

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

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Applicable System TAS7500

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1 Edition

Apr 16/12 Printed in Japan TAS7x00 Series Terahertz Spectroscopy & Imaging System System Software Operation Manual (Quantitative Analysis Option)

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

Option)

Revision History

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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^{\mathbb{R}} 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^{$\ensuremath{\mathbb{R}}$} X.

The operating procedures for The Unscrambler^(R) X described in this manual are the minimum procedures for creating a quantification model file that can be used for this option.</sup>

→ 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. 1 Installation

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.

tion input screen. Enter the Activation Key sent by Advantest on this screen.

- 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 Informa-
- 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. Installation and Uninstall

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.

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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)

```
LicensePasswordSheet
                                          Date of issue: 2012/02/17
Serial#: C050012
# Product Number
# License Type
                         -> PYSI75-02M
                         -> CpuFixed
# Expiration Client License -> 000
           -> AA9DCC963F0B685A9FDF710091C164E9A
# Password
                          -> 2017/03/22
# Expiration Date
# Number of License
                           -> 1
#**** license *****
CpuFixed 000 AA9DCC963F0B685A9FDF710091C164E9A 00000edcba98 PYSI75-02M
2017/03/22 1 00000edcba98 \leftarrow Enter this one line.
```

- 2) Select [Start] \rightarrow [All Programs] \rightarrow [Accessories] \rightarrow [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:

The following shows an example execution:

4–2

4. License Management

Figure 4-2 Example Execution of License Registration

```
C:\>%PLMS_ROOT%\bin\License_Add CpuFixed 000 AA9DCC963F0B685A9FDF710091C164E9A0
00000edcba98 PYSI75-02M 2017/03/22 1 00000edcba98J
License Added
C:\>
```

4–3

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] \rightarrow [All Programs] \rightarrow [Accessories] \rightarrow [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_RemJ
(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]:1J
(1):CpuFixed 000 AA9DCC963F0B685A9FDF710091C164E9A00000edcba98 PYSI75-02M 2017/0
3/22 1 00000edcba98
Will be Deleted. [Y/N]:yJ
License Removed
C:\>
```

5 - 1

5. Operating Procedures

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



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].

5–2

5. Operating Procedures





– 🚺 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] \rightarrow [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.

5. 1 Saving Spectrum Files

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

🖳 Save data tab	ble					x		
Name	Vertical axis	Horizontal axis	Number of points	Interval	Range			
🔽 sample01	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973	-		
▼ sample02	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973	=		
✓ sample03	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973			
🔽 sample04	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973			
📝 sample05	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973			
📝 sample06	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973	-		
•								
			Select All	Save	Close			

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. Operating Procedures

5. 2 Creating Quantification Model Files

1) Start The Unscrambler[®] X

Execute [Start] \rightarrow [All Programs] \rightarrow [The Unscrambler[®] X 10.1 (64-bit)] \rightarrow [The Unscrambler[®] X 10.1 (64-bit)].

2) Load the spectrum file

Click **[File]** \rightarrow **[Import Data]** \rightarrow **[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.

ASCII Impor	t								? x	
Separator			Headers	Headers			(٦	
💿 Comma	0:	space 💿 Ta	ь		Rows	s		l	<u>O</u> K	
🔘 Semicolo	n 🔿 (Custom		Rows 1	÷			ſ	Cancel	
				0-1	Colu	mns		l	_	
Process (Process double quotes									
Ireat cor	nsecuti	ve separators	as one							
Import as	; text									
		0.0000	0.0076	0.0153	0.0229	0.0305	0.0381	0.0458	0.0534	
		1	2	3	4	5	6	7	8	1
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	2
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!	,
< <p>1 11</p>									•	
12 X 656									.:	

Figure 5-3 ASCII Import Dialog Box

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

5–4

5. 2 Creating Quantification Model Files

U New Project [Not Save	d] - The Unsc	rambl	ler X						• X
File Edit View In	isert Plot	Task	s Tools	Help					
i 🖪 💜 🔡 🔞 i 🗠 (× & b B	×	📥 🤏 🛃	🔜 💥 i 🗠	∎洪[]∠ 🕏	ム チ 🍡			
	SpectraTable		0	0.007629395	0.01525879	0.02288818	0.03051758	0.03814697	0.04577637
Spectra Table			1	2	3	4	5	6	7
	sample01	1	-113.5911	-94.4663	-95.7448	-100.7643	-91.2941	-92.5533	-124.536
	sample02	2	-116.2613	-94.6092	-96.0213	-100.2582	-91.3093	-92.0176	-111.822
	sample03	3	-116.0037	-95.4350	-95.7033	-99.9597	-91.5252	-92.8448	-121.254
	sample04	4	-111.3704	-95.7516	-95.6163	-100.0374	-91.4403	-92.5900	-110.840
	sample05	5	-111.2046	-95.3422	-95.9535	-99.3964	-91.5312	-92.6062	-112.508
	sample06	6	-112.5031	-94.3761	-95.5986	-99.4638	-90.8869	-92.2288	-113.549
.	sample07	7	-114.7058	-95.6176	-95.5574	-99.3409	-91.1601	-92.6277	-113.863
Name : SpectraTable	sample08	8	-113.0888	-95.3518	-95.1734	-100.0577	-91.0007	-93.0360	-119.429
Size : 12 X 656	sample09	9	-112.7333	-95.3319	-95.3674	-99.6162	-91.2698	-93.2644	-121.928
Created :2012/02/29 20	sample10	10	-113.1878	-94.5687	-96.1239	-99.9312	-91.3998	-92.7368	-119.223
Source file : C:¥Spectru	sample11	11	-116.6966	-94.6756	-95.6410	-99.3444	-91.6523	-93.2274	-113.655
	sample12	12	-114.4981	-96.0685	-96.4415	-99.6937	-92.1692	-93.0845	-119.218
· · · ·	∢ 📃								۱.
Info Notes	🇰 Spectra	Table							▼ ×
							Value: -113.	5911	12X656;

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
rigule 5-5	Wall Window III winch Thickness has been Added

U New Project [Not Save	ed] - The Unscramb	ler X						
File Edit View I	nsert Plot Task	ks Tools H	lelp					
i 🖪 🧳 🔡 🔞 i 🔊 (ሮዛ 🔏 🗅 🛍 ⊁		- XX 122	∎兆⊵⊚	▲ <i>f</i> ■			
E-U New Project	SpectraTable	Thickness		0.007629395	0.01525879	0.02288818	0.03051758	0.03814697
SpectraTable		1	2	3	4	5	6	7
	sample01 1	10.0000	-113.5911	-94.4663	-95.7448	-100.7643	-91.2941	-92.5533
	sample02 2	10.0000	-116.2613	-94.6092	-96.0213	-100.2582	-91.3093	-92.0176
	sample03 3	10.0000	-116.0037	-95.4350	-95.7033	-99.9597	-91.5252	-92.8448
	sample04 4	29.0000	-111.3704	-95.7516	-95.6163	-100.0374	-91.4403	-92.5900
	sample05 5	29.0000	-111.2046	-95.3422	-95.9535	-99.3964	-91.5312	-92.6062
	sample06 6	29.0000	-112.5031	-94.3761	-95.5986	-99.4638	-90.8869	-92.2288
[▼	sample07 7	39.0000	-114.7058	-95.6176	-95.5574	-99.3409	-91.1601	-92.6277
Name : SpectraTable	sample08 8	39.0000	-113.0888	-95.3518	-95.1734	-100.0577	-91.0007	-93.0360
Size : 12X657 Created :2012/02/29 16	sample09 9	39.0000	-112.7333	-95.3319	-95.3674	-99.6162	-91.2698	-93.2644
0100100 2012, 02, 20 10	sample10 10	506.0000	-113.1878	-94.5687	-96.1239	-99.9312	-91.3998	-92.7368
Source file : C:#Spectru	sample11 11	506.0000	-116.6966	-94.6756	-95.6410	-99.3444	-91.6523	-93.2274
	sample12 12	506.0000	-114.4981	-96.0685	-96.4415	-99.6937	-92.1692	-93.0845
< >	•							•
Info Notes	# SpectraTable							+ X
						Valu	e: 506	12X657

* 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)

5. Operating Procedures

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.

New Project [Not Save	U New Project [Not Saved] - The Unscrambler X								
File Edit View Ir	nsert Plot	Task	s Tools	Help					
E 🖪 🧳 🔡 🔞									
🖃 😈 New Project	Х		0	0.007629395	0.01525879	0.02288818	0.03051758	0.03814697	0.04577637
🖮 📄 Spectra Table		A	1	2	3	4	5	6	7
📔 📋 📴 Column	sample01	1	-113.5911	-94.4663	-95.7448	-100.7643	-91.2941	-92.5533	-124.5365
· · · · · D 🔀	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
Column range : X 🔺	sample08	8	-113.0888	-95.3518	-95.1734	-100.0577	-91.0007	-93.0360	-119.4298
Size : 656 Pange : 2=657	sample09	9	-112.7333	-95.3319	-95.3674	-99.6162	-91.2698	-93.2644	-121.9282
Matrix : SpectraTable	i 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
K	• • • • • • • • • • • • • • • • • • •								
Info Notes	🗰 SpectraT	able	## X						- x
							Value: -113	3.5911	12X656

Figure 5-6 Input Variable Table

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



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5. 2 Creating Quantification Model Files

7) Execute partial least squares regression (PLSR)

Execute [Tasks] \rightarrow [Analyze] \rightarrow [Partial Least Squares Regression ...]. The Partial Least Squares dialog box opens.

Figure 5-8	Partial Le	east Squares	Dialog	Box
------------	------------	--------------	--------	-----

Partial Lea	ast Squares	? X	
Model Inpu	uts X Weights Y Weights \	/alidation Algorithm Warning Lim 💶 🗎	
Predict	ors		
X	SpectraTable {12x657}	•	
Rows	All Cols	X {656}	
			Select the input variable X.
Respon	ises		
Y:	SpectraTable {12x657}	•	Select the output variable Y.
Rows	All 🗸 Cols	Y {1} Define	
Ma <u>x</u> imum	n components 7	Algorithm used: NIPALS	
 <u>M</u> ean	center data	X Weights: All1.00 Y Weights: All1.00	
🔽 <u>I</u> denti	ify outliers	-	
	<u>O</u> K	Cancel	

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

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5. Operating Procedures



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.

5. 2 Creating Quantification Model Files

Figure 5-10	Save Model	Dialog Box
-------------	------------	------------

Save Model	
Entire model	
© <u>P</u> rediction	
 Eull With Inliers Short 	
© <u>C</u> lassification	
Number of components: 1	
<u>O</u> K <u>C</u> ancel	čti.

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^{\mathbb{R}} X.

5. Operating Procedures

5. 3 Performing Quantification

- 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

Quantification						×
Quantification Re	esult					
Quantification mo	del				Browse	»
Model path: C:¥S; Model name: PLS Components: Thic Components user Number of points	bectrum2¥PLSunsb skness ± 3 : 656					
Name	vertical axis	Horizontal axis	Number of points	Interval	Range	*
▼ sample207	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	
✓ sample208	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	
🔽 sample209	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	
🔽 sample210	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	=
✓ sample211	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	
📝 sample212	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	-
•	i		i	1	•	
				Select All	Quantit	y
L					Clos	se

- 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.

5–10

5. 3 Performing Quantification

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.
Overtification results are here each tage to the total tage. I how the spectra was a set of the spectra tage.

Quantification results can be saved to a text file by pressing the **[Save...]** button.

Figure 5-12 Result Tab of Quantification Dialog Box

Quantification re	sult	\frown			
Name	Component	Y-Predicted	/-Deviation	Hotelling's T2	X Sample Q-Residuals
sample207	Thickness	37.62444	88.52362	2.908494	4942.253
sample208	Thickness	51.3661	85.79897	2.133701	4403.703
sample209	Thickness	31.73347	88.22329	3.083449	4601.193
sample210	Thickness	504.4057	37.84107	2.727063	4784.501
sample211	Thickness	498.6058	87.06681	2.642933	4483.791
sample212	Thickness	512.9326	86.47749	2.871362	3949.378

6. 1 Graph Window of Analyze Window

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] \rightarrow [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.

6–1

6. Menu Details

◆ [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

6–3

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] \rightarrow [Save data table...] in 6. 1 "Graph Window of Analyze Window" on page 6-1.

Figure 6-2 Save data table Dialog Box

Name	Vertical axis	Horizontal axis	Number of points	Interval	Range	
🗸 sample01	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973	
✓ sample02	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973	=
🔽 sample03	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973	-
🔽 sample04	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973	
V sample05	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973	
🔽 sample06	Power(Log) [d	Frequency[THz]	656	0.0076294	0 - 4.9973	-
•					•	

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.

6. Menu Details

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]** \rightarrow **[Quantification]** in 6. 1 "Graph Window of Analyze Window" on page 6-1.

Figure 6-3 Quantification Dialog Box

Quantification						X
Quantification Re	esult					
Quantification mo	del				Browse	·
Model path: C:¥Spectrum2¥PLSunsb Model name: PLS Components: Thickness Components used: 3 Number of points: 656						
Name	vertical axis	Horizontal axis	Number of points	Interval	Range	*
🔽 sample207	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	
▼ sample208	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	
🔽 sample209	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	
🔽 sample210	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	=
📝 sample211	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	
📝 sample212	Power(Log) [d	Frequency[THz]	656	0.00762939	0 - 4.99725	-
•				1	•	
				Select All	Quantif	y)
					Clos	se

6–4

6–5

6. 3 Quantification Dialog Box

Quantification tab

[Browse] button		Loads a quantification model file.
Quantific	ation 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 condi- tions 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. Menu Details

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 \rightarrow [**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

6–6

7. 1 Spectrum File

7–1

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 $\textsc{Unscrambler}^{\ensuremath{\mathbb{R}}}$ X.

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

7. Glossary

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.

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