.

This dialog box is opened from right click → **[Properties...]** in 6. 1 "Graph Window of Analyze Window" on page 6-1.

Figure 6-4 Quantification Tab in Properties Dialog Box



Model path	Name of the path of the quantification model file used for quantification
Hotelling's T2	T2 statistic (an index that indicates the validity of a quantification model)
X Sample Q-Residuals	Residual (an index that indicates the validity of a quantification model)
Component	Name of the quantified component
Y-Predicted	Quantitative value
Y-Deviation	Deviation

7. Glossary

This chapter describes the terms used in this manual.

7. 1 Spectrum File

This is a file which stores multiple spectra.

The file format is CSV (comma separated value).

This file is used to create a quantification model using The Unscrambler® X.

This file is created from the **[File]** → **[Save data table...]** menu in a graph window in the Analyze window.

7. 2 Quantification Model File

This is a file which stores models used for executing quantification.

The file format is the standard file format of The Unscrambler® X (the extension is .unsb).

This file is loaded by using the System Software and is used to execute quantification.

List of Figures