# J-1000 series

# **CD Spectrometer**

**Software Manual** 

Spectra Manager<sup>™</sup> CFR



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#### **Preface**

This instruction manual serves as a guide for using this software. It is intended to instruct first-time users on how to properly use the software, and to serve as a reference for experienced users.

Before using the software, read this instruction manual carefully, and make sure you fully understand its contents. This manual should be easily accessible to the operator at all times during software operation. When not using the software, keep this manual stored in a safe place. Should this instruction manual be lost, order a replacement from your local JASCO distributor.

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# **Notation Used**

The following notational conventions are used throughout this manual:

#### **General Notation**

Notation	Meaning
[Measurement] menu	Names of menus, commands, and text boxes are enclosed in
[Parameters] command	square brackets '[]', followed by a description indicating whether the function is a menu, command, text box, etc. Shortcut keys used to select menus or commands are underlined.
<ok>, <cancel></cancel></ok>	Names of buttons are enclosed in angular brackets '< >'.

**Keyboard Operations** 

Notation	Meaning
Shift Ctrl	The key is enclosed in a square and shown in boldface.
Alt, F	Keys that are to be pressed in succession are separated by commas. In the example shown on the left, the Alt key is to be pressed and released, followed by the F key.
Shift + →	Keys that are pressed simultaneously are separated by a "plus" sign. In the example shown on the left, press the key while holding down the <b>Shift</b> key.

**Mouse Operations** 

Notation	Meaning
Point	Move the mouse pointer to the specified item.
Click	Quickly press and release the mouse button.
Double-click	Click the mouse button twice in rapid succession.
Drag	Point to an item, click and hold down the mouse button.
	Move the mouse with the button held down, and release
	the button when the pointer is in the desired position.

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#### 1. Introduction

#### 1.1 How to Use This Manual

This manual is for the JASCO J-1000 series CD spectrometer measurement program that runs on *Microsoft Windows*. The J-1000 series CD spectrometer measurement program consists of [Spectra Manager CFR-Compliant Program], which conforms to FDA regulation 21 CFR Part 11 concerning electronic records and electronic signatures, and [Spectra Manager v.2-Compliant Program], which does not conform to these standards. This instruction manual refers to [Spectra Manager CFR-Compliant Program] and [Spectra Manager v.2-Compliant Program] as [CFR Version Program] and [Non-CFR Version Program], respectively.

This chapter describes the structure and use of this manual. The manual consists of 7 chapters including this one. An explanation of each chapter is given below. For this manual, *Microsoft Windows* is referred to as *Windows* and a personal computer as a PC.

#### 1. Introduction

This chapter describes how to use this manual and gives an overview of each program and menu. Read this chapter first.

#### 2. Starting and Exiting Programs and the [Spectra Manager] Program Reference

This chapter describes detailed procedures ranging from turning on/off the CD spectrometer and PC to starting/exiting the programs. Refer to Chapter 3 for details about program operations. In addition, this chapter provides the [Spectra Manager] program reference.

#### 3. Accessory Registration Reference

This chapter describes how to register accessories used with the CD spectrometer.

#### 4. Introduction to the [Spectra Measurement] Program

This chapter describes the [Spectra Measurement/Analysis] programs with examples of basic procedures. Users unfamiliar with *Windows* or first-time users of the CD spectrometer should follow the procedures described in this chapter for a general overview of how to operate the program.

#### 5. Introduction to the [Time Course Measurement/Analysis] Programs

This chapter describes the [Time Course Measurement/Analysis] programs with examples of basic procedures.

#### 6 to 9. Measurement Program References

These chapters describe common toolbar and menu commands for the [Spectra Measurement], [Time Course Measurement] and [Data Monitor] programs, in addition to the parameters used in these programs. Read the relevant chapters as required.

- 6. Toolbar and menu reference.
- 7. [Spectra Measurement] program reference
- 8. [Time Course Measurement] program reference

#### 9. [Data Monitor] program reference

#### 10. Appendix

This chapter provides useful suggestions for specifying parameters for CD measurements.

#### 1.2 FDA 21CFR Part 11

FDA 21 CFR Part 11 is a set of regulations regarding digital archiving of data and data records for GLP, GCP, and GMP procedures. These regulations cover a number of areas, including: 1) access control and electronic signature requirements for data recorded by any computer-controlled analytical system in which the results are digitally archived; 2) the provision of security functions that can only be accessed by authorized personnel to ensure the security and integrity of data; and 3) a data auditing mechanism with the automatic creation of an Audit Trail to maintain a record of any creation, modification or deletion of instrument data.

# 1.3 Features of [Spectra Manager] Compatible with FDA 21CFR Part 11

JASCO Spectra Manager<sup>TM</sup> is an integrated software package that acts as a common platform for the range of JASCO analytical instruments, including UV/Vis, near-infrared, infrared, fluorescence, Raman, polarimetry, and circular dichroism spectrometers. The Spectra Manager<sup>TM</sup> software provides functionality ranging from analytical instrument control and spectral data processing to sophisticated and specialized data analysis programs. JASCO Spectra Manager<sup>TM</sup> CFR provides security and auditing functionality that ensures the security, integrity and confidentiality of electronic records by enforcing the use of electronic signatures and other security measures as described in the regulations outlined in 21 CFR Part 11.

JASCO Spectra Manager<sup>TM</sup> CFR consists of three core modules: Administrative Tools and Security Manager modules; intrinsic components of the Spectra Manager<sup>TM</sup> CFR software; and a database, which is an external component to the Spectra Manager<sup>TM</sup> CFR software. In addition, there are two broad classes of add-on modules: instrument drivers, which are spectrometer, or accessory-specific; and spectral analysis modules, which provide a range of sophisticated analytical and data processing tools. These add-on modules integrate seamlessly with the three core components of the Spectra Manager system to provide compliance with 21 CFR Part 11 regulations over the entire range of JASCO products. Figure 1.1 illustrates the system organization.

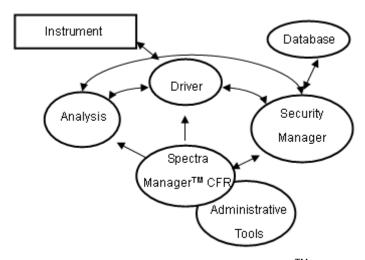


Figure 1.1 Structure of Spectra Manager™ CFR

All of the security management functions of JASCO Spectra Manager<sup>TM</sup> CFR are accessed through the Administrative Tools interface. The Security Manager components of the system are not directly accessible by a user, and thus the operation of these modules is not described. For secure management of data and data records, JASCO Spectra Manager<sup>TM</sup> CFR has two levels of security: system-level security and workgroup-level security.

When a user is registered in JASCO Spectra Manager<sup>TM</sup> CFR, the user must be assigned to one of four possible System Access Levels: "Administrators", "Power Users", "Users", or "Limited Users". The level of control that a user has over the management functions of the software system is determined by the System Access Level assigned to that user. Table 1.1 outlines the different rights assigned to the different types of users depending on their System Access Levels. Users with an "Administrators" system access level are referred to as "[Spectra Manager CFR] administrators". In contrast, users belonging to the "Administrators" group in *Windows* are referred to as "*Windows* administrators".

Note: An "Administrators" access level has no relation to "Windows administrator" and means administrator privileges for the [Spectra Manager CFR] program.

Table 1.1 Rights of each System Access Level

	Administrators	Power Users	Users	Limited Users
Display/modify system policy	OK			
Add/delete users	OK			
Modify user properties (incl. System Access Level)	OK			
Add a workgroup	OK			
Delete a workgroup	Workgroup Ma	anagers only		
Modify workgroup users	Workgroup Ma	anagers only		
Add/delete instruments	OK			
Modify instrument configuration	OK			
Add/delete programs	OK			
Display log management	OK	OK		

Workgroups correspond to actual groupings of users within the organization and may represent divisions such as projects, departments, or research groups. Each workgroup has a set of users, instruments, accessories, and analysis programs associated with it; only users registered with a specific workgroup may access the instruments and programs of that workgroup. Within a workgroup, users are granted access as either a "Manager", "Analyst", or "Operator", with authorities to modify instrument and analysis settings and use resources within the workgroup determined by the Workgroup User Rights granted. Selectable Workgroup User Rights vary depending on the system access level of the user. Table 1.2 outlines the relationship between the System Access Levels and Workgroup User Rights.

Table 1.2 Qualified access levels by Workgroup User Rights

	Administrators	Power Users	Users	Limited Users
Managers	OK	OK		
Analysts	OK	OK	OK	
Operators	OK	OK	OK	OK

By employing a two-level security model, global security authorization is independent of instrument, accessory, and application authorization, resulting in a highly flexible security system. Table 1.3 outlines the different rights assigned to the different types of users depending on their Workgroup User Rights.

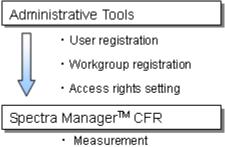
Table 1.3 Rights of each Workgroup User Rights

	Managers	Analysts	Operators
Register/unregister workgroup users	OK		
Change Workgroup user authorities	OK		
Register/unregister instruments for the workgroup	OK		
Register/unregister programs for the workgroup	OK		
Use a registered instrument	OK	OK	OK
Use a registered instrument application	OK	OK	OK
Modify measurement parameters	OK	OK	
Use a registered analysis program	OK	OK	OK
Modify analysis parameters	OK	OK	
Electronically sign data	OK	OK	OK

Figure 1.2 shows the typical operational flow of the JASCO Spectra Manager<sup>TM</sup> CFR. First, a user is created (registered) and their System Access Level is assigned using Administrative Tools. A Workgroup is created (registered), and individual users and analytical instruments are assigned to the Workgroup. Detailed access to instrument control and analysis programs can be set at the User and Workgroup levels. Access control levels as required by FDA 21 CFR Part 11 regulations are determined by the Administrative Tools settings.

Routine analyses can then be conducted by the operator using the measurement/analysis programs in JASCO Spectra Manager<sup>TM</sup> CFR. Since all levels of access are managed by Security Manager, individual users are only able to execute procedures that are allowed by their assigned access level. Access control ranges from declaring measurement parameters to conducting measurements and performing data analysis.

Analytical data obtained using any of the procedures described above can be saved as an electronic record with an electronic signature.



- · Analysis
- · Save with electronic signature
- · Review and Approval signature

Figure 1.2 Operational flow

## 1.4 Overview of [Spectra Manager]

[Spectra Manager] refers to the entire suite of measurement/analysis and administrative programs for JASCO CD spectrometers.

Specifically, [Spectra Manager] is a software program that communicates with the CD Spectrometer to start various measurement and analysis programs. Common programs that are used include programs for performing measurements using the CD Spectrometer, the [Validation] program for checking the performance of the CD spectrometer, and the [Spectra Analysis], [JASCO Canvas] and [Administrative Tools] programs.

Spectra Measurement Controls the CD spectrometer and measures samples.

Validation Checks the performance of the CD spectrometer.

Spectra Analysis Displays, processes, and prints the data obtained by [Spectra

Measurement].

JASCO Canvas Customizes the format of spectral data for printing.

Administrative Tools Controls the administration of the CD spectrometer and

measurement/analysis programs including the assignment of user

authority.

This manual mainly explains how to use several of the measurement programs. Refer to [Hardware Manual] for details about how to use the CD spectrometer. Refer to the individual instruction manuals for details about the [Validation], [Interval Scan Measurement], [Spectra Analysis], [Interval Data Analysis], and [JASCO Canvas] programs.

# 2. Starting and Exiting Programs and the [Spectra Manager] Program Reference

## 2.1 Starting the program

#### 2.1.1 Turning on the CD Spectrometer

- (1) Confirm that the standard detector is installed in the J-1000 series CD spectrometer. If another detector has been installed, replace it with the standard detector. Refer to the hardware manual "Model J-1100/1500 CD Spectrometer" or "Model J-1700 CD Spectrometer" for instructions on removing or installing the detector.
- (2) Supply nitrogen gas at a flow rate of at least 2 L/min. Absorption due to oxygen increases with decreasing wavelength, which reduces the light intensity reaching the detector. Please increase the flow rate to optimize the intensity within the desired wavelength range.

Nitrogen flow rate for different measurement wavelength ranges:

Up to 185 nm 2 L/min
Up to 180 nm 5 L/min
Up to 175 nm 15 L/min

Less than 175 nm More than 15 L/min

Note: Depending on the residual amount of nitrogen gas present when the spectrometer is first turned on, it is possible for absorption due to oxygen to be high even if the recommended nitrogen flow rate is used. In this case, pre-purge at a nitrogen flow rate of 15 L/min before performing measurements. The recommended pre-purge times are: 10 min for wavelengths up to 185 nm, 30 min for wavelengths up to 180 nm and 60 min for wavelengths up to 175 nm.

- (3) When using the 450 W Xe lamp, feed cooling water to the light source at a flow rate of about 2 L/min.
- (4) Turn on the "Power" switch at the left side of the CD spectrometer.

**WARNING!**: Running the xenon (Xe) lamp in air will generate ozone gas, which is harmful to humans. Always supply nitrogen gas for a few minutes before turning on the light source.

- Note 1: When performing measurements at wavelengths shorter than 180 nm, to maintain the effect of the nitrogen purge, after inserting or removing samples close the sample compartment lid as soon as possible.
- Note 2: A high nitrogen flow rate is necessary when performing measurements at wavelengths shorter than 175 nm because of the sharp increase in absorption due to oxygen.
- Note 3: Ozone gas absorbs light at wavelengths of 200 to 300 nm and 600 to 700 nm. This makes it difficult to perform measurements in these wavelength regions and can also damage optical parts due to corrosion. Always supply nitrogen gas before turning on the light source.

- Note 4: Never use helium gas. It will permeate into the photomultiplier tube, reducing the vacuum level and the functionality of the tube.
- Note 5: If a PC-controlled nitrogen gas flow meter (an optional accessory) is installed, all that is necessary to do is to simply open the main valve of the gas cylinder.

  Nitrogen will start flowing when the spectrometer is started. The flow rate can be controlled via the measurement program.
- Note 6: Step (3) is not necessary with the 150 W Xe lamp, which is cooled with air.
- Note 7: Just turning ON the "Power" switch does not result in the light source being turned on. The light source will be turned on automatically when the measurement program is started.

# 2.1.2 Starting the PC and Windows and Registering a J-1000 Series CD spectrometer

Turn on the PC and monitor to start *Windows*. When a J-1000 series CD spectrometer is connected for the first time, registration of the CD spectrometer is required in [Spectra Manager].

Note: The operations described in this section can be performed only by Administrators.

Start [Administrative Tools], right-click [Instrument] and select [Register Instrument...] from the shortcut menu to display the window in Fig. 2.2.

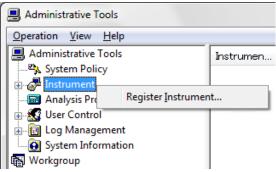


Figure 2.1 [Administrative Tools] window

(1) Select the check box for the JASCO J-1000 series control driver and click the <<u>N</u>ext> button to display the dialog box in Fig. 2.3.

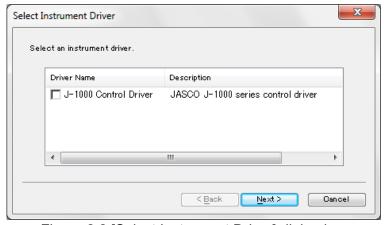


Figure 2.2 [Select Instrument Driver] dialog box

(2) Enter the CD spectrometer name, model name and serial number and then click the <Finish> button to register the CD spectrometer. The model name and serial number are inscribed on the name plate on the rear panel of the CD spectrometer.

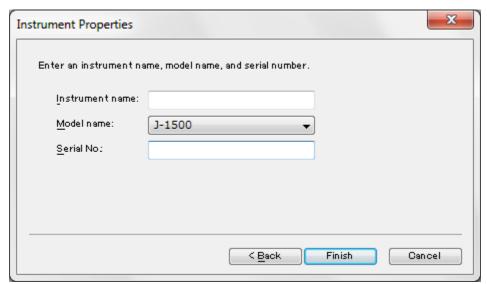


Figure 2.3 [Instrument Properties] dialog box

The CD spectrometer is registered and the name is displayed in the right pane of the [Administrative Tools] window.

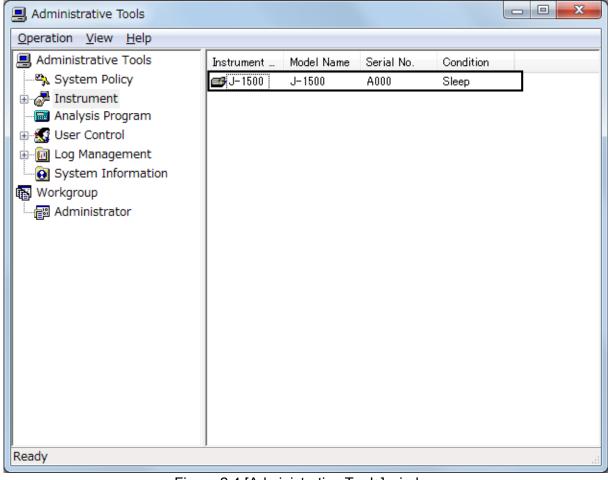


Figure 2.4 [Administrative Tools] window

Note: After registering the CD spectrometer, exit the program and perform the following operations after logging on again.

(3) Restart [Spectra Manager] and start [Administrative Tools]. Right-click the registered CD spectrometer name and select [Properties...] to display the dialog box in Fig. 2.5. First, check that [Model name], [Display name], [Serial number], and [Driver version] are displayed in the [General] tab.



Figure 2.5 [General] tab in [Properties] dialog box

(4) Click the [Composition] tab to set parameters for the nitrogen gas flow meter and the light source.

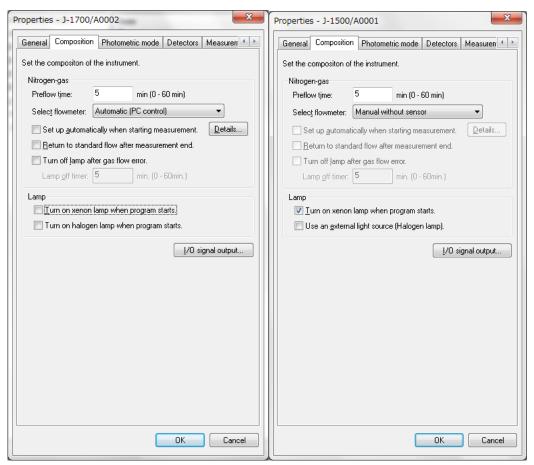


Figure 2.6 [Composition] tab in [Properties] dialog box J-1700 (left), J-1500 (right)

Nitrogen-gas		
[Preflow time]	Specifies the nitrogen gas preflow time before the light	
	source is turned on.	
[Select flowmeter]	Selects the nitrogen gas flow meter.	
	[Manual without sensor]: Select this when using a manual	
	flow meter with no sensor.	
	[Manual with sensor]: Select this when using a manual flow	
	meter with a sensor.	
	[Automatic (PC control)]: Select this when using a	
	PC-controlled automatic flow meter.	
[Set up <u>a</u> utomatically at	Specifies the nitrogen gas flow rate for the idling or	
measurement]	measurement state. The flow rate is automatically	
	controlled. This function is only available when the	
	[Automatic (PC control)] flow meter is selected.	

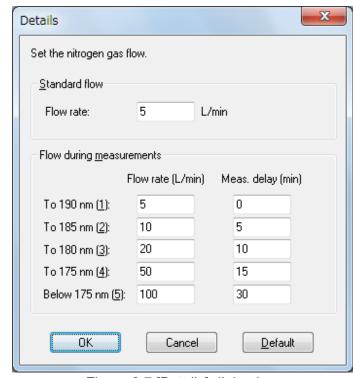


Figure 2.7 [Details] dialog box

[Return to standard flow after a measurement end]	Specifies that the flow rate is automatically returned to the standard flow rate after measurement. This function is only available when the [Automatic (PC control)] flow meter is selected.
[Turn off <u>l</u> amp after gas flow error]	Specifies that the lamp is automatically turned off after a gas flow error has occurred. This function is only available when the [Automatic (PC control)] or [Manual with sensor] flow meter is selected.
[Lamp <u>o</u> ff timer]	Specifies the time before the light source is automatically turned off after a nitrogen gas flow error has occurred. This function is only available when the [Automatic (PC control)] or [Manual with sensor] flow meter is selected.
Lamp	
[Turn on xenon lamp when program starts]	Specifies that the Xe lamp is automatically turned on when the measurement program is started.
[Turn on halogen lamp when program stars]	Specifies that the WI lamp is automatically turned on when the measurement program is started. (only for J-1700)
[Use an <u>e</u> xternal light source (Halogen lamp)]	Specifies that the external halogen lamp is used. (only for J-1500)
< <u>I</u> /O signal output>	Specifies that the drain and external start signals from the CD spectrometer are sent to the accessory attached to the I/O ports. Select the desired check boxes. When the accessory is made by JASCO, these settings are

I/O Signal Output

Enable drain signal.

I/O Port Num.: I/O 1 16 I/O 2 12 I/O Signal level: Positive Negative
Output time: 1000 msec

Enable external start signal.

OK Cancel

Figure 2.8 [I/O Signal Output] dialog box

(5) Click the [Photometric mode] tab to register the photometric mode.

The electric signals except other than CD signals can be detected using the J-1000 series CD spectrometer. The photometric modes selected in this dialog box are displayed in the measurement program. For J-1100, the available photometric modes are limited.

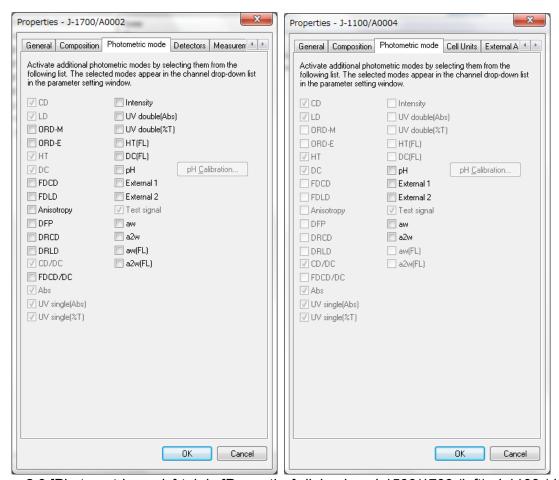


Figure 2.9 [Photometric mode] tab in [Properties] dialog box J-1500/1700 (left), J-1100 (right)

CD	Measures the circular dichroism signal
LD	Measures the linear dichroism signal
ORD-M	Measures the optical rotational dispersion signal. The
OND W	ORD-M accessory is required. (Not available for J-1100)
ORD-E	Measures the optical rotational dispersion signal. The
OND-L	ORD-E accessory is required. (Not available for J-1100)
HT	Measures the high-tension (HT) voltage applied to the
111	CD photomultiplier tube in the transmission
	configuration.
DC	Measures the direct current (DC) voltage applied to
DC	` ,
	the CD photomultiplier tube in the transmission
	configuration.
FDCD	Measures the fluorescence detected circular dichroism
	signal. The FDCD accessory is required. (Not available for
	J-1100)
	$\Delta F = F_1 - F_r$
	F <sub>I</sub> : Fluorescence intensity excited by left circularly polarized
	light
	F <sub>r</sub> : Fluorescence intensity excited by right circularly
	polarized light
FDLD	Measures the fluorescence detected linear dichroism
	signal. The FDCD accessory is required. (Not available for
	J-1100)
	$\Delta F = F_{//} - F_{\perp}$
	F <sub>//</sub> : Fluorescence intensity excited by horizontally linear
	polarized light
	F ⊥: Fluorescence intensity excited by vertically linear
	polarized light
Anisotropy	Measures the fluorescence anisotropy signal. (Not
	available for J-1100).
D.F.P.	Measures the degree of fluorescence polarization signal.
	(Not available for J-1100).
DRCD	Measures the circular dichroism signal using detector for
	fluorescence configuration  Measures the linear dichroism signal using detector for
DRLD	fluorescence configuration
CD/DC	Measures the CD and DC signals and displays the CD
33,50	signal divided by the DC signal.
FDCD/DC	Measures the FDCD and DC signals and displays the
1 000/00	FDCD signal divided by the DC signal. (Not available for
	J-1100).
Abs.	Measures the absorption spectrum. The absorption signal
ANG.	is obtained by conversion of the HT signal. Select this when
	is obtained by conversion of the FT signal. Select this when

	the HT voltage for the photomultiplier tube in the
LIV single (Abs.)	transmission configuration is set to Auto.
UV single (Abs.)  UV single (%T)	Measures the absorption spectrum. The absorption signal
	is obtained by conversion of the DC signal. Select this when
	the HT voltage for the photomultiplier tube in the
	transmission configuration is set to Manual.
	Measures the transmittance (%T) spectrum. The %T signal
	is obtained by conversion of the DC signal. Select this when
	the HT voltage for the photomultiplier tube in the
Intensity	transmission configuration is set to Manual.
	Measures the fluorescence intensity. Select this when the
	HT voltage for the photomultiplier tube in the fluorescence
	configuration (90 degrees with respect to the measurement
	beam direction) is set to Auto.
UV double (Abs.)	(Not available for J-1100)
	Measures the absorption spectrum using a UV double
	beam attachment. (Not available for J-1100)
UV double (%T)	Measures the transmittance spectrum using a UV double
	beam attachment. (Not available for J-1100)
HT(FL)	Measures the applied voltage (HTV) to the photomultiplier
	tube in the fluorescence configuration (90 degrees with
	respect to the measurement beam direction). (Not available
	for J-1100)
DC(FL)	Measures the direct current (DC) voltage to the
	photomultiplier tube in the fluorescence configuration (90
	degrees with respect to the measurement beam direction).
I	(Not available for J-1100)
pH	Measures the direct current signal from the pH meter. The
	pH meter is required.
External 1	Measures the signal from external signal input 1 ("EXT 1"
	terminal on the rear panel of the amplifier).
External 2	Measures the signal from external signal input 2 ("EXT 2"
	terminal on the rear panel of the amplifier).
Test signal	This is mainly used for checking the instrument.
aw	Measures the 50 kHz signal from the detector in the
	transmission configuration for the measurement beam.
	(Used for JASCO service engineers.)
a2w	Measures the 100 kHz signal from the detector in the
	transmission configuration for the measurement beam.
	(Used for JASCO service engineers.)
aw(FL)	Measures the 50 kHz signal from the detector in the
	fluorescence configuration (90 degrees with respect to the
	measurement beam direction) for the measurement beam.

	(Used for JASCO service engineers. Not available for J-1100)
a2w(FL)	Measures the 100 kHz signal from the detector in the fluorescence configuration (90 degrees with respect to the measurement beam direction) for the measurement beam.  Used for JASCO service engineers. (Not available for J-1100)

#### The example of combination in accessories and photometric mode

FDCD unit: FDCD, FDLD, DC(FL), FL Detector (manual)

Integrating sphere: DRCD, DRLD, HT(FL)

Emission monochromator: Intensity, FL Detector (manual)
Stopped flow: CD/DC, DC, CD Detector (manual)

ORDM-520 ORD-M, HT ORDE-521 ORD-E, HT

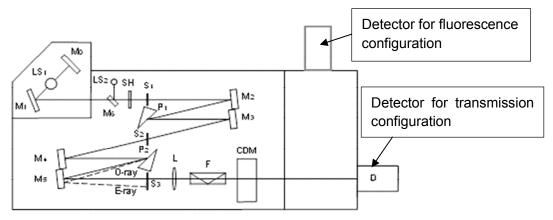


Figure 2.10 Configuration of detectors

- (6) Click the [Detectors], [Measurement Units], [Cell Units] and [External Accessories] tabs to register detectors, measurement units, cell units, and external accessories, respectively. Refer to Chapter 4 for details about registering accessories.
- (7) Click the [Adjustments] tab to perform CD spectrometer adjustments.

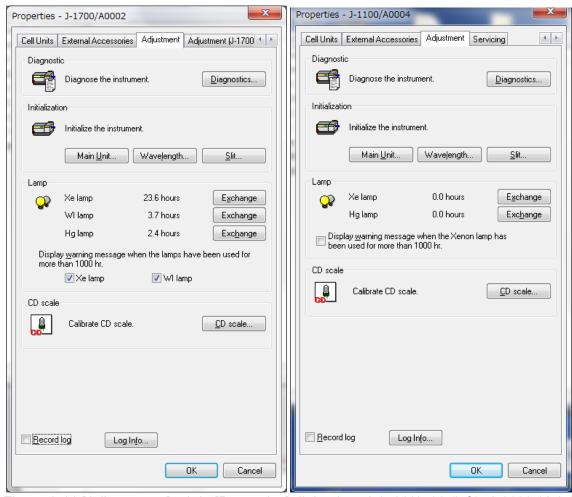


Figure 2.11 [Adjustments] tab in [Properties] dialog box J-1500/1700 (left), J-1100 (right)

Diagnostic	
< <u>D</u> iagnostics>	Confirms whether the CD spectrometer is functioning
	correctly.
Initialization	
<main unit=""></main>	Initializes the instrument settings.
<wavelength></wavelength>	Initializes the wavelength settings.
< <u>S</u> lit>	Initializes the slit width settings.
Lamp	
[Xe lamp]	Displays the number of hours the xenon lamp has been
	used. When the xenon lamp is exchanged, click the
	<exchange> button to reset the number of hours used to 0.</exchange>
[WI lamp]	Displays the number of hours the halogen lamp has been
	used. When the halogen lamp is exchanged, click the
	<exchange> button to reset the number of hours used to 0.</exchange>
	(only for J-1700)
[Hg lamp]	Displays the number of hours the mercury lamp has been
	used. When the mercury lamp is exchanged, click the
	<exchange> button to reset the number of hours used to 0.</exchange>

[Display warning message when the lamps have been used for more than 1000 hr]

Displays a warning message when the xenon and/or halogen lamp have been used for more than 1000 hours (see Fig. 2.12). Halogen lamp can be selected only for J-1700.



Figure 2.12 Warning message for xenon lamp usage time

Note: The lifetime of the xenon lamp is approximately 1000 hours. When it has been used for more than 1000 hours, the decrease in intensity of the light source will effect measurements.

CD scale

Record log

Calibrates the scale for CD signal. Used for users.

Records a log of J-1000. When error occurs, send a log to JASCO service engineers.

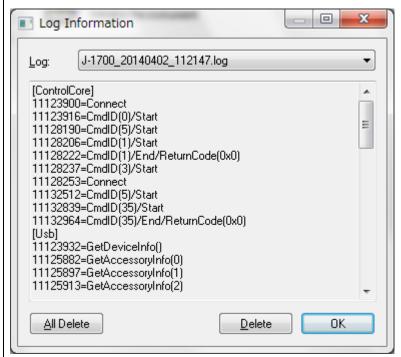


Figure 2.13 [Log Information] dialog box

Click the <<u>D</u>iagnostics...> button to display the [Diagnostics] dialog box. This function confirms whether the CD spectrometer is functioning correctly.

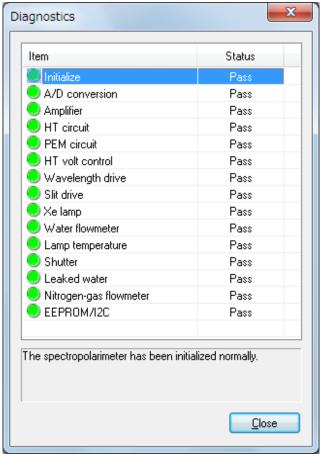


Figure 2.14 [Diagnostics] dialog box

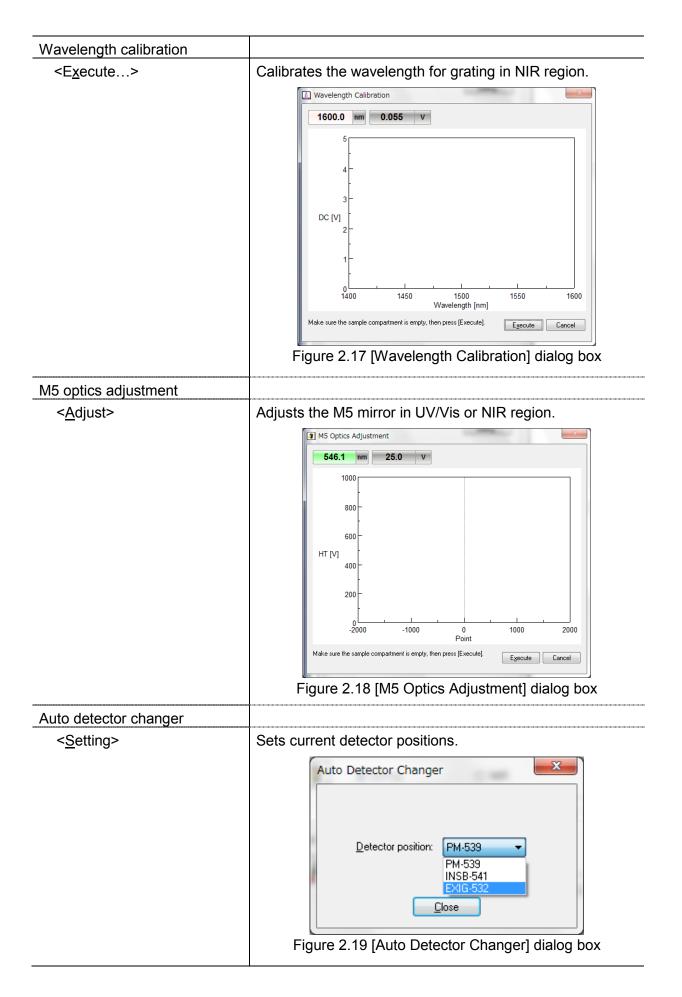
If an error message is displayed in the message area in Fig 2.13, contact your local JASCO distributor.

(8) Click the [Adjustment (J-1700)] tab to perform CD spectrometer adjustments. (Only J-1700)



Figure 2.15 [Diagnostics] dialog box

# Changeover wavelengths Sets the changeover wavelengths for light source, grating and detectors. Changeover Wavelength Settings Light source / Grating: Detector 1: Detector 2: 300 Nm Figure 2.16 [Changeover Wavelength Settings] dialog box



(9) Click the [Servicing] tab to calibrate CD spectrometer conditions such as the detector sensitivity. If calibration is required, contact your local JASCO distributor.

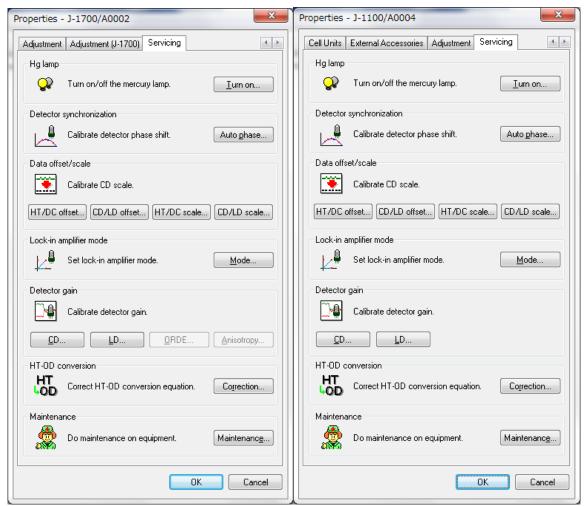


Figure 2.20 [Calibrations] tab in [Properties] dialog box

Hg lamp	Turns the mercury lamp on or off.
Detector synchronization	Calibrates the phase shift of the CD and FL detectors. Used for JASCO service engineers.
Data offset/scale	Calibrates the offset and scale of Main unit (J-1000). Used for JASCO service engineers.
Lock-in amplifier mode	Selects the lock-in amplifier mode. Used for JASCO service engineers.
Detector gain	Calibrates the scale for CD, LD, ORDE and anisotropy signals. Used for JASCO service engineers.
HT-OD conversion	Calibrates the HT-OD conversion equation. Used for JASCO service engineers.
Maintenance	Used for JASCO service engineers.

Note: In the CFR version, J-1000 must be registered to Workgroup before use. Refer to the [Spectra Manager CFR Administrative Tools] manual for details about registering the CD spectrometer to Workgroup.

### 2.1.3 Starting [Spectra Manager]

(1) After starting *Windows*, double-click the [Spectra Manager] icon located on the *Windows* desktop. Type the username and password in the logon dialog box to display the window in Fig. 2.21.

Note: [Spectra Manager] can also be started by selecting [Start] - [All Programs] - [JASCO] - [Spectra Manager] from the Windows [Start] menu.

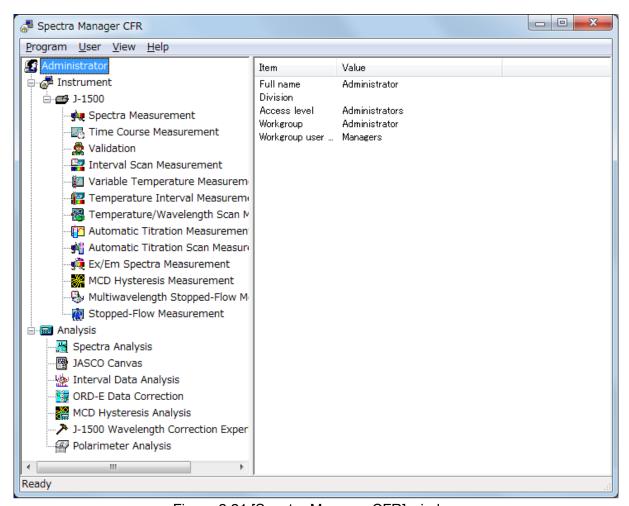


Figure 2.21 [Spectra Manager CFR] window

(2) Start the [Spectra Measurement] program to measure a sample.
Double-click [Spectra Measurement] from the [Instrument] list of [Spectra Manager] to start the program. The window in Fig. 2.22 is displayed.

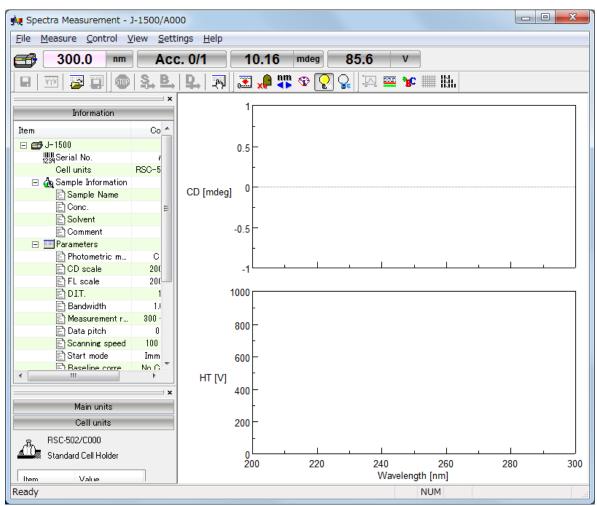


Figure 2.22 [Spectra Measurement] window

#### 2.1.4 Components of the Program Window

In this section, the [Spectra Analysis] program window is used as an example to explain program operation components. The names of the various components (windows and dialog boxes) are also described.

#### View window

[Spectra Analysis] shows multiple spectrum display windows (called "Views") in the main program window. Views have no dedicated menu bar, toolbar or status bar. Instead, the toolbar buttons and other components in the [Spectra Analysis] program window can be used for the active View window.

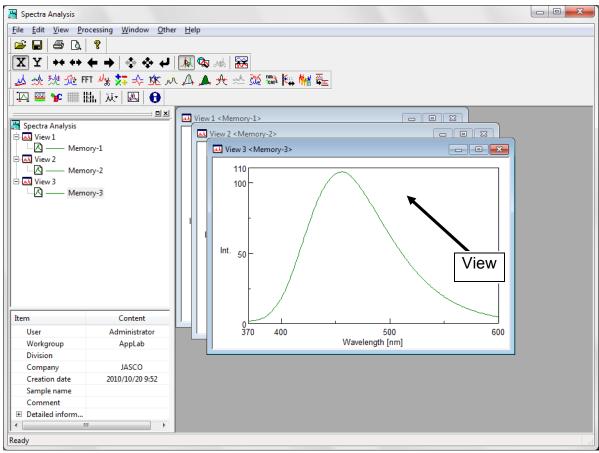


Figure 2.23 "Views" in [Spectra Measurement] program window

#### Dialog boxes

Commands and menu items ending with an ellipsis (...) open a dialog box when clicked. The opened dialog box usually contains parameters that must be specified. The [Styles] dialog box from the  $[\underline{V}]$  menu is used as an example to explain the names and functions, as well as the operational rules for various sections of the dialog box.

To display the [Styles] dialog box in Fig. 2.24, select [Styles...] from the [View] menu in the [Spectra Analysis] program. The names of various sections of the dialog box are indicated below.

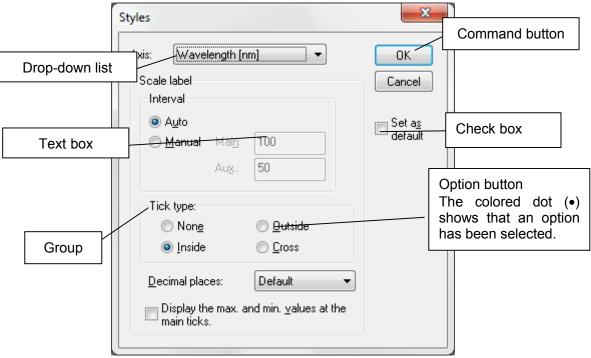


Figure 2.24 [Styles] dialog box

## 2.2 Exiting the Program

## 2.2.1 Exiting [Spectra Manager]

(1) Select  $[E\underline{x}it]$  from the  $[\underline{P}rogram]$  menu to close [Spectra Manager].

Note: [Spectra Manager] can also be exited by clicking the <Close> button.

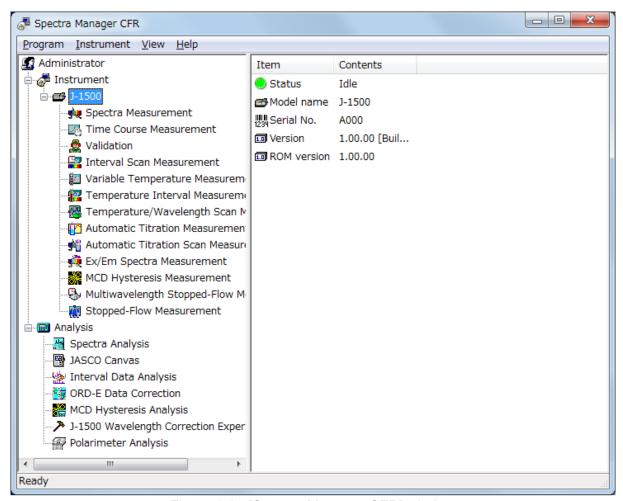


Figure 2.25 [Spectra Manager CFR] window

[Spectra Manager] cannot be exited before closing the running measurement/analysis programs. If programs are running, the dialog box in Fig. 2.26 is displayed. After clicking the <OK> button, close the running programs.

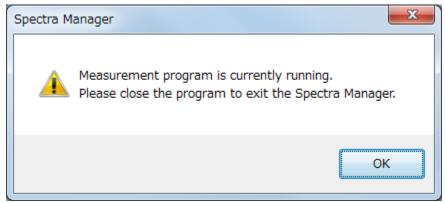


Figure 2.26 Message when a program is still running

### (2) Exiting Windows

Exit Windows in accordance with standard Windows operation procedures.

## 2.2.2 Turning off the PC and CD Spectrometer

- (1) First, turn off the PC and monitor. Do not forget to turn off the monitor.
- (2) Ensure that the sample compartment is empty, and then turn off the CD spectrometer.

# 2.3 [Spectra Manager CFR] Program Reference

[Spectra Manager CFR] is an integrated software package that acts as a common platform for the entire range of JASCO analytical instruments.

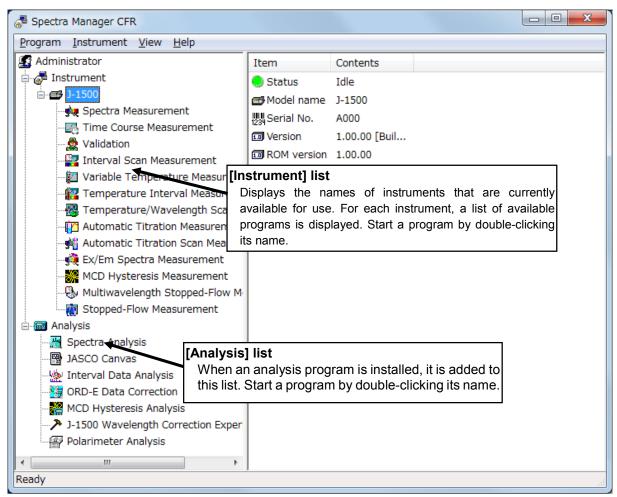


Figure 2.27 [Spectra Manager CFR] window

The standard measurement and analysis programs are displayed in Fig. 2.27. When an optional program is installed, it is added to one of these lists.

- Note 1: The CD Spectrometer is also referred to as the "instrument" in this manual.
- Note 2: "Communication" refers to sending a control signal from the PC to the CD spectrometer or transferring measured data from the CD spectrometer to the PC.

### Menu

[Program] menu		
[Administrative <u>T</u> ools]	Starts the [Administrative Tools] program.	
[Change <u>P</u> assword]	Changes the current password.	
[ <u>L</u> ogoff]	Logs off the current user.	
[E <u>x</u> it]	Exits [Spectra Manager].	
[ <u>U</u> ser] menu		
[Change <u>W</u> orkgroup]	Changes the Workgroup.	
[ <u>V</u> iew] menu		
[ <u>S</u> tatus Bar]	Shows/hides the status bar.	
[Help] menu		
[Contents]	Displays the Help contents window.	
[ <u>S</u> earch Topic]	Displays the Help search function window.	
[ <u>A</u> bout]	Displays version information about the CD spectrometer	
	control driver.	

# 3. Accessory Registration Reference

The J-1000 series CD spectrometers and software automatically recognize an attached accessory, display information about the accessory, and start registered programs based on recognized accessories. This chapter provides information of installing and registering accessories, the program that is started when an accessory is recognized, and the actions of [Spectra Manager CFR] when recognizing an accessory.

# 3.1 Installing/Attaching an Accessory

Accessories for J-1000 series CD spectrometers are automatically recognized. Information about the respective accessory is contained within the accessory itself. The accessory is recognized when its cable is connected to the sample compartment connector. When installing a J-1000 accessory, confirm that the accessory cable is properly connected to the CD spectrometer connector.

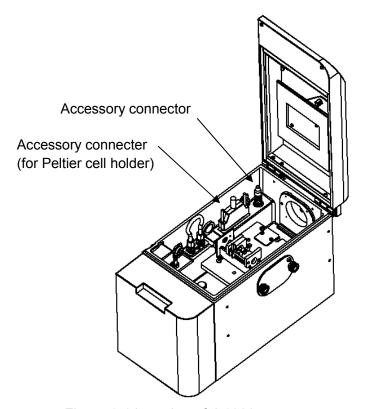


Figure 3.1 Location of J-1000 accessory connectors

## 3.2 Precautions for Peltier Thermostatic Cell Holder

The electrical power for the Peltier thermostatic cell holder is supplied from the J-1000 series CD spectrometer when this accessory is connected and detected by the instrument. When power is being supplied, an icon is displayed on the status bar.

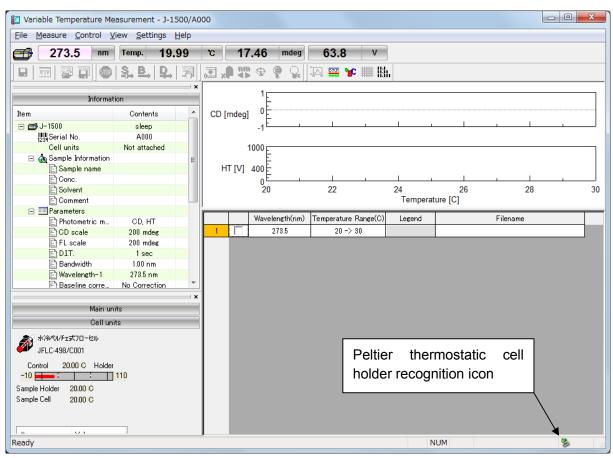


Figure 3.2 Icon displayed on the status bar after the Peltier thermostatic cell holder has been recognized

## 3.2.1 Removing the Peltier Thermostatic Cell Holder

This section describes how to remove the Peltier thermostatic cell holder while the J-1000 series instrument is running.

(1) Click the cursor on the accessory icon to display the [Safely Remove Temp unit] pop-up menu.

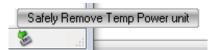


Figure 3.3 Pop-up prompt for safely removing the thermostatic unit

(2) Left-click the command to display the [Safely Remove Thermostatic Unit] dialog box.

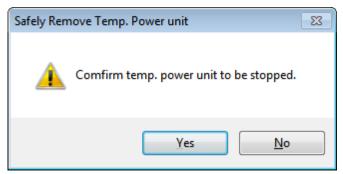


Figure 3.4 [Safely Remove Thermostatic Unit] dialog box

(3) Click the < Yes> button. The electrical power supply for the Peltier thermostatic cell holder will be stopped and the cell holder can now be safely removed.

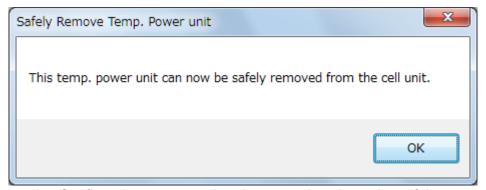


Figure 3.5 Confirmation message that thermostatic unit can be safely removed

To use the Peltier thermostatic cell holder again, reconnect its accessory cable to the J-1000 series instrument.

# 3.3 Registering Accessories

This section describes the procedure for registration of accessories used with the CD spectrometer.

## 3.3.1 Registering an Automatically-Recognized Accessory

- (1) Confirm that the instrument is turned on and that [Spectra Manager] is running.
- (2) Connect the automatically-recognized accessory to the sample compartment. The accessory name, accessory ID and serial number are automatically registered.

## 3.3.2 Registering an Accessory Requiring Manual Registration

Note: This operation can be performed only by Administrators.

(1) Confirm that the CD spectrometer is turned on and that [Spectra Manager] is running. After starting [Administrative Tools], right-click the instrument name and select [Properties...] (see Fig. 3.6).

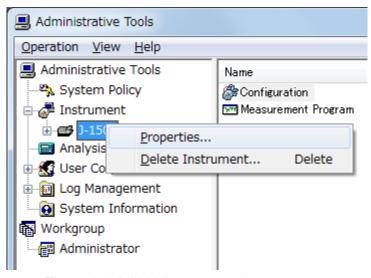


Figure 3.6 J-1000 instrument shortcut menu

### 3.3.2.1 Detectors

This section describes the procedure for registration of detectors used with the CD spectrometer.

(1) Click the [Detectors] tab in Fig. 3.7. Select the type of detector from the [Type] drop-down list.

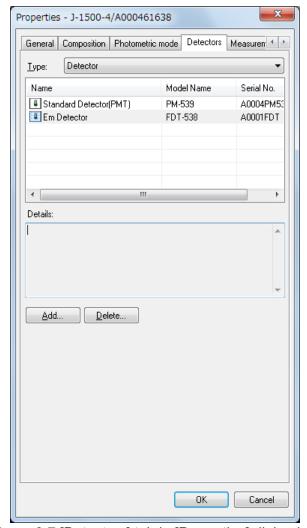


Figure 3.7 [Detectors] tab in [Properties] dialog box

Table 3.1 Accessories

1 45.6 6.1 7 10000001.00		
Туре		
Standard WL Detector (PMT): PM-539		
Extended WL Detector (ExPMT): EXPM-531		
Extended WL Detector (InGaAs):		
InGaAs-532		
Extended WL Detector (APD) : EXAP-533		
FDCD Detector (PMT): PMJ-534		
FDCD Detector (ExPMT): EXPML-535		
FDCD Detector (InGaAs): EXLGL-536		
FDCD Detector (APD) : EXAPL-537		
FL Intensity Detector : FDT-538		
Em Detector: FDT-455		
ORD-M Detector (PMT): PM-540		
Extended WL Detector (InSb) : INSB-541		
(only for J-1700)		

For J-1100, only the dedicated wavelength range expansion detector (PMT) can be selected.

(2) Click the <<u>A</u>dd...> button to display the dialog box in Fig. 3.8.

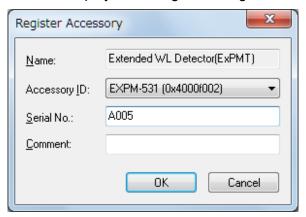


Figure 3.8 [Register Accessory] dialog box

(3) [Name] is automatically entered by selecting the accessory in the [Accessory ID] drop-down list. Type the serial number and a comment as required, and then click the <OK> button to register the accessory and display it in the list of registered accessories (see Fig.3.9).

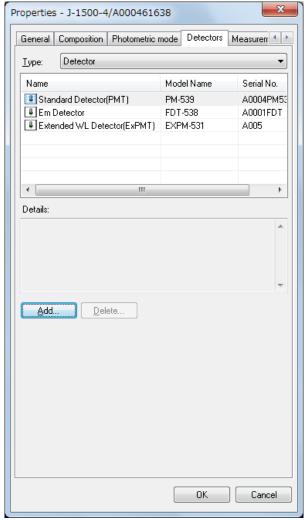


Figure 3.9 [Detectors] tab in [Properties] dialog box

### 3.3.2.2 Measurement Units

This section describes the procedure for registration of measurement units used with the CD spectrometer. For J-1100, this tab is not displayed.

(1) Click the [Measurement Units] tab in Fig. 3.10. Select the type of measurement unit from the [Type] drop-down list.

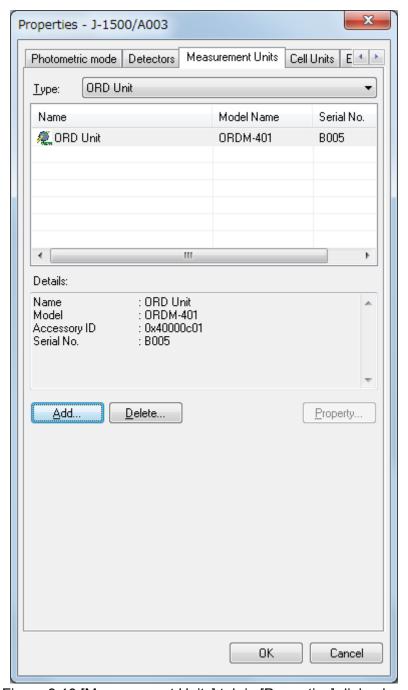


Figure 3.10 [Measurement Units] tab in [Properties] dialog box

Table 3.2 Accessories		
Туре		
ORD Attachment		
Fluorescence Monochromator		

(2) Click the <Add...> button to display the dialog box in Fig. 3.11.



Figure 3.11 [Register Accessory] dialog box

(3) [Name] is automatically entered by selecting the accessory in the [Accessory ID] drop-down list. Type the serial number and a comment as required, and then click the <OK> button to register the accessory and display it in the list of registered accessories (see Fig. 3.12).

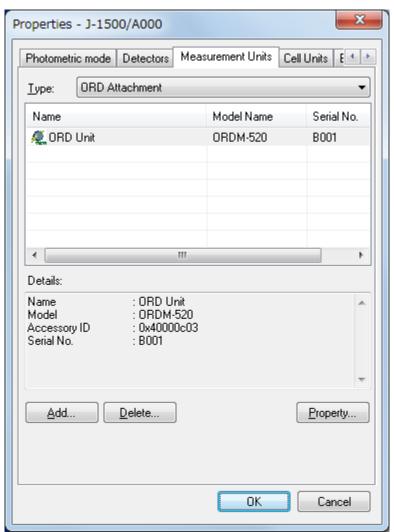


Figure 3.12 [Measurement Units] tab in [Properties] dialog box

#### 3.3.2.3 **Cell Units**

This section describes the procedure for registration of cell units used with the CD spectrometer.

(1) Click the [Cell Units] tab in Fig. 3.13. Select the type of cell unit from the [Type] drop-down list.

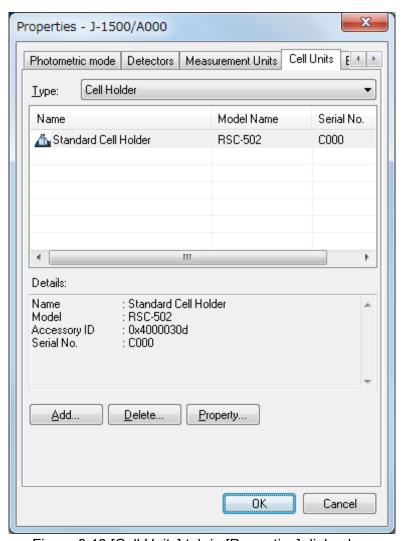


Figure 3.13 [Cell Units] tab in [Properties] dialog box

Table 3.3 Accessories

Туре
Cell Holder
Temperature Controller
Flow Cell
Integration Sphere
FDCD Attachment
Double Beam UV Attachment
MCD Controller
Stopped Flow Controller
Cryostat Holder
High Temp. Cell Unit

For J-1100, only the cell holder and temperature controller can be selected.

(2) Click the  $\leq Add... >$  button to display the dialog box in Fig. 3.14.

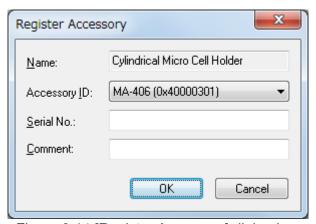


Figure 3.14 [Register Accessory] dialog box

(3) [Name] is automatically entered by selecting the accessory in the [Accessory ID] drop-down list. Type the serial number and a comment as required, and then click the <OK> button to register the accessory and display it in the list of registered accessories (see Fig. 3.15).

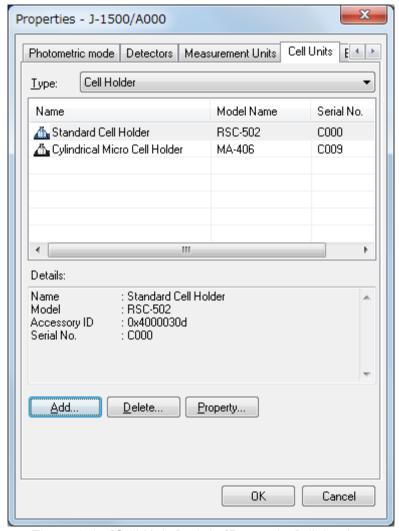


Figure 3.15 [Cell Units] tab in [Properties] dialog box

#### 3.3.2.4 External Accessories

This section describes the procedure for registration of external accessories used with the CD spectrometer. For J-1100, this tab is not displayed.

(1) Click the [External Accessories] tab in Fig. 3.16. Select the type of external accessory from the [Type] drop-down list. For-1100, the [External Accessories] tab is not displayed.

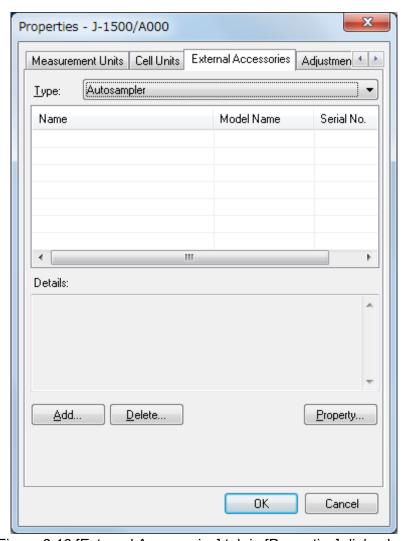


Figure 3.16 [External Accessories] tab in [Properties] dialog box

Table 3.4 Accessories
Туре
Automatic Titrator
Circulator
Autosampler
PAI Unit

(2) Click the <Add...> button to display the dialog box in Fig. 3.17.

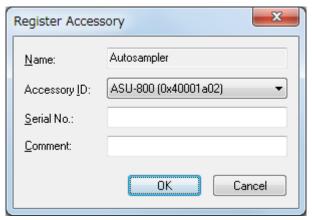


Figure 3.17 [Register Accessory] dialog box

(3) [Name] is automatically entered by selecting the accessory in the [Accessory ID] drop-down list. Type the serial number and a comment as required, and then click the <OK> button to register the accessory and display it in the list of registered accessories (see Fig.3.18).

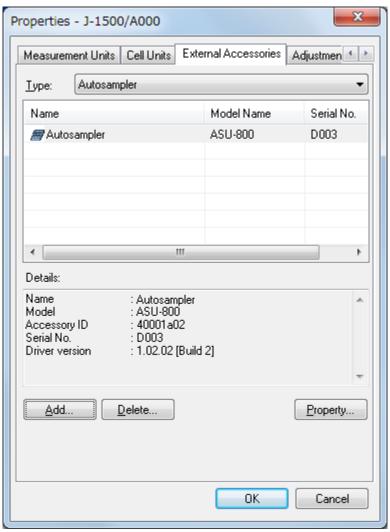


Figure 3.18 [External Accessories] tab in [Properties] dialog box

# 3.4 Actions of [Spectra Manager] When Recognizing an Accessory

This section describes the actions of [Spectra Manager] running a measurement program when an automatically-recognized accessory with registered programs is attached to or removed from the CD spectrometer.

Note: Do not attach/remove an automatically-recognized accessory while the program is displaying a dialog box or message.

## 3.4.1 When an Automatically-Recognized Accessory is Attached

When an automatically-recognized accessory is attached, a dialog box stating "An accessory has been attached" is displayed, and information on that accessory is displayed on the accessory bar.

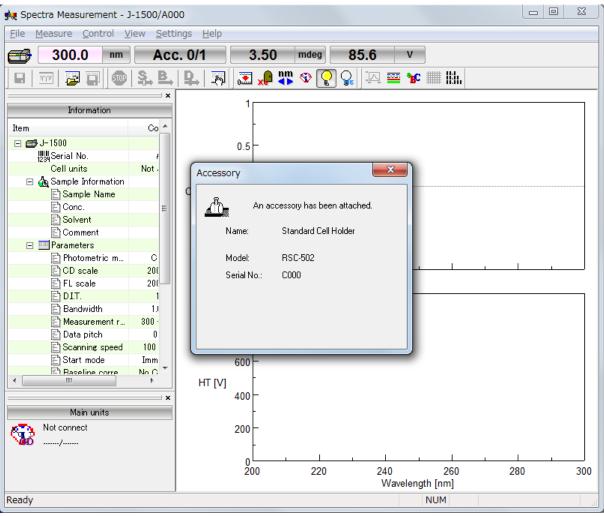


Figure 3.19 Message when an automatically-recognized accessory is being attached while [Spectra Manager] and a measurement program are running

## 3.4.2 When the Automatically-Recognized Accessory is Removed

When an automatically-recognized accessory is removed, a dialog box stating "An accessory was removed" is displayed, and information on that accessory disappears from the accessory bar.

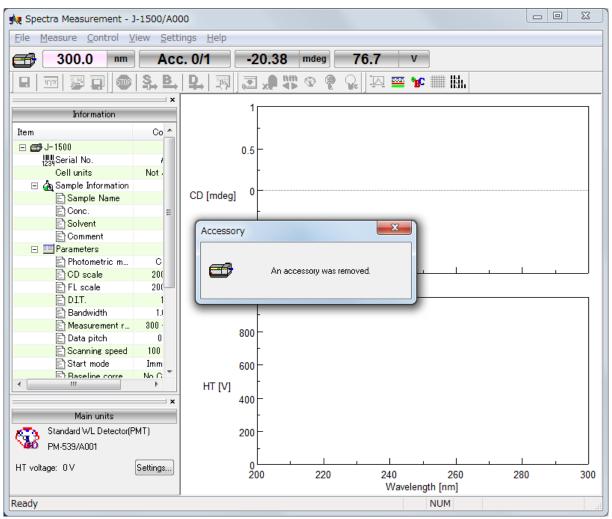


Figure 3.20 Message when an automatically-recognized accessory is removed while [Spectra Manager] and a measurement program are running

# 3.5 Status Display for the CD Spectrometer

This section describes the display of the CD spectrometer status in a measurement program.

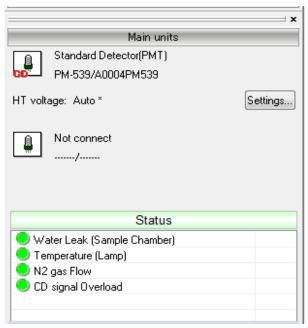


Figure 3.21 Status of CD spectrometer

Water Leak (Sample Chamber)	When water leakage occurs in the sample compartment, the green indicator in the status box turns red. A stop valve, an optional accessory, automatically prevents water from leaking.
Temperature (Lamp)	When the light source temperature exceeds 80 °C, the green indicator turns red and the light source is turned off automatically.
N <sub>2</sub> gas Flow	When the nitrogen flow rate is less than the specified value, the green indicator turns red. This item is displayed only when the [Manually with sensor] or [Automatic (PC control)] flow meter is used.  Note 1: For the [Manually with sensor] type, the sensor position can be changed and the flow rate can be specified.  Note 2: For the [Automatic (PC control)] type, when the flow rate is less than the idling flow rate specified in the [Administrative Tools] program, the green indicator turns red.
CD signal Overload	When the CD signal exceeds the upper limit of the measurement range specified by [CD scale] or [FL scale] in the [Parameters] dialog box, the green indicator turns red. Specify a larger CD or FL scale.

# 4. Introduction to the [Spectra Measurement] Program

This chapter describes how to use the [Spectra Measurement] program, including procedures for starting the [Spectra Measurement] program, measuring the spectrum of a sample, and saving and printing data, for practice in operating a JASCO CD spectrometer.

Explanations of the parameters have been kept to a minimum, with a focus on the flow of operations. Follow the measurement procedures outlined below for practice in operating the CD spectrometer. Refer to Chapter 6 "Measurement Program Reference" for details about toolbar icons and menus, and to Chapter 7 "[Spectra Measurement] Program Menu Reference" for details about the [Parameters...] command.

# 4.1 Procedures for the [Spectra Measurement] Program

This section describes procedures ranging from measuring a CD spectrum of an ammonium d-10-camphorsulfonate solution to saving and printing the measurement data.

Starting the [Spectra Measurement] Program	Refer to Section 4.2
$\downarrow$	
Specifying Measurement Parameters	Refer to Section 4.3
$\downarrow$	
Measuring the Sample	Refer to Section 4.4
$\downarrow$	
Saving Spectra	Refer to Section 4.5
$\downarrow$	
Printing Results	Refer to Section 4.6
$\downarrow$	
Exiting the Program	Refer to Section 4.7

# 4.2 Starting the [Spectra Measurement] Program

To start the program, double-click [Spectra Measurement] from the [Instrument] list of [Spectra Manager]. The window in Fig. 4.1 is displayed.

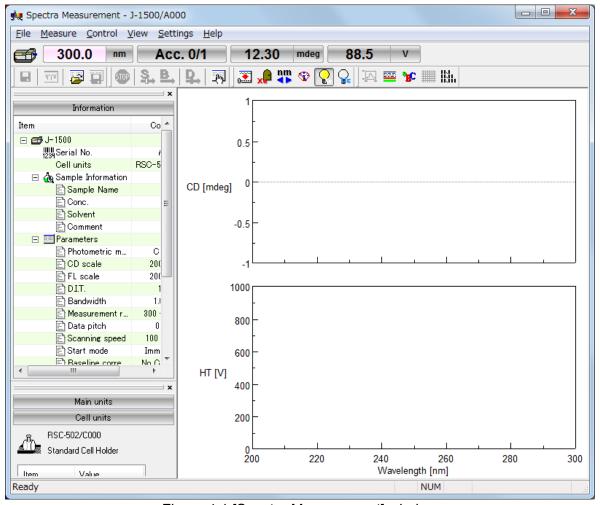


Figure 4.1 [Spectra Measurement] window

# 4.3 Specifying Measurement Parameters

- (1) Select [Parameters...] from the [Measure] menu (or click the button) to display the dialog box in Fig. 4.2. The [Parameters] dialog box contains the [General], [Control], [Information], and [Data] tabs. The [General] tab is open by default in the [Parameters] dialog box. The page can be changed by clicking each tab at the top of the dialog box.
- Note 1: In the CFR version, parameter history is automatically saved. It is therefore necessary to specify or open the parameters before measurement.
- Note 2: In the CFR version, Managers or Analysts authority is required to specify parameters.
- (2) The parameters can be switched between two modes: Basic mode and Advanced mode. In Basic mode, the choice of parameters is partially limited. In Advanced mode, each parameter is specified individually. The parameters described in this section are specified in Basic mode. To switch between Basic and Advanced modes, click the <Basic Mode> or <Advanced Mode> button.
- (3) Specify the measurement parameters in the [General] tab as follows.

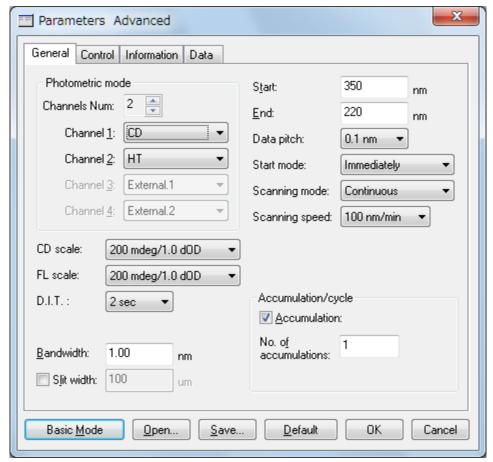


Figure 4.2 [General] tab in [Parameters] dialog box

Photometric mode [Channels Num]

[Channel <u>1</u>] [CD]
[Channel <u>2</u>] [HT]

[CD scale] 200 mdeg/1.0 dOD [FL scale] 200 mdeg/1.0 dOD

 [D. I. T.]
 2 sec

 [Bandwidth]
 1 nm

 [Start]
 350 nm

 [End]
 220 nm

 [Data pitch]
 0.1 nm

[Start mode] [Immediately]
[Scanning mode] [Continuous]
[Scanning speed] 100 nm/min

Accumulation/cycle

[Accumulation] Deselected

[No. of accumulations]

Note: Select the appropriate [CD scale] for the sample to be measured.

Parameters can be set by using two methods: selecting from available options and specifying numeric values and characters. An example of setting parameters by using each method is given below.

#### 1) Selecting from available options

The following example describes how to select the CD scale. Select the CD scale from the available options in the [CD scale] drop-down list. Click the arrow to the right of the box to display the full list of [CD scale] options (see Fig. 4.3). Select the desired CD scale (in this example, 200 mdeg/1.0 dOD).



Figure 4.3 [CD scale] drop-down list

#### 2) Specifying numeric values and characters

The following example describes how to specify the start wavelength. Click the [Start] text box to edit the start wavelength. When the cursor appears in the text box, values can be entered. Type the desired wavelength (in the example in Fig. 4.2, 350 nm) in the text box to set the start wavelength.

(4) Specify the measurement parameters in the [Control] tab as follows.

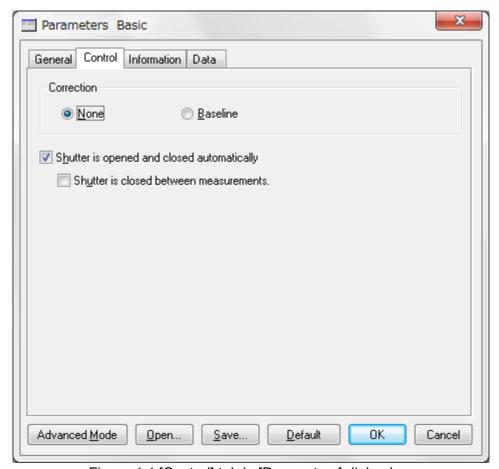


Figure 4.4 [Control] tab in [Parameters] dialog box

Correction [None]
[Shutter is opened and closed automatically] Selected
[Shutter is closed between measurements.] Deselected

(5) Click the [Information] tab. Type information in the [Sample <u>n</u>ame], [O<u>p</u>erator], [Di<u>v</u>ision], [<u>C</u>omment], [Concentration] and [Solvent] text boxes as desired. The information entered here is saved as comment information together with the spectral data when the spectra are saved.

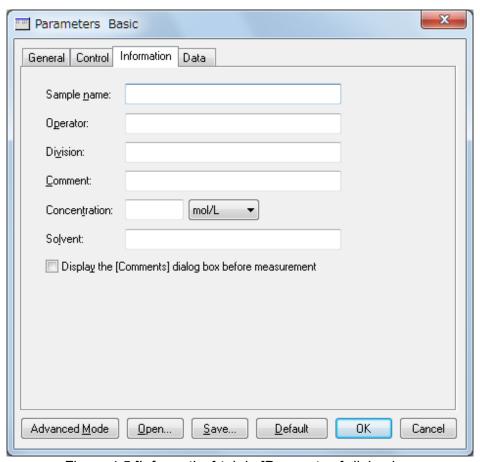


Figure 4.5 [Information] tab in [Parameters] dialog box

[Sample <u>name</u>] Enter as desired (maximum 63 characters).

[Operator] Enter an operator name (maximum 63 characters).

[Di<u>v</u>ision] Enter a division name for the operator (maximum 127

characters).

[Comment] Enter a comment (maximum 127 characters).

[Concentration] Enter a sample concentration.

[Solvent] Enter a solvent name (maximum 127 characters).

[Display the [Comments] Deselected

dialog box before measurement]

Note: In the CFR version, the [Operator] and [Division] text boxes cannot be changed by the user.

(6) Click the [Data] tab. Specify the [Save data], [Send data], and [Print] options for the measured spectrum. In this example, select the [To Spectra Analysis] check box.

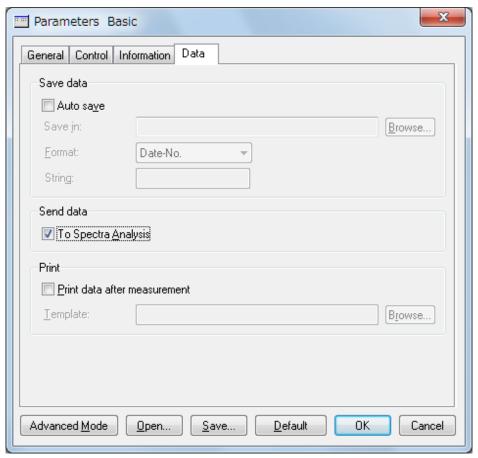


Figure 4.6 [Data] tab in [Parameters] dialog box

[Auto save]Deselected[To Spectra Analysis]Selected[Print data after measurement]Deselected

(7) In the CFR version, always save changes to the parameters. Click the <<u>S</u>ave...> button to display the dialog box in Fig. 4.7.

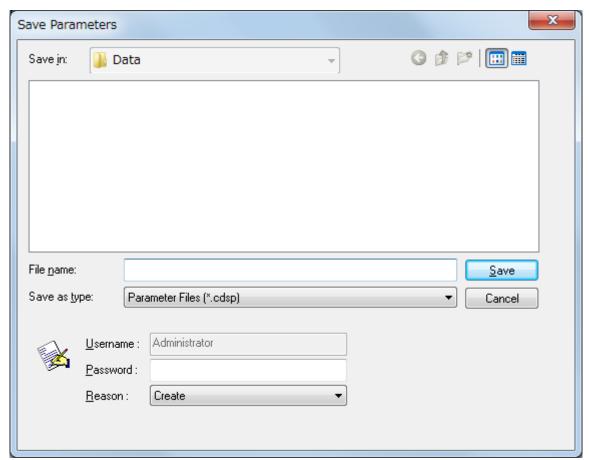
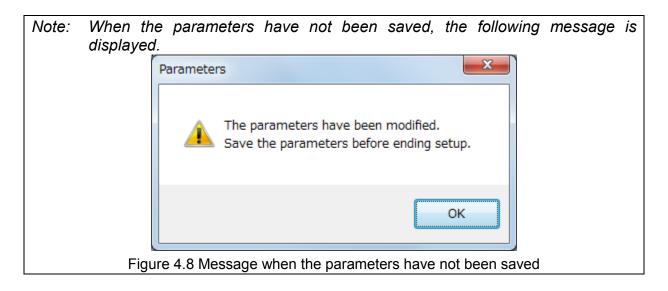


Figure 4.7 [Save Parameters] dialog box

(8) After entering the file name, type a password and then click the <Save> button.



## 4.4 Measuring the Sample

(1) Inserting the sample

Fill the cell with the sample, place it in the cell holder, and then close the lid of the sample compartment.

(2) Measuring the sample

Select [Sample Measurement] from the [Measure] menu (or click the button) to measure the spectrum for the sample. The progress of the measurement is displayed in the window (see Fig. 4.9).

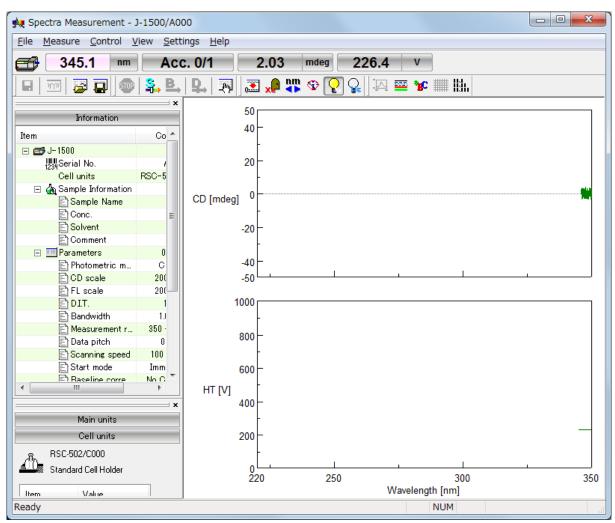


Figure 4.9 [Spectra Measurement] window

After measurement, the [Spectra Analysis] program starts and the measured data is displayed in a window. This window is called a "View". Figure 4.10 shows an example of a measured spectrum that has not yet been saved (Title bar: View <Memory-1>).

Note 1: When the [Spectra Analysis] program is already running, it is not automatically displayed as the active window after measurement. Click [Spectra Analysis] on the Windows task bar to display the program as the active window.

Note 2: Data is not automatically transferred unless the [To Spectra Analysis] check box is selected in the [Data] tab of the [Parameters] dialog box. To transfer data, select [Send to Analysis] from the [File] menu (or click the button).

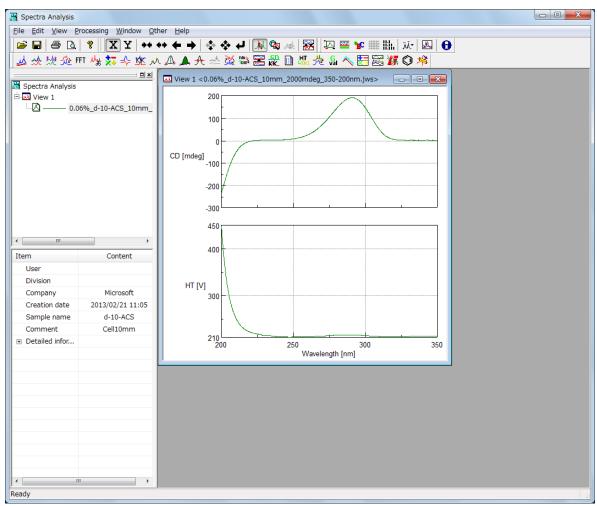


Figure 4.10 Spectrum View

# 4.5 Saving Spectra

This section describes the procedure for saving spectra using the [Spectra Analysis] program.

Note: Spectra can also be saved by selecting [Save <u>Data...</u>] from the [<u>File</u>] menu (or by clicking the <u>lab</u> button) in the [Spectra Measurement] program.

(1) Select [Save As...] from the [File] menu in the [Spectra Analysis] program to display the dialog box in Fig. 4.11.

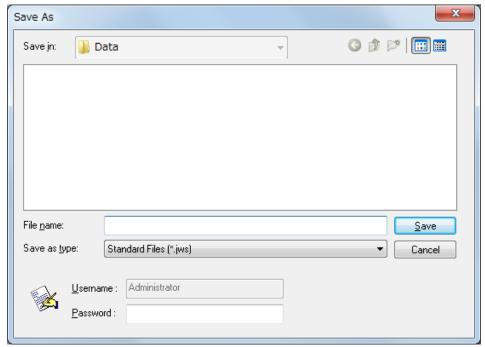


Figure 4.11 [Save As] dialog box

(2) From the [Save in] drop-down list, select the folder in which to save the spectrum.

Note: In the CFR version, the [Save in] drop-down list cannot be used to select a folder in which to save the data. Folder selection is limited by Administrators using the [Administrative Tools] program. Refer to the [Administrative Tools] program manual for details.

- (3) Type the file name in the [File <u>name</u>] text box. In this example, type "d-10-ACS" as the file name.
- (4) After entering the file name, type a password and then click the <Save> button.
- (5) The file name is appended with the extension ".jws" ("d-10-ACS.jws"), which is the standard file type.
- (6) After saving the data, the title bar of the View changes to "View (d-10-ACS.jws)".

Note: Refer to the [Spectra Analysis] program manual for details about saving spectra.

# 4.6 Printing Results

Print the measured spectra using a connected printer as follows.

(1) Select [Print Setup...] from the [File] menu to display the dialog box in Fig. 4.12. The content of this dialog box varies depending on the connected printer. Configure the printer settings if necessary.

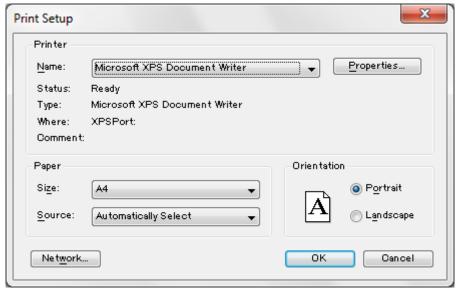


Figure 4.12 Example of [Print Setup] dialog box

- (2) Select [Print...] from the [File] menu to print the data.
- Note 1: Refer to the [Spectra Analysis] program manual for details about printing a spectrum.
- Note 2: In the CFR version, "Unsigned" will be watermarked on the printed page when no creation signature is assigned to the measurement data.

# 4.7 Exiting the Program

(1) Exiting the [Spectra Analysis] program

Select  $[E\underline{x}it]$  from the  $[\underline{F}ile]$  menu. The [Spectra Analysis] window closes, leaving the [Spectra Measurement] window displayed.

Note: When there are unsaved spectra in the window, a warning message is displayed. Perform the action recommended by the message. A message is displayed for each unsaved spectrum.

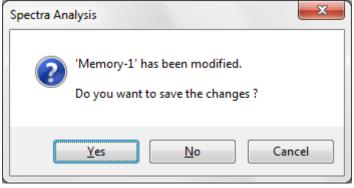


Figure 4.13 Message when data has not been saved

(2) Exiting the [Spectra Measurement] program

Select  $[E\underline{x}it]$  from the  $[\underline{F}ile]$  menu to close the [Spectra Measurement] program, leaving the [Spectra Manager] window displayed.

- (3) Exiting the [Spectra Manager] program
  - Select [Exit] from the [Program] menu.
- (4) Exiting Windows

Exit Windows in accordance with standard Windows operation procedures.

(5) Turning off the PC and CD spectrometer

First, turn off the PC and monitor. Do not forget to turn off the monitor.

Ensure that the sample compartment is empty, and then turn off the CD spectrometer.

# 5. Introduction to the [Time Course Measurement] Program

This chapter describes how to use the [Time Course Measurement] program, including procedures for starting the [Time Course Measurement] program, measuring the spectrum of a sample, and saving and printing data, for practice in operating a JASCO CD spectrometer. Explanations of the parameters have been kept to a minimum, with a focus on the flow of operations. Follow the measurement procedures outlined below for practice in operating the CD spectrometer. Refer to Chapter 6 "Measurement Program Reference" for details about toolbar icons and menus, and refer to Chapter 8 "[Time Course Measurement] Program Menu Reference" for details about the [Parameters...] command.

# 5.1 Procedures for the [Time Course Measurement] Program

This section describes procedures ranging from measuring CD time-course data for an ammonium d-10-camphorsulfonate solution to saving and printing the measurement data.

Starting the [Time Course Measurement] Program	Refer to Section 5.2
$\downarrow$	
Specifying Measurement Parameters	Refer to Section 5.3
$\downarrow$	
Measuring the Sample	Refer to Section 5.4
$\downarrow$	
Saving Data	Refer to Section 5.5
$\downarrow$	
Printing Results	Refer to Section 5.6
$\downarrow$	
Exiting the Program	Refer to Section 5.7

# 5.2 Starting the [Time Course Measurement] Program

To start the program, double-click [Time Course Measurement] from the [Instrument] list of [Spectra Manager]. The window in Fig. 5.1 is displayed.

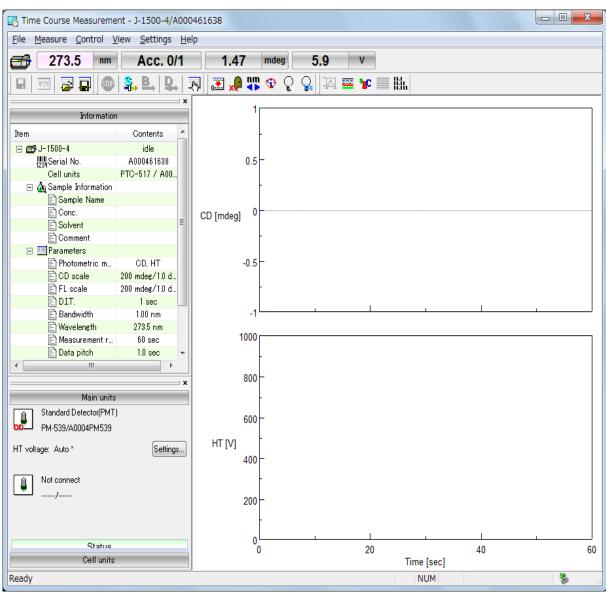


Figure 5.1 [Time Course Measurement] window

# 5.3 Specifying Measurement Parameters

- (1) Select [Parameters...] from the [Measure] menu (or click the button) to display the dialog box in Fig. 5.2. The [Parameters] dialog box contains the [General], [Control], [Information], and [Data] tabs. The [General] tab is open by default in the [Parameters] dialog box. The page can be changed by clicking each tab at the top of the dialog box.
- Note 1: In the CFR version, parameter history is automatically saved. It is therefore necessary to specify or open the parameters before measurement.
- Note 2: In the CFR version, Managers or Analysts authority is required to specify parameters.
- (2) The parameters can be switched between two modes: Basic mode and Advanced mode. In Basic mode, the choice of parameters is partially limited. In Advanced mode, each parameter is specified individually. The parameters described in this section are specified in Basic mode. To switch between Basic and Advanced modes, click the <Basic Mode> or <Advanced Mode> button.
- (3) Specify the measurement parameters in the [General] tab as follows.

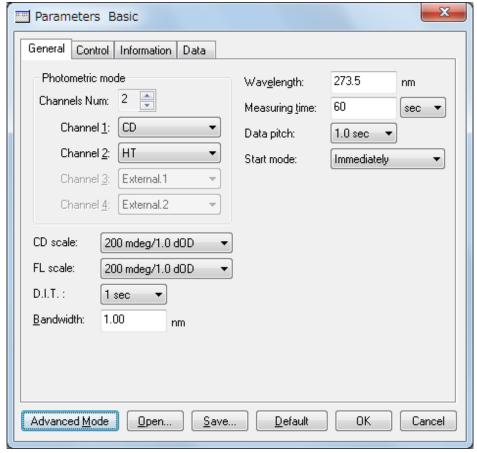


Figure 5.2 [General] tab in [Parameters] dialog box

Photometric mode
[Channels Num] 2
[Channel 1] [CD]

[Channel <u>2</u>] [HT]

[CD scale] 200 mdeg/1.0 dOD [FL scale] 200 mdeg/1.0 dOD

 [D. I. T. ]
 1 sec

 [Bandwidth]
 1 nm

 [Wavelength]
 291 nm

 [Measuring time]
 60 sec

 [Data pitch]
 1 sec

[Start mode] [Immediately]

Note: Select the appropriate [CD scale] for the sample to be measured.

Parameters can be set by using two methods: selecting from available options and specifying numeric values and characters. An example of setting parameters using each method is given below.

#### 1) Selecting from available options

The following example describes how to select the CD scale. Select the CD scale from the available options in the [CD scale] drop-down list. Click the arrow to the right of the box to display the full list of [CD scale] options (see Fig. 5.3). Select the desired CD scale (in this example, 200 mdeg/1.0 dOD).



Figure 5.3 [CD scale] drop-down list

#### Specifying numeric values and characters

The following example describes how to specify the wavelength. Click the [Wavelength] text box to edit the wavelength. When the cursor appears in the text box, values can be entered. Type the desired wavelength (in the example in Fig. 5.2, 291 nm) in the text box to set the wavelength.

(4) Specify the measurement parameters in the [Control] tab as follows.

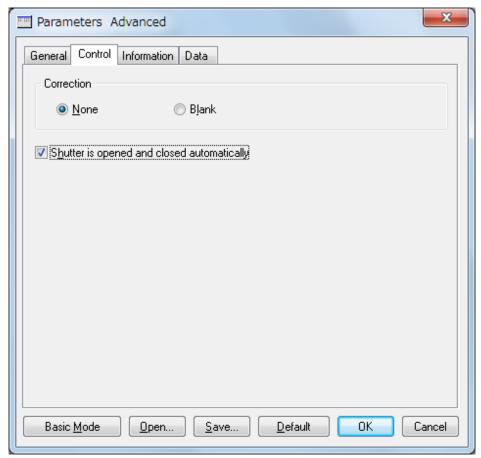


Figure 5.4 [Control] tab in [Parameters] dialog box

Correction [None] [Shutter is opened and closed automatically] Selected

(5) Click the [Information] tab. Type information in the [Sample <u>n</u>ame], [O<u>p</u>erator], [Di<u>v</u>ision], [<u>C</u>omment], [Concentration] and [Solvent] text boxes as desired. The information entered here is saved as comment information together with the time-course data when the data are saved.

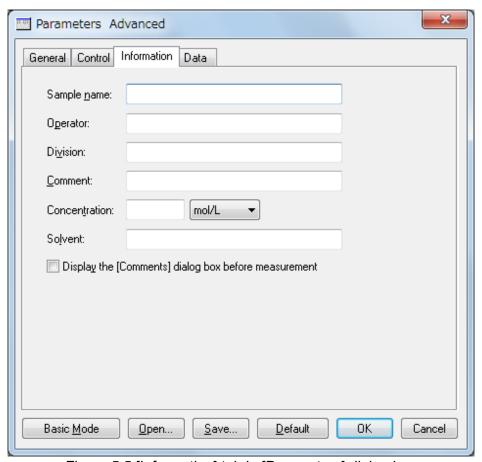


Figure 5.5 [Information] tab in [Parameters] dialog box

[Sample <u>name</u>] Enter as desired (maximum 63 characters).

[Operator] Enter an operator name (maximum 63 characters).

[Di<u>v</u>ision] Enter a division name for the operator (maximum 127

characters).

[Comment] Enter as desired (maximum 127 characters).

[Concentration] Enter as desired.

[Solvent] Enter as desired (maximum 127 characters).

[Display the [Comments] Deselected

dialog box before measurement]

Note: In the CFR version, the [Operator] and [Division] text boxes cannot be changed by the user.

(6) Click the [Data] tab. Specify the [Save data], [Send data], and [Print] options for the measured data. In this example, select the [To Spectra Analysis] check box.

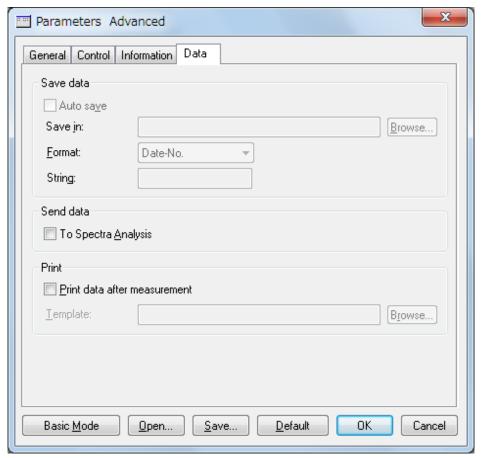


Figure 5.6 [Data] tab in [Parameters] dialog box

[Auto save]Deselected[To Spectra Analysis]Selected[Print data after measurement]Deselected

(7) In the CFR version, always save changes to the parameters. Click the <<u>S</u>ave...> button to display the dialog box in Fig. 5.7.

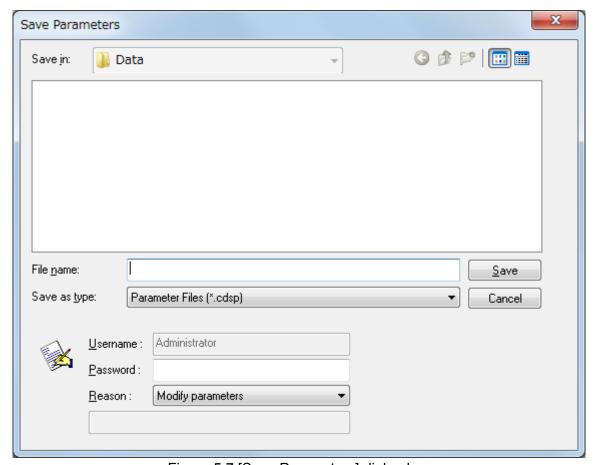
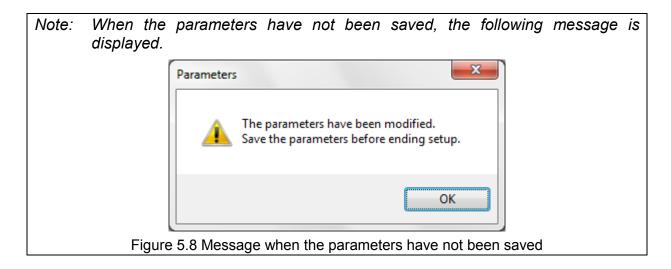


Figure 5.7 [Save Parameters] dialog box

(8) After entering the file name, type a password and then click the <<u>S</u>ave> button.



### 5.4 Measuring the Sample

#### (1) Inserting the sample

Fill the cell with the sample, place it in the cell holder, and then close the lid of the sample compartment.

#### (2) Measuring the sample

Select [Sample Measurement] from the [Measure] menu (or click the button) to measure the time-course data for the sample. The progress of the measurement is displayed in the window (see Fig. 5.9).

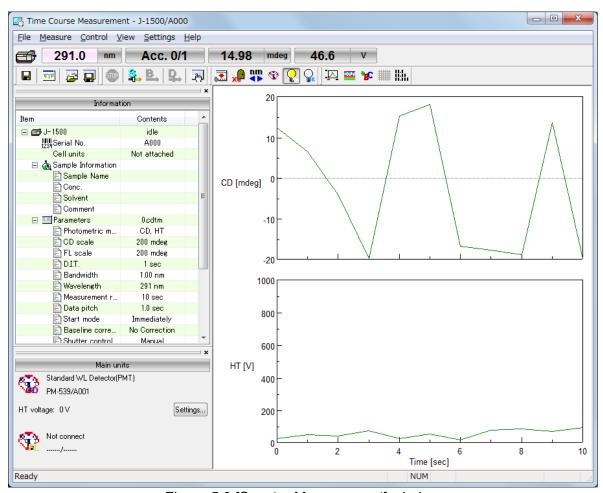


Figure 5.9 [Spectra Measurement] window

After measurement, the [Spectra Analysis] program starts and the measured data is displayed in the window. This window is called a "View". Figure 5.10 shows an example of a measured spectrum that has not yet been saved (Title bar: View <Memory-1>).

Note 1: When the [Spectra Analysis] program is already running, it is not automatically displayed as the active window after measurement. Click [Spectra Analysis] on the Windows task bar to display the program as the active window.

Note 2: Data is not automatically transferred unless the [To Spectra <u>A</u>nalysis] check box is selected in the [Data] tab of the [Parameters] dialog box. To transfer data, select [Send to Analysis] from the [File] menu (or click the button).

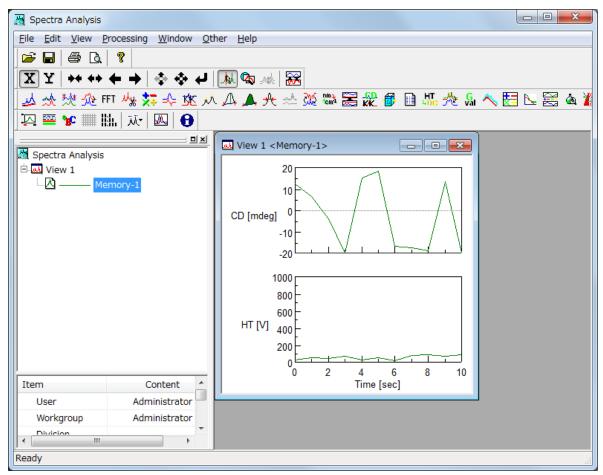


Figure 5.10 Spectrum View (fluorescence spectra)

# 5.5 Saving Time-Course Data

This section describes the procedure for saving time-course data using the [Spectra Analysis] program.

Note: Data can also be saved by selecting [Save <u>Data...</u>] from the [<u>File</u>] menu (or by clicking the <u>lab</u> button) in the [Spectra Measurement] program.

(1) Select [Save As...] from the [File] menu in the [Spectra Analysis] program to display the dialog box in Fig. 5.11.

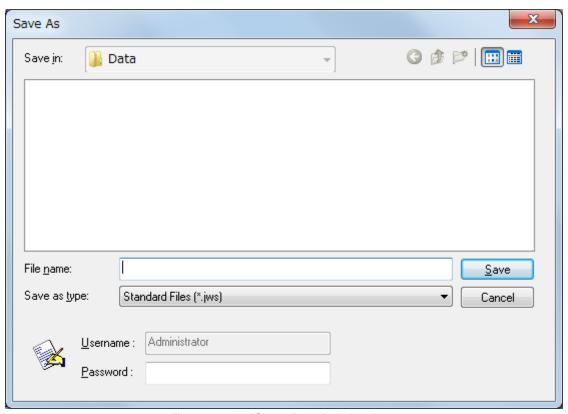


Figure 5.11 [Save Data] dialog box

(2) From the [Save in] drop-down list, select the folder in which to save the data.

Note: In the CFR version, the [Save in] drop-down list cannot be used to select a folder in which to save the data. Folder selection is limited by Administrators using the [Administrative Tools] program. Refer to the [Administrative Tools] program manual for details.

- (3) Type the file name in the [File name] text box. In this example, type "d-10-ACS" as the file name.
- (4) After entering the file name, type a password and then click the <Save> button.
- (5) The file name is appended with the extension ".jws" ("d-10-ACS.jws"), which is the standard file type.
- (6) After saving the data, the title bar of the View changes to "View (d-10-ACS.jws)".

Note: Refer to the [Spectra Analysis] program manual for details about saving spectra.

## 5.6 Printing Results

Print the measured spectra using a connected printer as follows.

(1) Select [Print Setup...] from the [File] menu to display the dialog box in Fig. 5.12. The content of this dialog box varies depending on the connected printer. Configure the printer settings if necessary.

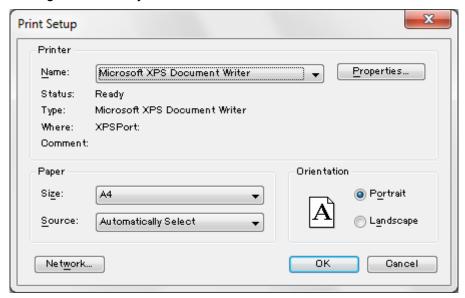


Figure 5.12 Example of [Print Setup] dialog box

- (2) Select [Print...] from the [File] menu to print the data.
- Note 1: Refer to the [Spectra Analysis] program manual for details about printing a spectrum.
- Note 2: In the CFR version, "Unsigned" will be watermarked on the printed page when no creation signature is assigned to the measurement data.

## 5.7 Exiting the Program

(1) Exiting the [Spectra Analysis] program

Select  $[E\underline{x}it]$  from the  $[\underline{F}ile]$  menu. The [Spectra Analysis] window closes, leaving the [Spectra Measurement] window displayed.

Note: When there are unsaved data in the window, a warning message is displayed. Perform the action recommended by the message. A message is displayed for each unsaved set of data.

Spectra Analysis

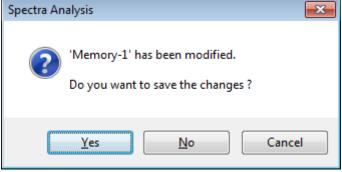


Figure 5.13 Message when data have not been saved

(2) Exiting the [Time Course Measurement] program

Select [Exit] from the [File] menu to close [Time Course Measurement], leaving the [Spectra Manager] window displayed.

(3) Exiting the [Spectra Manager] program

Select [Exit] from the [Program] menu.

(4) Exiting Windows

Exit Windows in accordance with standard Windows operation procedures.

(5) Turning off the PC and CD spectrometer

First, turn off the PC and monitor. Do not forget to turn off the monitor.

Ensure that the sample compartment is empty, and then turn off the CD spectrometer.

## 6. Measurement Program Reference

This chapter describes common toolbar and menu commands for the [Spectra measurement], [Time Course Measurement] and [Data Monitor] programs. Refer to Chapters 7 to 9 or the [Help] menu for details about specific parameters for each measurement program.

- Note 1: Refer to Table 6.1 for information about the availability of toolbar and menu commands in the three programs.
- Note 2: All toolbar and menu commands are not necessarily available for every program.

The [Spectra Measurement] program reference describes the features of the [Spectra Measurement] program for measuring a sample spectrum.

### 6.1 Overview of Measurement Programs

Starting the measurement program displays the window in Fig. 6.1.

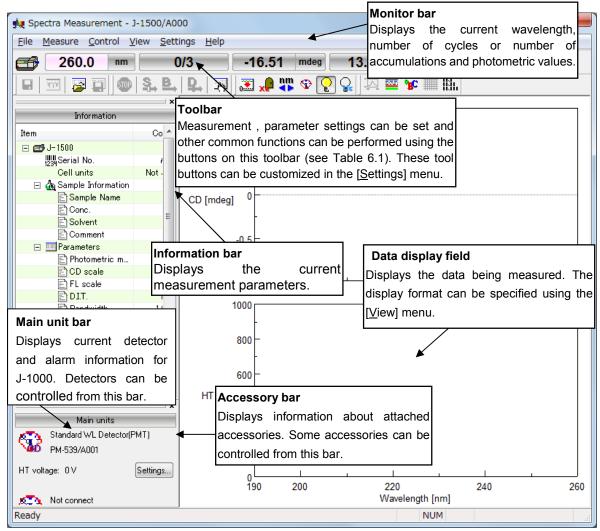


Figure 6.1 Measurement program window ([Spectra Measurement])

Table 6.1 Toolbar buttons and names

Button	Name	Reference Section	Spectra	Time Course	Data
			•	Measurement	
	[Save]	6.2.1 [Save Data]	<b>✓</b>	•	
m	[Send to Analysis]	6.2.2 [Send to Analysis]	<b>✓</b>	✓	
	[Open Parameters]	6.2.3 [Open Parameters]	<b>✓</b>	•	
	[Save Parameters]	6.2.4 [Save Parameters]	<b>✓</b>	•	
<b>500</b>	[Cancel]	6.3.1 [Cancel]	<b>✓</b>	<b>✓</b>	
<b>3</b>	[Sample Measurement]	6.3.2 [Sample Measurement]	<b>✓</b>	•	
	[Blank/Baseline	6.3.3 [Baseline Measurement]	<b>✓</b>	<b>✓</b>	
₽.	Measurement]	6.3.4 [Blank Measurement]			
	[DC Dark Measurement]	6.3.5 [DC Dark Measurement]	•	V	
_{h/y}]	[Parameters]	6.3.6 [Parameters]	<b>✓</b>	<b>✓</b>	<b>~</b>
<u></u>	[ <u>Z</u> ero Clear]	6.4.1 [Zero Clear]	<b>✓</b>	<b>✓</b>	<b>~</b>
	[Shutter]	6.4.2 [Shutter]	<b>✓</b>	<b>✓</b>	<b>✓</b>
nm	[Move Wavelength]	6.4.3 [Move Wavelength]	<b>✓</b>	<b>✓</b>	<b>✓</b>
<	[Detector]	6.4.4 [Detector]	<b>✓</b>	<b>✓</b>	<b>✓</b>
	[Xe Lamp]	6.4.5 [Light Source]	<b>✓</b>	<b>✓</b>	<b>✓</b>
	[WI Lamp]	Note: Turns the xenon lamp on or off.			
96	[Hg Lamp]	6.4.5 [Light Source]	<b>✓</b>	•	V
		Note: Indicates the status of the mercury lamp. The lamp cannot be turned on or off by clicking the button.			
	[Scales]	6.5.1 [Scales]	~	•	
	[Patterns]	6.5.2 [Patterns]	<b>✓</b>	<b>✓</b>	•
*BC	[Fonts]	6.5.3 [Fonts]	<b>✓</b>	<b>✓</b>	<b>✓</b>
	[Gridlines]	6.5.4 [Gridlines]	<b>✓</b>	<b>✓</b>	•
	[Styles]	6.5.5 [Styles]	<b>✓</b>	<b>✓</b>	<b>✓</b>
1.00	[Digital]	6.5.12 [View Mode]			<b>✓</b>
	[Graph]	6.5.12 [View Mode]			•

#### Window

Title bar	Displays the program name.	
Menu bar	Displays the menus for operation.	
Monitor bar	Displays from left to right the current wavelength, number of cycles or number of accumulations and photometric values.	
Toolbar	Displays available tool buttons. These tool buttons can be customized in the [Settings] menu.	
Information bar	Displays the current measurement parameters.	
Main unit bar	Displays current detector information and alarm information for the J-1000 CD spectrometer.	
Accessory bar	Displays information about the attached accessory.	
Spectrum display field	Displays the spectrum or time-course data being measured.	
Status bar	Displays the current state of the instrument and an explanation of the selected menu.	

#### Menu

[ <u>F</u> ile] menu		Spectra Measure- ment	Time Course Measure- ment	Data Monitor
[Save D <u>a</u> ta]	Saves the spectrum with a new file name.	•	•	
[Send to Analysis]	Transfers the measured data to the [Spectra Analysis] program.	✓	<b>✓</b>	
[ <u>O</u> pen Parameters]	Selects a parameter file and opens those parameters.	✓	<b>✓</b>	
[Save <u>P</u> arameters]	Saves the currently specified measurement parameters with the entered file name.	•	•	
[Open <u>B</u> aseline]	Selects a baseline file and opens that baseline spectrum.  Note: In the CFR version, this function is not available.	•		
[Save Base <u>l</u> ine]	Saves the currently measured baseline spectrum with the entered file name.  Note: In the CFR version, this function is not available.	<b>✓</b>		
[E <u>x</u> it]	Exits the measurement program and returns to [Spectra Manager].	<b>✓</b>	✓	<b>√</b>

	Note: This command is in the [Measure] menu in the [Data Monitor] program.			
[Measure] menu				
[Cancel]	Cancels the measurement.	✓	1	
[Sample Measurement]	Measures the spectrum or time-course data for the sample.	<b>/</b>	<b>/</b>	
[Baseline Measurement]	Measures the baseline spectrum for baseline correction.	<b>/</b>		
[Blank Measurement]	Measures the blank for blank correction.		<b>/</b>	
[DC Dark Measurement]	Measures the dark spectrum for dark correction.	<b>✓</b>	<b>/</b>	
[Parameters]	Specifies parameters and saves or opens the measurement parameters.	✓	•	•
[Control] menu				
[Zero Clear]	Sets the photometric value of ORD-M or fluorescence intensity at the current wavelength to zero.	•	•	•
[Shutter]	Opens/closes the shutter.	✓	<b>✓</b>	1
[Move Wavelength]	Moves the CD spectrometer wavelength to the desired wavelength.	/	<b>✓</b>	<b>✓</b>
[Detector]	Sets the detector sensitivity.	✓	1	•
[Light Source]	Turns on or off the xenon lamp.	✓	✓	1
[N <u>i</u> trogen Flowrate]	Specifies the flow rate of nitrogen gas. This command is only displayed when [Automatic (PC control)] is selected for the nitrogen flow meter.	•	<b>'</b>	<b>'</b>
[Selec <u>t</u> Detector]	Selects a detector.	•	•	1
[Se <u>l</u> ect Accessory]	Selects an accessory.	•	•	1
[View] menu				
[Scales]	Specifies the display scale for the spectrum or time-course data.	<b>✓</b>	<b>/</b>	
[Patterns]	Selects the display color and line style for the spectrum or time-course data.	•	•	
[Fonts]	Specifies the display font for the spectrum or time-course data.	✓	<b>/</b>	

[Gridlines]	Shows/hides the gridlines for the spectrum or time-course data.	1	•	
[Styles]	Specifies the display style for the spectrum or time-course data.	✓	<b>✓</b>	
[Overlay]	Overlays spectra or time-course data when cycle measurement is selected.	•	<b>'</b>	
[Select Graph]	Selects the graph to be displayed on the CD spectrum display field.	✓	✓	
[Information Bar]	Shows/hides the information bar.	1	1	1
[Accessory Bar]	Shows/hides the accessory bar.	1	1	•
[ <u>T</u> oolbars]	Shows/hides toolbars.	1	1	1
[Status Bar]	Shows/hides the status bar.	1	1	•
[View Mode]	Displays the photometric value in digital or graph mode.			1
[Graph View]	Selects the graph to be displayed when graph mode is selected for the photometric value display.			•
[Settings] menu				
[Default Parameters]	Specifies measurement parameters for running the [Spectra Measurement] and [Time Course Measurement] programs based on the currently recognized accessory.  Note: In the CFR version, this function is not available.	*	•	
[Customize Toolbar]	Customizes and shows/hides toolbars.	✓	<b>✓</b>	1
[Monitor Bar]	Customizes the style of the monitor bar.	<b>'</b>	<b>✓</b>	1
[Help] menu				
[About]	Displays version information for the program.	•	•	•

# 6.2 [File] Menu

Saves or opens a measured data or parameter file.

## 6.2.1 [Save Data...]

Saves the measured data with a new file name.

Note: This operation can also be performed by clicking the tool button 📳 [Save].

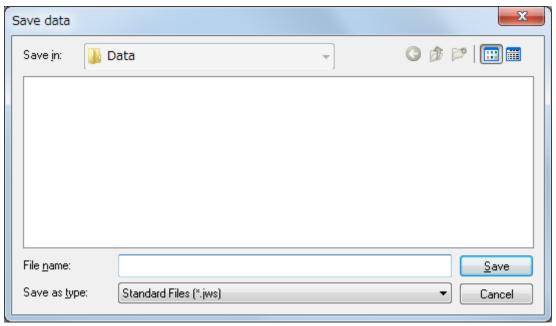
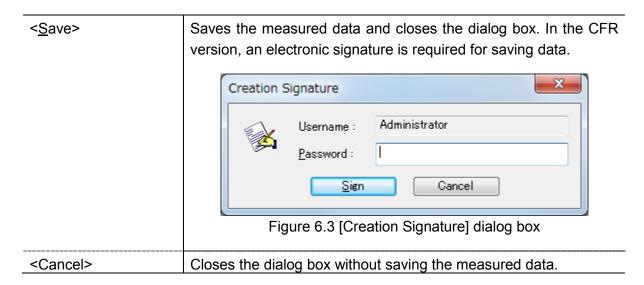


Figure 6.2 [Save data] dialog box

[Save <u>i</u> n] list	Selects a drive or folder to browse using the drop-down list. Files saved in the currently opened folder are displayed in the file name list.
File name list	Lists the files in the currently opened folder. Use as a reference when naming a file.
[File <u>n</u> ame]	Enters a file name for saving the measured data.  An extension may be omitted.
[Save as <u>t</u> ype]	Selects the files (type of extension) to display in the file name list. Files other than Standard Files (*.jws) cannot be selected.



Note: In the CFR version, the [Save in] drop-down list cannot be used to select a folder. However, a subfolder within the prespecified folder can be selected.

#### 6.2.2 [Send to Analysis]

Transfers the measured data to the [Spectra Analysis] program. Selecting the [To Spectra Analysis] check box in the [Data] tab of the [Parameters] dialog box from the [Measure] menu automatically transfers the measured spectrum to the [Spectra Analysis] program after measurement.

When a value of 2 or more is specified for the number of cycles in the [Parameters] dialog box, the dialog box in Fig. 6.4 is displayed.

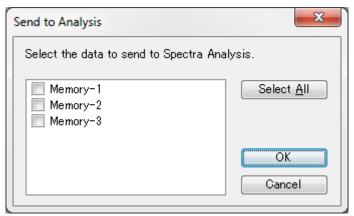


Figure 6.4 [Send to Analysis] dialog box

Select the check boxes for the data to send to the [Spectra Analysis] program (or click the <Select All> button to send all data), and then click the <OK> button.

Note: This operation can also be performed by clicking the tool button [Send to Analysis].

### 6.2.3 [Open Parameters...]

Selects a parameter file and opens those parameters.

Note 1: This operation can also be performed by clicking the tool button [2] [Open Parameters].

Note 2: The dialog box in Fig. 6.5 displays only the parameter files for the currently attached accessory.

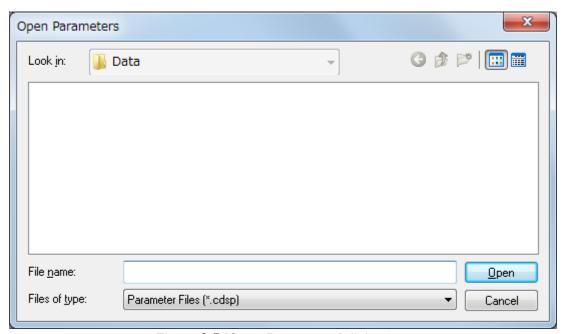


Figure 6.5 [Open Parameters] dialog box

[Look <u>i</u> n] list	Selects a drive and folder to browse using the drop-down list. Files saved in the currently opened folder are displayed in the file name list.	
File name list	Lists the files in the currently opened folder. Selects the file name	
	of the parameters to open.	
[File <u>n</u> ame]	Enters the file name for the parameters to open.	
	An extension may be omitted since the appropriate extension for	
	the measurement program is automatically appended.	
[Files of type]	Selects the files (type of extension) to display in the file name list.	
	Files other than Parameter Files (having the appropriate	
	extension for the measurement program) cannot be selected.	
< <u>O</u> pen>	Opens a parameter file and closes the dialog box.	
<cancel></cancel>	Closes the dialog box without opening a parameter file.	

Note: In the CFR version, the [Look in] drop-down list cannot be used to select a folder. However, a subfolder within the prespecified folder can be selected.

## 6.2.4 [Save Parameters...]

Saves the currently specified measurement parameters with the entered file name.

Note: This operation can also be performed by clicking the tool button [ [Save Parameters].

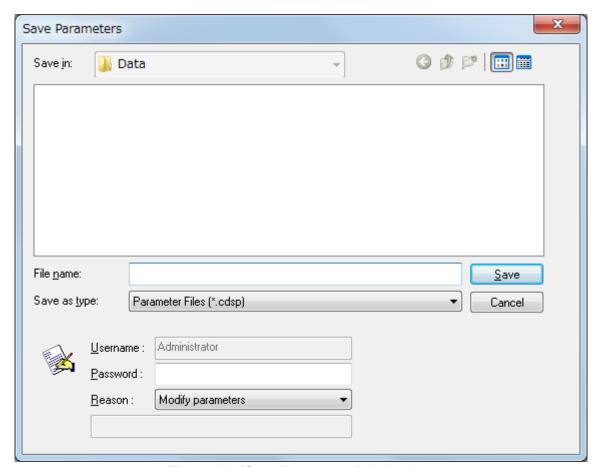


Figure 6.6 [Save Parameters] dialog box

[Save <u>i</u> n] list	Selects a drive or folder to browse using the drop-down list. Files saved in the currently opened folder are displayed in the file name list.
File name list	Lists the files in the currently opened folder. Use as a reference
	when naming a file.
[File <u>n</u> ame]	Enters a file name for saving parameters.
	An extension may be omitted since the appropriate extension for
	the measurement program is automatically appended.
[Save as type]	Selects the files (type of extension) to display in the file name list.
	Files other than Parameter Files (having the appropriate extension
	for the measurement program) cannot be selected.
[ <u>U</u> sername]	Displays the name of the logged-on user. This cannot be edited.
[ <u>P</u> assword]	In the CFR version, an electronic signature is required for saving
	parameters. Type a password in the text box.

[ <u>R</u> eason]	Selects a reason for saving the parameters. This cannot be selected when new parameters are created. After modifying parameters, select [Other] from the drop-down list to activate the text box for typing the reason.	
< <u>S</u> ave>	Saves the parameter file and closes the dialog box.	
<cancel></cancel>	Closes the dialog box without saving the parameter file.	

Note: In the CFR version, the [Save in] drop-down list cannot be used to select a folder. However, a subfolder within the prespecified folder can be selected.

#### 6.2.5 [Open Baseline...]

Selects a baseline file and opens that baseline. When a baseline file is opened, the sample spectrum is corrected by using the opened baseline spectrum.

- Note 1: In the CFR version, this function is not available.
- Note 2: The following dialog box displays only the baseline files for the currently attached accessory.

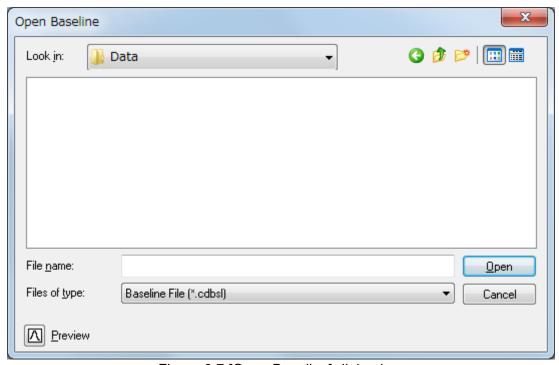


Figure 6.7 [Open Baseline] dialog box

Click the <a> <b style="color: blue;">Preview> button in Fig. 6.6 to display the spectrum of the selected baseline file (see Fig. 6.7).</a>

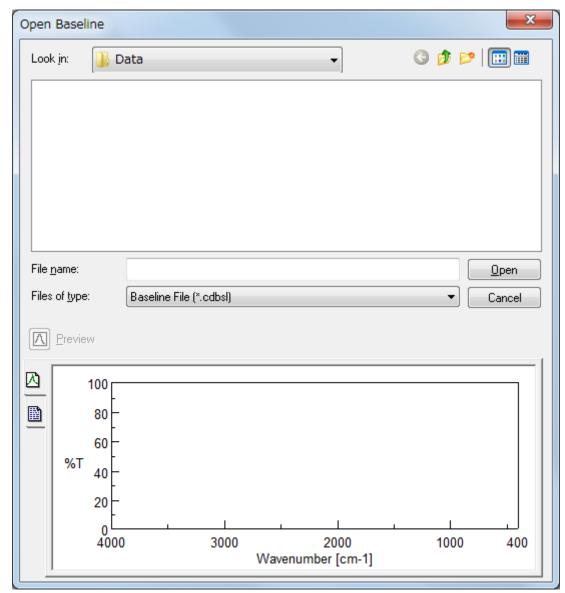


Figure 6.8 [Open Baseline] dialog box

[Look in] list	Selects a drive or folder to browse using the drop-down list. Files saved in the currently opened folder are displayed in the file name list.
File name list	Lists the files in the currently opened folder. Selects the file name of the baseline spectrum to open.
[File <u>n</u> ame]	Enters the file name of the baseline spectrum to open.  An extension may be omitted since the extension ".cdbsl" is automatically appended.
[Files of type]	Selects the files (type of extension) to display in the file name list. Files other than Baseline Files (*.cdbsl) cannot be selected.
< <u>P</u> review>	Displays the baseline spectrum and information about the selected file (see Fig. 6.8).
< <u>O</u> pen> <cancel></cancel>	Opens the baseline file and closes the dialog box.  Closes the dialog box without opening a baseline file.

## 6.2.6 [Save Baseline...]

Saves the currently measured baseline spectrum with the entered file name.

Note: In the CFR version, this function is not available.

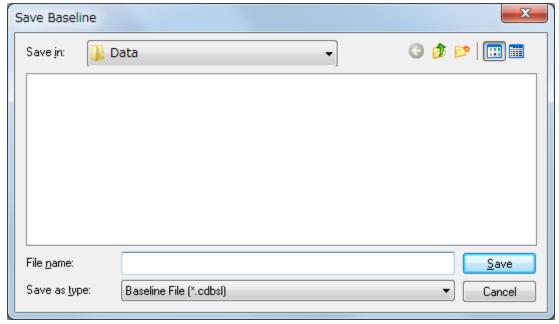


Figure 6.9 [Save Baseline] dialog box

[Save <u>i</u> n] list	Selects a drive or folder to browse using the drop-down list. Files saved in the currently opened folder are displayed in the file name list.
File name list	Lists the files in the currently opened folder. Use as a reference when naming a file.
[File <u>n</u> ame]	Enters a file name for saving the baseline spectrum.  An extension may be omitted since the extension ".cdbsl" is automatically appended.
[Save as <u>t</u> ype]	Selects the files (type of extension) to display in the file name list. Files other than Baseline Files (*.cdbsl) cannot be selected.
< <u>S</u> ave>	Saves the measured baseline spectrum and closes the dialog box.
<cancel></cancel>	Closes the dialog box without saving the measured baseline spectrum.

## 6.2.7 [Exit]

Exits the [Spectra Measurement] program.

### 6.3 [Measure] Menu

Starts or cancels the measurement, and specifies the measurement parameters.

#### 6.3.1 [Cancel]

Cancels the measurement. A dialog box to confirm whether to keep the measurement data is displayed.

Note: This operation can also be performed by clicking the tool button [ [Cancel].

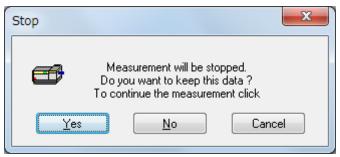


Figure 6.10 [Cancel] dialog box

< <u>Y</u> es>	Keeps the measured spectrum.
< <u>N</u> o>	Discards the measured spectrum.
<cancel></cancel>	Continues the measurement.

## 6.3.2 [Sample Measurement]

Measures the CD spectrum of the sample. Selecting the [To Spectra Analysis] check box in the [Data] tab of the [Parameters] dialog box from the [Measure] menu automatically transfers the measured data to the [Spectra Analysis] program after measurement. The measured data is displayed in a new View.

Note: This operation can also be performed by clicking the tool button [Sample] or pressing the measurement start button of the CD spectrometer.

#### 6.3.3 [Baseline Measurement]

Measures the baseline spectrum for baseline correction. Available if [Baseline] is selected in the [Control] tab of the [Parameters] dialog box.

Baseline correction removes the effects of solvents and additional agents other than the target sample. The true sample spectrum is obtained by subtracting the baseline spectrum from the measured spectrum.

Confirm that the sample for baseline measurement has been inserted, and then click the <Measure> button.

Note: This operation can also be performed by clicking the tool button [24] [Baseline Measurement]. When the dialog box in Fig. 6.11 is displayed, the baseline measurement can also be started by pressing the < Measure button.

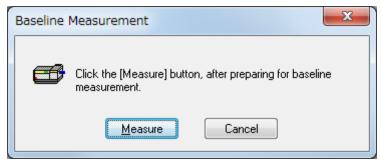


Figure 6.11 [Baseline Measurement] dialog box

< <u>M</u> easure>	Measures the baseline spectrum for baseline correction.
<cancel></cancel>	Closes the [Baseline Measurement] dialog box without measuring the
	baseline

### 6.3.4 [Blank Measurement]

Measures the blank data for blank correction. Available if [Blank] is selected in the [Control] tab of the [Parameters] dialog box.

Blank correction removes the effects of solvents and additional agents other than the target sample. The sample signal is obtained by subtracting the blank data from the data obtained during measurement of the sample.

Confirm that the blank has been inserted, and then click the < Measure > button.

Note: This operation can also be performed by clicking the tool button [2] [Blank Measurement]. When the dialog box in Fig. 6.12 is displayed, the blank measurement can also be started by pressing the <Measure> button.

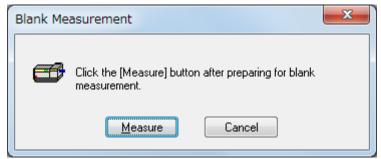


Figure 6.12 [Blank Measurement] dialog box

< <u>M</u> easure>	Measures the blank spectrum for blank correction.
<cancel></cancel>	Closes the [Blank Measurement] dialog box without measuring the
	blank.

#### 6.3.5 [DC Dark Measurement]

Measures the photometric value for dark correction. Available if the InGaAs photoconductive detector is used.

Note: This operation can also be performed by clicking the tool button [IDC Dark Measurement].

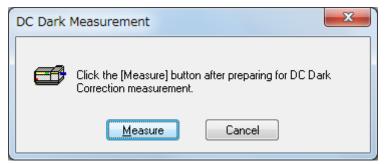


Figure 6.13 [DC Dark Measurement] dialog box

< <u>M</u> easure>	Measures the photometric value for dark correction.
<cancel></cancel>	Closes the [DC Dark Measurement] dialog box without measuring the
	dark current.

### **6.3.6** [Parameters...]

Specifies the measurement parameters. Refer to each measurement program reference.

# 6.4 [Control] menu

### 6.4.1 [Zero Clear]

Sets the photometric value of the ORD-M or fluorescence intensity to zero. Available if an ORD-M or fluorescence detector is connected.

Note: This operation can also be performed by clicking the tool button [Zero Clear].

### **6.4.2** [Shutter]

Opens/closes the shutter.

Note: This operation can also be performed by clicking the tool button Place [Shutter].

#### 6.4.3 [Move Wavelength...]

Moves the wavelength of the CD spectrometer to the desired wavelength. When the measurement is started, data acquisition begins once the wavelength returns to the value specified in [Parameters].



Figure 6.14 [Move Wavelength] dialog box

[Move to]	Specifies the wavelength.
	J-1100: 180 to 600 nm
	J-1500: 163 to 1600 nm
	J-1700: 163 to 2500 nm
<ok></ok>	Moves the wavelength of the CD spectrometer to the specified
	wavelength and closes the dialog box.
<cancel></cancel>	Closes the dialog box without applying any changes to the [Move
	Wavelength] settings.

Note: This operation can also be performed by clicking the tool button [Move Wavelength].

## 6.4.4 [Detector ...]

Specifies the sensitivity for monitoring the photometric value.

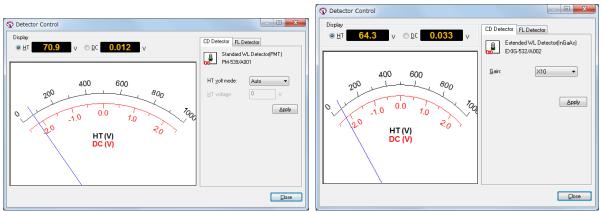


Figure 6.15 [Detector Control] dialog box (left: PMT, APD) (right: InGaAS, InSb)

Display	
[ <u>H</u> T]	Displays the HT voltage for the detector.
[ <u>D</u> C]	Displays the DC voltage for the detector.
[HT volt mode]	
[Auto]	Automatically sets the applied voltage for the photomultiplier tube.
[Manual]	Manually sets the applied voltage for the photomultiplier tube.
[Off]	Sets the detector voltage off.
[ <u>H</u> T voltage]	Specifies the photomultiplier tube voltage when [Manual] is selected
	for [HT volt mode].
	Setting range: 0 to 1000 V
[ <u>G</u> ain]	Selects the voltage gain for the InGaAs or InSb detector.
	Options: ×1, ×10, ×100
< <u>A</u> pply>	Sets the sensitivity of the CD spectrometer to the specified
111111111111111111111111111111111111111	sensitivity.
<cancel></cancel>	Closes the dialog box without applying any changes to the [Detector
	Control] settings.

Note: This operation can also be performed by clicking the tool button

#### 6.4.5 [Light Source...]

Turn on/off the light source.

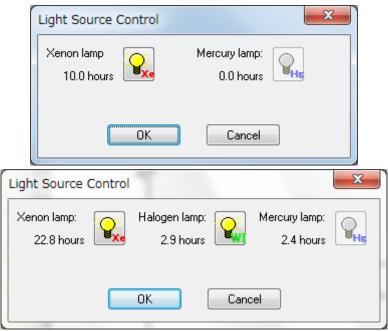


Figure 6.16 [Light Source Control] dialog box J-1100/1500 (top) J-1700 (bottom)

Note 1: This operation can also be performed by clicking the tool button [Light Source].

Note 2: indicates the status of the mercury lamp. The lamp cannot be turned on or off by clicking the button.

### 6.4.6 [Nitrogen Flowrate...]

Controls the nitrogen gas flow rate. Available if a PC-controlled nitrogen-gas auto flow meter is selected.

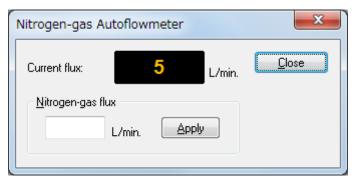


Figure 6.17 [Nitrogen Gas Auto Flow Meter] dialog box

Note: This command is displayed when the PC-controlled nitrogen gas auto flow meter is selected in [Administrative Tools].

### 6.4.7 [Select Detector...]

Recognizes a detector manually. Select the detector to use and click the <OK> button. A dialog box stating "Connecting to the detector..." is displayed.

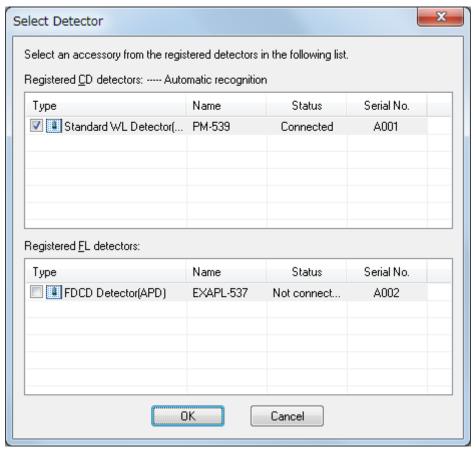


Figure 6.18 [Select Detector] dialog box

### 6.4.8 [Select Accessory...]

Selects an accessory (cell unit, external accessories or measurement units) to be used. After clicking the <OK> button, the message "The accessory was attached successfully." is displayed.

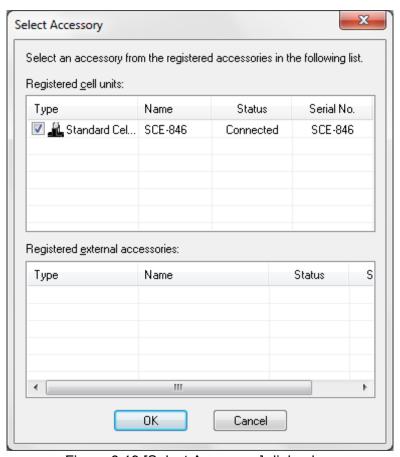


Figure 6.19 [Select Accessory] dialog box

Note: In the CFR version, the function for automatically starting registered programs for accessories is not provided.

#### 6.4.9 [Accessory Model Number]

When an accessory that has been registered is attached, the accessory name is displayed as a command on the [Control] menu (see Fig. 6.20). Select the command to control the attached accessory.

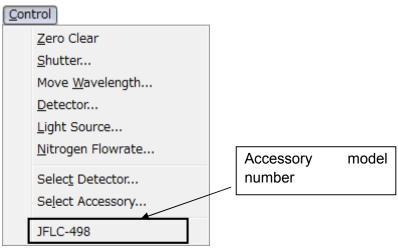


Figure 6.20 [Control] dialog box

- Note 1: Use this function to return the temperature of the Peltier device to room temperature after measuring data at high or low temperatures to set a target temperature after inserting a sample.
- Note 2: This operation can also be performed by clicking the <Setting...> button in the accessory bar.

# 6.5 [View] Menu

Specifies the view options.

# 6.5.1 [Scales...]

Specifies the display scale for the spectrum.

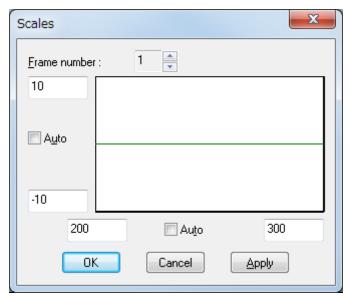


Figure 6.21 [Scales] dialog box

[Frame number]	Selects the graph for which to change the scales.
Horizontal axis	Enters the scale for the horizontal axis. Selecting the [Auto]
	check box displays the entire range irrespective of the entered values.
Vertical axis	Enters the scale for the vertical axis. Selecting the [Auto] check
	box displays the graph at the optimal scale for the specified
	horizontal axis range.
<ok></ok>	Applies the changes to the [Scales] settings and closes the dialog box.
<cancel></cancel>	Closes the dialog box without applying any changes to the
	[Scales] settings.
< <u>A</u> pply>	Applies the specified scales to the graph selected in [Frame number].

Note: This operation can also be performed by clicking the tool button [A] [Scales].

# 6.5.2 [Patterns...]

Selects the display color and line style for the spectrum.

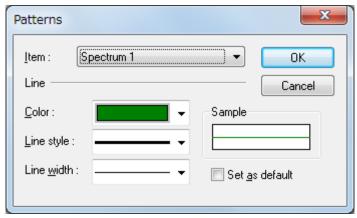


Figure 6.22 [Patterns] dialog box

[ <u>l</u> tem]	Selects an item from spectra 1 to 16, frame, gridlines, and auxiliary gridlines to change its color and line style.
[ <u>C</u> olor]	Shows the available colors for the selected item in the drop-down list.
[ <u>L</u> ine style]	Shows the available line styles. The currently selected item in the [Item] drop-down list is displayed with the selected line style.
[Line <u>w</u> idth]	Shows the available line widths. The currently selected item in the [Item] drop-down list is displayed with the selected line width.
Sample	Displays a sample of the selected pattern.
[Set as default]	Applies the selected patterns to all subsequently opened Views.
<ok></ok>	Applies the changes to the [Patterns] settings and closes the dialog box.
<cancel></cancel>	Closes the dialog box without applying any changes to the [Patterns] settings.

Note: This operation can also be performed by clicking the tool button [Patterns].

# 6.5.3 [Fonts...]

Specifies the display font for the data.

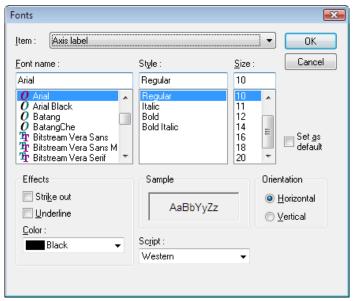


Figure 6.23 [Fonts] dialog box

[ <u>l</u> tem]	Selects an item to change its font settings.
	[Axis label]: Character ([CD (mdeg)], [nm], or other)
	[Scale label]: Numeric value
[Font name]	Lists available font names.
[St <u>y</u> le]	Lists available styles.
[ <u>S</u> ize]	Lists available sizes.
Effects	Selects strikeout and underline effects.
	[Strike out]: Draws a line through the middle of the text.
	[Underline]: Underlines the text.
Sample	Displays a sample of the specified font.
Orientation	Selects the orientation for displaying the axis label.
	[Horizontal]: Displays the y-axis label horizontally
	[Vertical]: Displays the y-axis label vertically
[Set as default]	Applies the specified fonts to all subsequently opened Views.
[ <u>C</u> olor]	Shows the available colors for the selected item in the drop-down
	list.
[Sc <u>r</u> ipt]	Selects the language for the specified font.
<ok></ok>	Applies the changes to the [Fonts] settings and closes the dialog
	box.
<cancel></cancel>	Closes the dialog box without applying any changes to the [Fonts]
	settings.

Note: This operation can also be performed by clicking the tool button [15].

# 6.5.4 [Gridlines...]

Shows/hides the gridlines for the data.



Figure 6.24 [Gridlines] dialog box

Main gridlines	
[ <u>H</u> orizontal]	Displays major horizontal axis gridlines.
[ <u>V</u> ertical]	Displays major vertical axis gridlines.
Auxiliary gridlines	
[H <u>o</u> rizontal]	Displays minor horizontal axis gridlines.
[V <u>e</u> rtical]	Displays minor vertical axis gridlines.
[Set as default]	Applies the selected gridlines to all subsequently opened Views.
<ok></ok>	Applies the changes to the [Gridlines] settings and closes the
	dialog box.
<cancel></cancel>	Closes the dialog box without applying any changes to the
	[Gridlines] settings.

Note: This operation can also be performed by clicking the tool button [Gridlines].

# 6.5.5 [Styles...]

Specifies the display style for the spectrum.



Figure 6.25 [Styles] dialog box

[ <u>A</u> xis]	Selects an item to change its display style.
Interval	
[A <u>u</u> to]	Automatically selects the gridline format.
[ <u>M</u> anual]	Manually specifies the gridline format for the main and auxiliary
	scales.
Tick type	
[Non <u>e]</u>	Displays no ticks on the axis
[Outside]	Displays ticks on the outside of the axis.
[Inside]	Displays ticks on the inside of the axis.
[ <u>C</u> ross]	Displays ticks on both sides of the axis.
[Decimal places]	Selects the number of decimal places for the display values on
	the horizontal and vertical axes.
[Display the max. and min.	Displays the maximum and minimum values at the main ticks.
values at the main ticks]	Values at the auxiliary ticks are not displayed.
[Set as default]	Applies the specified styles to all subsequently opened Views.
<ok></ok>	Applies the changes to the [Styles] settings and closes the
	dialog box.
<cancel></cancel>	Closes the dialog box without applying any changes to the
	[Styles] settings.

Note: This operation can also be performed by clicking the tool button [1]. [Styles].

### 6.5.6 [Overlay]

Overlays the spectra in the spectrum measurement display field when cycle measurement is selected.

# 6.5.7 [Select Graph...]

Selects the graphs to display in the data display field.

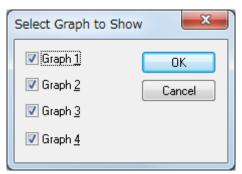


Figure 6.26 [Select Graph to Show] dialog box

[Graph <u>1</u> ]	Displays the graph for photometric mode 1 as graph 1 in the data display field.
[Graph <u>2</u> ]	Displays the graph for photometric mode 2 as graph 2 in the data display field.
[Graph <u>3</u> ]	Displays the graph for photometric mode 3 as graph 3 in the data display field.
[Graph <u>4</u> ]	Displays the graph for photometric mode 4 as graph 4 in the data display field.
<ok></ok>	Selects the graphs to display and closes the dialog box.
<cancel></cancel>	Closes the dialog box without selecting a graphs to display.

## 6.5.8 [Information Bar]

Shows/hides the information bar.

# 6.5.9 [Accessory Bar]

Shows/hides the accessory bar.

## 6.5.10 [Toolbars]

Shows/hides toolbars.

[ <u>F</u> ile]	Shows/hides the toolbar corresponding to the [File] menu.
[ <u>M</u> easure]	Shows/hides the toolbar corresponding to the [Measure] menu.
[Control]	Shows/hides the toolbar corresponding to the [Control] menu.
[ <u>V</u> iew]	Shows/hides the toolbar corresponding to the [View] menu.

# 6.5.11 [Status Bar]

Shows/hides the status bar.

# 6.5.12 [View Mode]

Displays the photometric value in digital or graph mode in the photometric value monitor.

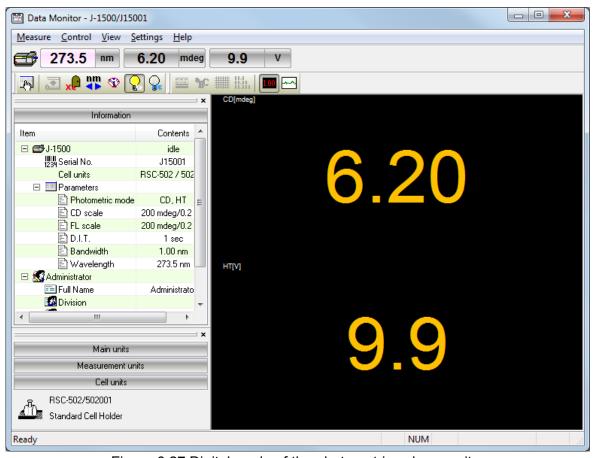


Figure 6.27 Digital mode of the photometric value monitor

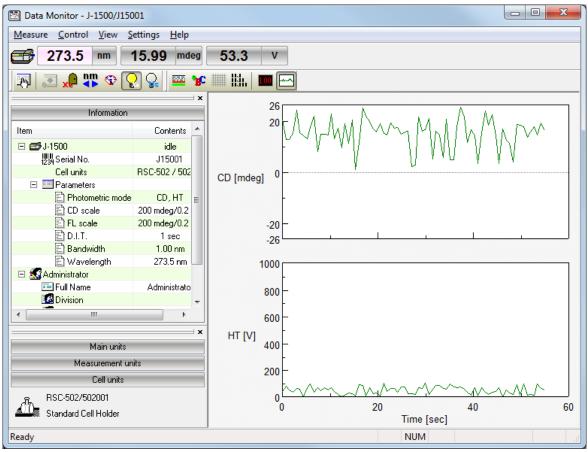


Figure 6.28 Graph mode of the photometric value monitor

#### **6.5.13** [Graph View]

Specifies [Patterns], [Fonts], [Gridlines] and [Styles] when graph mode is selected for the photometric value monitor. Refer to Sections 6.5.2 [Patterns...], 6.5.3 [Fonts...], 6.5.4 [Gridlines...] and 6.5.5 [Styles...] for details about setting each command.

## 6.6 [Settings] Menu 6.6.1 [Default Parameters...]

Note: In the CFR version, this function is not available.

Specifies measurement parameters for running the measurement program based on the currently recognized accessory. Default parameters can be specified for each accessory. Attach the accessory to be used and specify its default parameters.

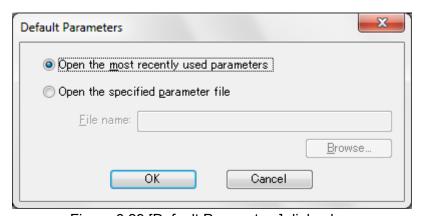


Figure 6.29 [Default Parameters] dialog box

[Open the most recently used parameters]	Starts with the parameters previously specified before exiting the measurement program.
[Open the specified <u>parameter</u> file]	Starts with a specified parameter file.
[ <u>F</u> ile name]	Displays the name of path to the parameter file when the [Open the specified parameter file] option button is selected.
< <u>B</u> rowse>	Selects the drive and file name for a saved parameter file (see Fig. 6.30).
<ok></ok>	Applies the changes to the [Default Parameters] settings and closes the dialog box.
<cancel></cancel>	Closes the dialog box without applying any changes to the [Default Parameters] settings.

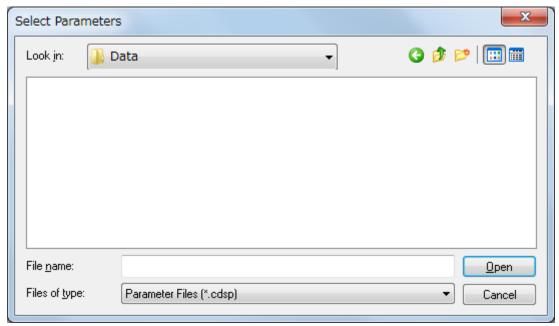


Figure 6.30 [Select Parameters] dialog box (when <<u>B</u>rowse...> is clicked in [Default Parameters])

### 6.6.2 [Customize Toolbar...]

Customizes and shows/hides toolbars.

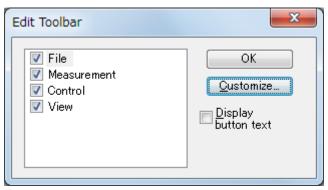


Figure 6.31 [Edit Toolbar] dialog box

[Measurement]	Shows/hides the toolbar corresponding to the [Measure] menu and adds/removes the following tool buttons.
	Button Name
	[Cancel]
	[Sample Measurement]
	[Baseline Measurement]/
	[Blank Measurement]
	[DC Dark Measurement]
	[Parameters]
[Control]	Shows/hides the toolbar corresponding to the [Control] menu and adds/removes the following tool buttons.
	Button Name
	[Auto Zero]
	[Shutter]
	[Move Wavelength]
	[Sensitivity]
	[Light Source][Hg Lamp]
[View]	Shows/hides the toolbar corresponding to the [View] menu and adds/removes the following tool buttons.
	Button Name
	[Scales]
	[Patterns]
	[Fonts]
	[Gridlines]
	[Styles]
	[Digital]
	[Graph]
[ <u>D</u> isplay button text]	Displays the button name under each tool button.
< <u>C</u> ustomize>	Displays the dialog box for customizing toolbars (see Fig. 6.32).

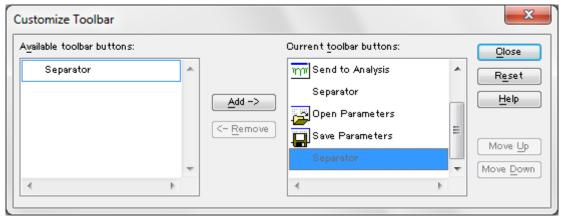


Figure 6.32 [Customize Toolbar] dialog box

#### 6.6.3 [Monitor Bar...]

Customizes the style for the monitor bar.

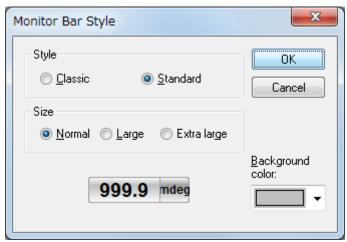
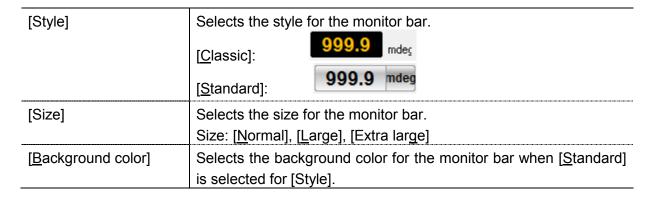


Figure 6.33 [Monitor Bar Style] dialog box



# 6.7 [Help] Menu

# 6.7.1 [About...]

Displays version information for each measurement program.

# 7. [Spectra Measurement] Program Reference

The [Spectra Measurement] program measures the change in the sample signal intensity while scanning the wavelength. This chapter describes specific measurement parameters for the [Spectra Measurement] program.

## 7.1 [Parameters...]

Specifies measurement parameters.

The window has four tabs for parameter settings, as shown in Figs 7.2 [General], Fig. 7.3 [Control], Fig. 7.4 [Information], and Fig. 7.5 [Data].

The [General] tab is open by default in the [Parameters] dialog box. The page can be changed by clicking each tab at the top of the dialog box.

The parameters can be switched between two modes: Basic mode and Advanced mode. In Basic mode, the choice of parameters is partially limited. In Advanced mode, each parameter is specified individually.

<basic advanced<="" mode="" th=""><th>Switches between Basic and Advanced modes. Advanced mode</th></basic>	Switches between Basic and Advanced modes. Advanced mode
Mode>	can only be used for J-1500.
< <u>O</u> pen>	Opens a measurement parameter file.
< <u>S</u> ave>	Saves the measurement parameters. In the CFR version, an electronic signature is required for saving parameters.
< <u>D</u> efault>	Restores the parameters of the [General] and [Control] tabs to their default values.
<0K>	Applies the changes to the [Parameters] settings and closes the dialog box.
<cancel></cancel>	Closes the dialog box without applying any changes to the [Parameters] settings.

- Note 1: This operation can also be performed by clicking the tool button [Parameters].
- Note 2: In the CFR version, Managers or Analysts authority is required to specify the parameters.
- Note 3: In the CFR version, when the parameters are specified or changed, a signature is required. Clicking the <OK> button when the parameters have not been saved displays the following message.

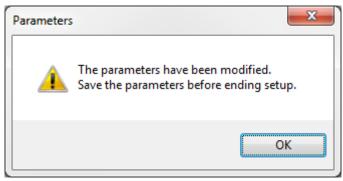


Figure 7.1 Message when the signature for the parameters is missing

## 7.1.1 [General] tab

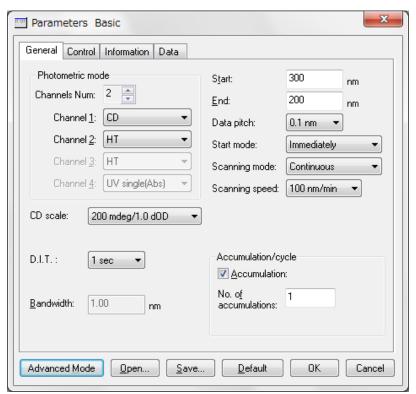


Figure 7.2(a) J-1100 [General] tab in [Parameters] dialog box

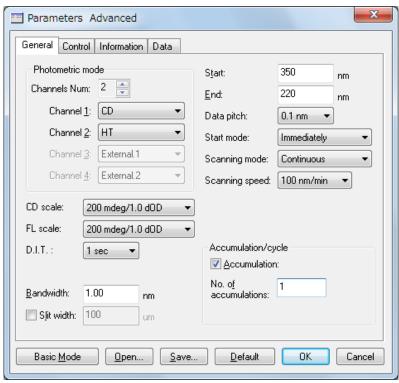


Figure 7.2(b) J-1500 [General] tab in [Parameters] dialog box

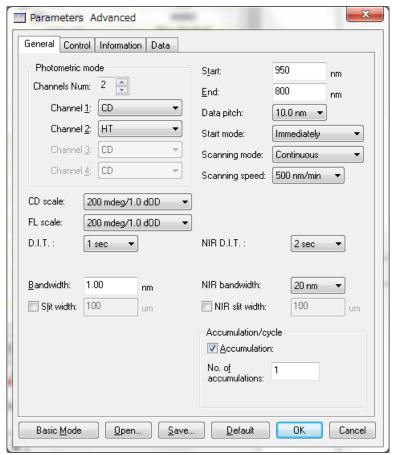


Figure 7.2(c) J-1700 [General] tab in [Parameters] dialog box

Photometric mode	Selects the desired measurement parameters for the photometric
	mode.
[Channels Num]	Selects the number of channels to display in the spectrum display
	field. Click the arrow (▼ or ▲) to select the number of channels.
	Options: 1 to 4
[Channel n]	Selects the photometric mode for each channel. Click the drop-down
-	list to select the photometric mode.
[CD scale]	Selects the CD/LD range for the detector in the transmission
-	configuration.
	[20 mdeg/0.05 dOD]: High sensitivity mode. Available when the
	CD range is within ±20 mdeg and the LD
	range is within ±0.05 dOD.
	[200 mdeg/1.0 dOD]: Standard sensitivity mode. Available when
	the CD range is within ±200 mdeg and the
	LD range is within ±1.0 dOD.
	[2000 mdeg/1.0 dOD]: Wide range mode. Available when the CD
	range is within ±2000 mdeg and the LD
	range is within ±1.0 dOD.
	[10000 mdeg/1.0 dOD]: Maximum range mode. Available when
	the CD range is within ±10000 mdeg and
	the LD range is within ±1.0 dOD.

[FL scale]	Selects the FDCD/FDLD configuration.	range for the C detector in the fluorescence
	[20 mdeg/0.05 dOD]:	High sensitivity mode. Available when the FDCD range is within ±20 mdeg and the FDLD range is within ±0.05 dOD.
	[200 mdeg/1.0 dOD]:	Standard sensitivity mode. Available when the FDCD range is within ±200 mdeg and the FDLD range is within ±1.0 dOD.
	[2000 mdeg/1.0 dOD]:	Wide range mode. Available when the FDCD range is within ±2000 mdeg and the FDLD range is within ±1.0 dOD.
	[10000 mdeg/1.0 dOD	]: Maximum range mode. Available when the FDCD range is within ±10000 mdeg and the FDLD range is within ±1.0 dOD.
[D.I.T.]	Selects the data acquisition	on time (integration time) per point.
ر ۱.۱۰۰۱	J-1100: 5 msec to 8 sec	on time (integration time) per point.
		30 sec
J-1500/1700: 0.1 msec to 30 sec  [Bandwidth] Selects the spectral bandwidth.		
[ <u>D</u> andwidth]	J-1100: 1 nm (fixed)	widti.
	J-1500/1700: 0.01 nm to	16 00 pm
[Clit width]		
[Slit width]	·	thin the range from 1 to 4000 µm. Selecting ext box for entering the slit width.
[Start]	Specifies the measureme	
[0]4.1]	J-1100: 180 to 600 nm	nt ctart may crong an
	J-1500: 163 to 1600 nm	
	J-1700: 163 to 2500 nm	
[ <u>E</u> nd]	Specifies the measureme	nt end wavelength
[ <u>=</u> ]	J-1100: 180 to 600 nm	nt ona wavolongui.
	J-1500: 163 to 1600 nm	
	J-1700: 163 to 2500 nm	
[Data pitch]		terval for data acquisition.
	Selects the wavelength interval for data acquisition.  Selects the measurement start condition.	
[Start mode]		
	Options: [Immediately], [V	
		r] when an optional accessory such as a
	stopped flow system is used.	
[Sca <u>n</u> ning mode]	Selects the scanning mod	le.
	Options:	Ocation of the contract
	[Continuous]:	Continuous scan. Scans the wavelength
		at the speed specified in [Scanning
	[045::1:	speed].
	[Step]:	Step scan. Increments the wavelength in
		steps corresponding to the data
		wavelength interval, and performs

	[Step (Auto)]:	measurements at each wavelength for a time specified by [D.I.T.] while the drive is stopped. The scanning speed depends on [D.I.T.]. In this case, the D.I.T. value is chosen automatically and cannot be selected.  Performs a step scan while automatically adjusting D.I.T. to obtain a constant signal-to-noise ratio. Selecting [Step (Auto)] displays [D.I.T. Upper] and [D.I.T. Lower] instead of [D.I.T.]. Click the arrows to display the drop-down lists and select the desired values. In the low signal-to-noise ratio region, the D.I.T. is automatically set between [D.I.T. Upper] and [D.I.T. Lower].
[Scanning speed]	Specifies the scanning	speed. Available if [Continuous] is selected for
[ <u>o</u> canning speed]	[Scanning mode].	speed. Available ii [Continuods] is selected for
	J-1100: 1 nm/min to 50	00 nm/min
	J-1500/1700: 1 nm/min	
[NIR D. I. T.]	Selects the data acquis	sition time (integration time) per point for NIR
	region.	
	J-1700: 016 msec to 30	sec
[NIR bandwidth]	Selects the spectral bar	ndwidth for NIR region.
	J-1700: 20 nm, 30 nm,	40 nm, 50 nm
[NIR slit width]	Specifies the slit width	within the range from 1 to 4000 $\mu m$ . Selecting
		s the text box for entering the slit width. (only
	for J-1700)	
Accumulation/cycle		
[No. of c <u>y</u> cles]	· ·	of measurements for each sample. When 2 or
	displayed.	are specified, the [Cycle interval] text box is
	Input range: 1 to 999	
	· · · · · · · · · · · · · · · · · · ·	cumulation] check box is selected, [No. of
	c <u>y</u> cles] is not	-
[ <u>A</u> ccumulation]	Specifies that cumulative	ve averaging should be used to measure the
	spectrum. Selecting [Ad	ccumulation] displays [No. of accumulations].
[No. o <u>f</u>	Specifies the number of	measurements used to average the spectrum.
accumulations]	If measurement is s	stopped, all completed accumulations are
	averaged.	

# 7.1.2 [Control] tab

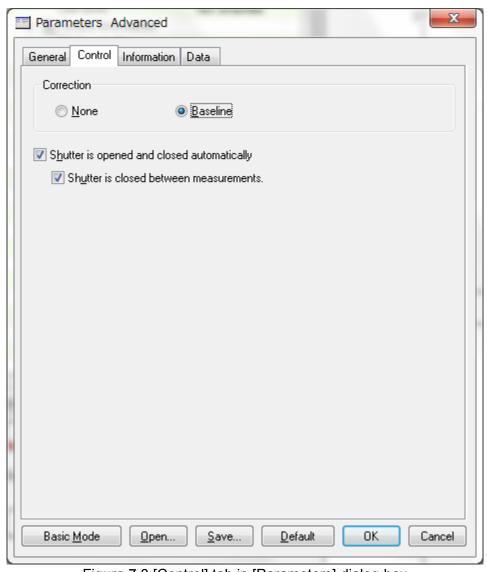


Figure 7.3 [Control] tab in [Parameters] dialog box

Correction	
[ <u>N</u> one]	Selects the use of no correction.
[ <u>B</u> aseline]	Selects baseline correction using a measured baseline.
[Shutter is opened and	Automatically opens the shutter just before the measurement
closed automatically]	starts and closes it after the measurement finishes, regardless
	of the current shutter status. Even when this option is selected,
	if cycle measurement is selected, the shutter is not closed
	between measurements.
[Sh <u>u</u> tter is closed	Automatically closes the shutter between measurements, if
between measurements]	cycle measurement is selected.

# 7.1.3 [Information] tab

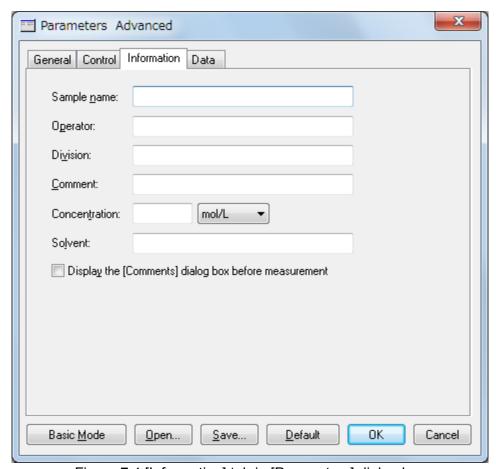


Figure 7.4 [Information] tab in [Parameters] dialog box

[Sample <u>n</u> ame]	Enters a sample name (maximum 63 characters).
[O <u>p</u> erator]	Enters an operator name (maximum 63 characters).
[Di <u>v</u> ision]	Enters a division name for the operator (maximum 127
	characters).
[Comment]	Enters a comment (maximum 127 characters).
[Concentration]	Enters a sample concentration. There is no character
	limit.
[So <u>l</u> vent]	Enters a solvent name (maximum 127 single-byte
	characters).
[Display the [Comments]	Displays the [Comments] dialog box for each
dialog box before	measurement.
measurement]	

Note: In the CFR version, the [Operator] and [Division] text boxes cannot be changed by the user.

#### 7.1.4 [Data] tab

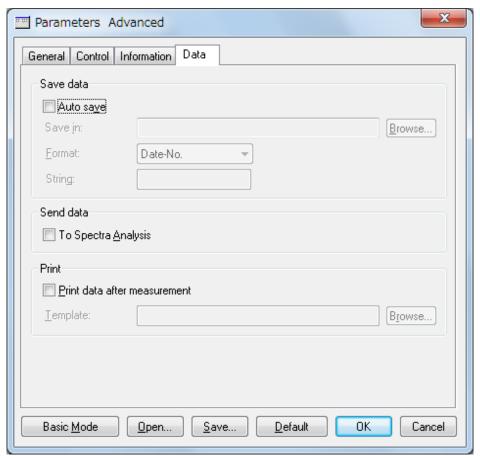


Figure 7.5 [Data] tab in [Parameters] dialog box

Save data

Selects to automatically save data. A file name is automatically allocated to the measured data and the data is saved to the specified directory.

Note: In the CFR version, when [Auto save] is selected, the following dialog box is displayed when the sample measurement starts. Start the measurement after typing a signature.

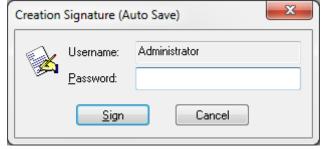


Figure 7.6 [Creation Signature (Auto Save)] dialog box

[Auto save] Automatically saves measured data.

[Save in] Displays the drive and folder name for saving data.

< <u>B</u> rowse>	Browses to the [Save in] drive and folder.
[ <u>F</u> ormat]	Selects the file name to be assigned during auto saving. The file
	format is Standard Files (*.jws).
[Date-No.]	Sets [Date] + [3-digit serial number] as the file name. The date
	and serial number are connected with a hyphen "-".
[Sample-No.]	Sets [Sample name] + [3-digit serial number] as the file name.
	[Sample name] is the name entered in the [Information] tab.
[Comment-No.]	Sets [Comment] + [3 digit serial number] as the file name.
	[Comment] is the comment entered in the [Information] tab.
[Sample-Comment-No.]	Sets [Sample name] + [Comment] + [3-digit serial number] as the
	file name. [Sample name] and [Comment] are the name and
	comment entered in the [Information] tab, respectively.
[String-No.]	Sets [String-No.] + [3-digit serial number] as the file name. Type
	the character string in the text box below the drop-down list
***************************************	(maximum 63 single-byte characters).
[String]	Enters a character string when [String-No.] is selected for
-	[Format] (maximum 63 single-byte characters).
Send data	Selects to automatically send measured data to the [Spectra
	Analysis] program after measurement.
[To Spectra Analysis]	Automatically sends measured data to the [Spectra Analysis]
	program after measurement.
Print	Selects to automatically print data after measurement.
[ <u>P</u> rint data after	Automatically prints data after measurement.
measurement]	
[ <u>T</u> emplate]	Displays the drive and file name of a saved template file.
<b<u>rowse&gt;</b<u>	Selects the drive and file name of a saved template file.

# 8. [Time Course Measurement] Program Reference

The [Time Course Measurement] program measures the temporal change in the sample signal intensity at a fixed wavelength. This chapter describes specific measurement parameters for the [Time Course Measurement] program.

# 8.1 [Parameters...]

Specifies the measurement parameters.

The window has four tabs for parameter settings, as shown in Figs 8.2 [General], Fig. 8.3 [Control], Fig. 8.4 [Information], and Fig. 8.5 [Data]. The [General] tab is open by default in the [Parameters] dialog box. The page can be changed by clicking each tab at the top of the dialog box.

The parameters can be switched between two modes: Basic mode and Advanced mode. In Basic mode, the choice of parameters is partially limited. In Advanced mode, each parameter is specified individually.

<basic <u="">Mode/Advanced <u>M</u>ode&gt;</basic>	Switches between Basic and Advanced modes. Advanced mode can only be used for J-1500.
< <u>O</u> pen>	Opens a measurement parameter file.
< <u>S</u> ave>	Saves the measurement parameters. In the CFR version, an electronic signature is required for saving parameters.
< <u>D</u> efault>	Restores the parameters of the [General] and [Control] tabs to their default values.
<0K>	Applies the changes to the [Parameters] settings and closes the dialog box.
<cancel></cancel>	Closes the dialog box without applying any changes to the [Parameters] settings.

- Note 1: This operation can also be performed by clicking the tool button [Parameters].
- Note 2: In the CFR version, Managers or Analysts authority is required to specify the parameters.
- Note 3: In the CFR version, when the parameters are specified or changed, a signature is required. Clicking the <OK> button when the parameters have not been saved displays the following message.

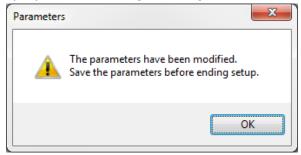


Figure 8.1 Message when the signature for the parameters is missing

### 8.1.1 [General] tab

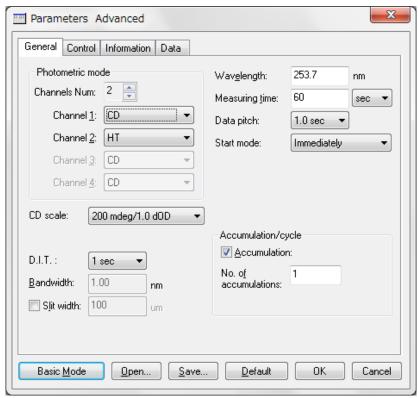


Figure 8.2(a) J-1100 [General] tab in [Parameters] dialog box

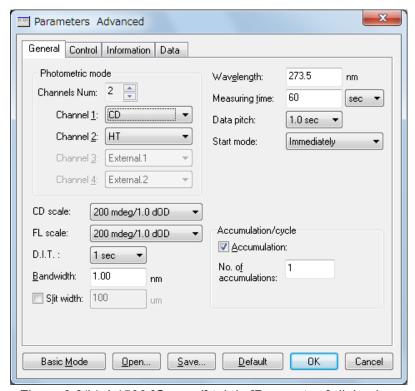


Figure 8.2(b) J-1500 [General] tab in [Parameters] dialog box

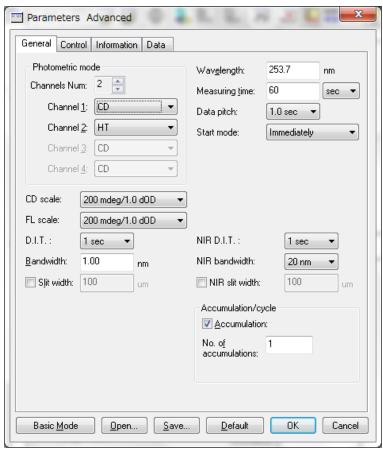


Figure 8.2(c) J-1700 [General] tab in [Parameters] dialog box

Photometric mode	Selects the desired measurement parameters for the photometric mode.	
[Channels Num]	Click the arrow (▼ or ▲) and select [Channels Num:] to display in the time-course data display field.  Options: 1 to 4	
[Channel n]	Selects the photometric mode for each channel. Click the drop-down list to select the photometric mode.	
[CD scale]	Selects the CD/LD scale range for the detector in the transmission configuration.	
	[20 mdeg/0.05 dOD]: High sensitivity mode. Available when the CD range is within ±20 mdeg and the LD range is within ±0.05 dOD.	
	[200 mdeg/1.0 dOD]: Standard sensitivity mode. Available when the CD range is within ±200 mdeg and the LD range is within ±1.0 dOD.	
	[2000 mdeg/1.0 dOD]: Wide range mode. Available when the CD range is within ±2000 mdeg and the LD range is within ±1.0 dOD.	
	[10000 mdeg/1.0 dOD]: Maximum range mode. Available when the CD range is within ±10000 mdeg and the LD range is within ±1.0 dOD.	

[FL scale]	Selects the FDCD/FDLD scale range for the C detector in the fluorescence configuration.		
	[20 mdeg/0.05 dOD]: High sensitivity mode. Available when the		
	FDCD range is within ±10 mdeg and the		
	FDLD range is within ±0.05 dOD.		
	[200 mdeg/1.0 dOD]: Standard sensitivity mode. Available when		
	the FDCD range is within ±200 mdeg and		
	the FDLD range is within ±1.0 dOD.		
	[2000 mdeg/1.0 dOD]: Wide range mode. Available when the		
	FDCD range is within ±2000 mdeg and the		
	FDLD range is within ±1.0 dOD.		
	[10000 mdeg/1.0 dOD]: Maximum range mode. Available when		
	the FDCD range is within ±10000 mdeg		
	and the FDLD range is within ±1.0 dOD.		
[D.I.T.]	Selects the data acquisition time (integration time) per point.		
[D.1.1.]	J-1100: 5 msec to 8 sec		
	J-1500/1700: 0.1 msec to 30 sec		
[ <u>B</u> andwidth]	Selects the spectral bandwidth.		
[ <u>D</u> anawath]	J-1100: 1 nm (fixed)		
	J-1500/1700: 0.01 nm to 16.00 nm		
[Slit width]			
[Oint Midth]	Specifies the slit width within the range from 1 to 4000 µm. Selecting		
[Wavelength]	[Slit width] activates the text box for entering the slit width.  Specifies the measurement start wavelength.		
[vvav <u>e</u> ierigiti]	J-1100: 180 to 600 nm		
	J-1500: 163 to 1600 nm J-1700: 163 to 2500 nm		
[Measuring time]	Specifies the measurement time.		
[Modeding <u>t</u> ime]	Input range: 2 to12002 sec		
[Data pitch]	Selects the wavelength interval for data acquisition.		
[Start mode]	Selects the measurement start condition.		
[Start mode]	Options: [Immediately], [Wait for ext trigger]		
	Use [Wait for ext. trigger] when an optional accessory such as a		
[NIR D. I. T.]	stopped flow system is used.  Selects the data acquisition time (integration time) per point for NIR		
[MIX D. I. 1.]	region.		
	J-1700: 016 msec to 30 sec		
[NIR bandwidth]	Selects the spectral bandwidth for NIR region.		
[Mix banawath]	J-1700: 20 nm, 30 nm, 40 nm, 50 nm		
[NIR slit width]	Specifies the slit width within the range from 1 to 4000 µm. Selecting		
[ till t ont mater]	[Slit width] activates the text box for entering the slit width. (only for		
	J-1700)		
Accumulation/cycle			
[No. of cycles]	Specifies the number of measurements for each sample. When 2 or		
[ 5. 5 <u>7</u> 5.55]	Tapatament and training of the desired for each earlies. Third 2 of		

	more measurements are specified, the [Cycle interval] text box is displayed.  Input range: 1 to 999	
	Note: When the [Accumulation] check box is selected, [No. of cycles] is not displayed.	
[ <u>A</u> ccumulation]	Specifies that cumulative averaging should be used to measure the spectrum. Selecting [Accumulation] displays [No. of accumulations].	
[No. o <u>f</u>	Specifies the number of measurements used to average the spectrum.	
accumulations]	If measurement is stopped, all completed accumulations are averaged. Input range: 1 to 999.	

# 8.1.2 [Control] tab

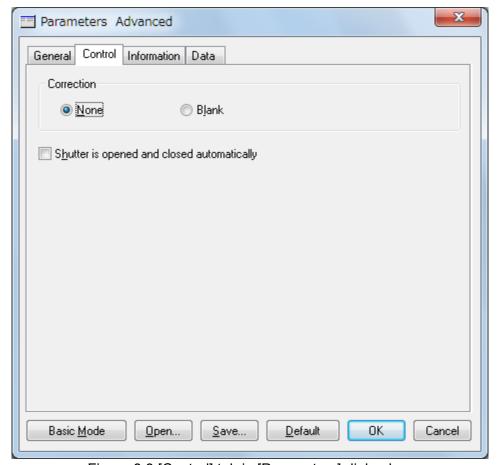


Figure 8.3 [Control] tab in [Parameters] dialog box

Correction		
[ <u>N</u> one]	Selects the use of no correction.	
[B <u>l</u> ank]	Selects blank correction using a measured blank.	
[Shutter is opened and closed automatically]	Automatically opens the shutter just before the measurement starts and closes it after the measurement finishes, regardless of the current shutter status. Even when this option is selected, if cycle measurement is selected, the shutter is not closed between measurements.	

### 8.1.3 [Information] tab

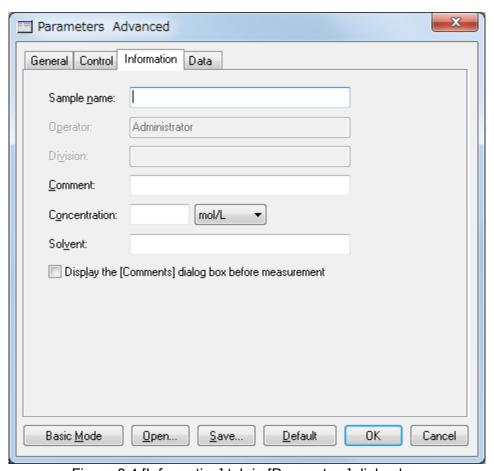


Figure 8.4 [Information] tab in [Parameters] dialog box

[Sample <u>n</u>ame] Enters a sample name (maximum 63 characters). [Operator] Enters an operator name (maximum 63 characters). [Division] Enters a division name for the operator (maximum 127 characters). [Comment] Enters a comment (maximum 127 characters). [Concentration] Enters a sample concentration. There is no character limit. [Solvent] Enters a solvent name (maximum 127 single-byte characters). [Display the [Comments] Displays the [Comments] dialog box for each dialog box before measurement. measurement]

Note: In the CFR version, the [Operator] and [Division] text boxes cannot be changed by the user.

#### 8.1.4 [Data] tab

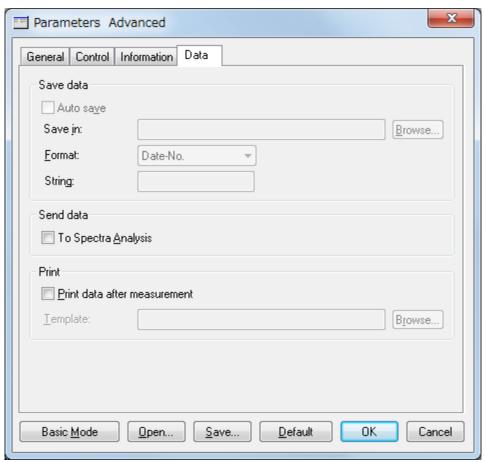


Figure 8.5 [Data] tab in [Parameters] dialog box

Save data

Selects to automatically save data. A file name is automatically allocated to the measured data and the data is saved to the specified directory.

Note: In the CFR version, when [Auto save] is selected, the following dialog box is displayed when the sample measurement starts. Start the measurement after typing a signature.

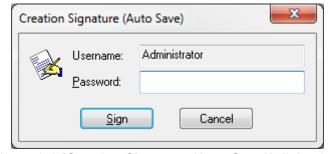


Figure 8.6 [Creation Signature (Auto Save)] dialog box

[Auto save] Automatically saves measured data
[Save in] Displays the drive and folder name for saving data.

< <u>B</u> rowse>	Browses to the [Save in] drive and folder.	
[ <u>F</u> ormat]	Selects the file name to be assigned during auto saving. The file	
	format is Standard Files (*.jws).	
[Date-No.]	Sets [Date] + [3-digit serial number] as the file name. The d	
	and serial number are connected with a hyphen "-".	
[Sample-No.]	Sets [Sample name] + [3-digit serial number] as the file name	
	[Sample name] is the name entered in the [Information] tab.	
[Comment-No.]	Sets [Comment] + [3 digit serial number] as the file name.	
	[Comment] is the comment entered in the [Information] tab.	
[Sample-Comment-No.]	Sets [Sample name] + [Comment] + [3-digit serial number] as the	
	file name. [Sample name] and [Comment] are the name and	
	comment entered in the [Information] tab, respectively.	
[String-No.]	Sets [String-No.] + [3-digit serial number] as the file name. Type	
	the character string in the text box below the drop-down list	
	(maximum 63 single-byte characters).	
[Strin <u>g]</u>	Enters a character string when [String-No.] is selected for	
	[Format] (maximum 63 single-byte characters).	
Send data	Selects to automatically send measured data to [Spectra	
	Analysis] program after measurement.	
[To Spectra Analysis]	Automatically sends measured data to the [Spectra Analysis]	
	program after measurement.	
Print	Selects to automatically print data after measurement.	
[Print data after	Automatically prints data after measurement.	
measurement]		
[ <u>T</u> emplate]	Displays the drive and file name of a saved template file.	
<browse></browse>	Selects the drive and file name of a saved template file.	

# 9. [Data Monitor] program reference

The [Data Monitor] program is used to provide an enlarged display of the photometric values when the CD spectrometer is being tested or calibrated. This chapter describes specific measurement parameters for the [Data Monitor] program.

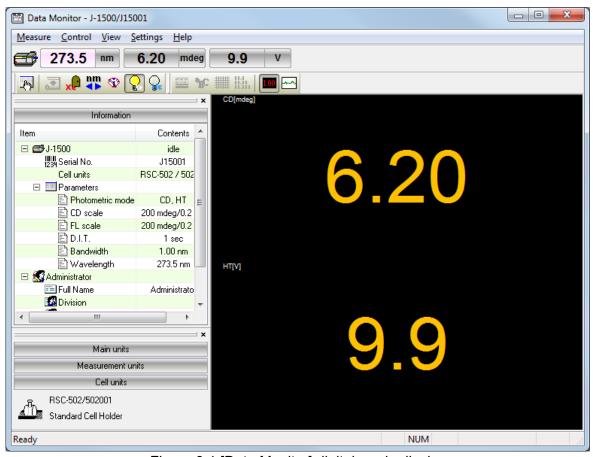


Figure 9.1 [Data Monitor] digital-mode display

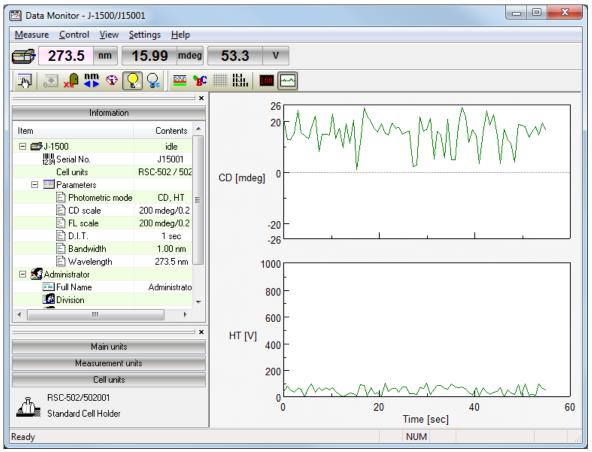


Figure 9.2 [Data Monitor] graph-mode display

# 9.1 [Parameters...]

Specifies the measurement parameters.

<ok></ok>	Applies the changes to the [Parameters] settings and closes the dialog box.		
<cancel></cancel>	Closes the dialog box without applying any changes to the [Parameters]		
	settings.		

Note: This operation can also be performed by clicking the tool button [Parameters].

# 9.1.1 [Parameters]

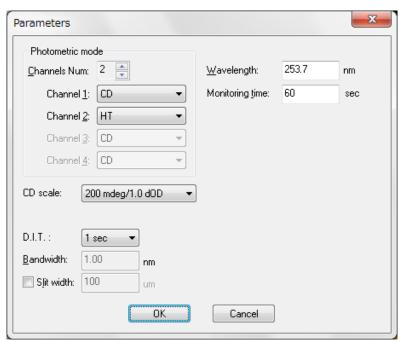


Figure 9.3(a) J-1100 [General] tab in [Parameters] dialog box

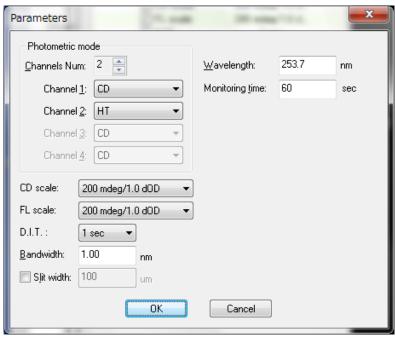


Figure 9.3(b) J-1500 [General] tab in [Parameters] dialog box

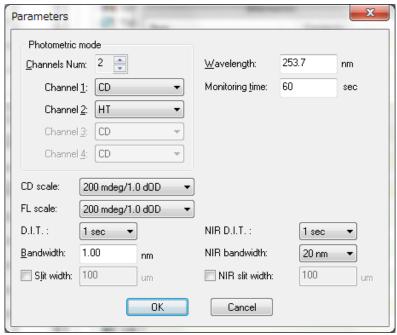


Figure 9.3(c) J-1700 [General] tab in [Parameters] dialog box

Photometric mode	Selects the desired measurement parameters for the photometric mode.	
[ <u>C</u> hannels Num]	Click the arrow (▼ or ▲) and select [Channels Num:] to display in the time-course data display field.  Options: 1 to 4	
[Channel n]	Selects the photometric mode for each channel. Click the drop-down list to select the photometric mode.	
[CD scale]	Selects the CD/LD scale range for the detector in the transmission configuration.  [20 mdeg/0.05 dOD]: High sensitivity mode. Available when the CD range is within ±20 mdeg and the	
	LD range is within ±0.05 dOD.  [200 mdeg/1.0 dOD]: Standard sensitivity mode. Available when the CD range is within ±200 mdeg and the LD range is within ±1.0 dOD.	
	[2000 mdeg/1.0 dOD]: Wide range mode. Available when the CD range is within ±2000 mdeg and the LD range is within ±1.0 dOD.	
	[10000 mdeg/1.0 dOD]: Maximum range mode. Available when the CD range is within ±10000 mdeg and the LD range is within ±1.0 dOD.	
[FL scale]	Selects the FDCD/FDLD scale range for the C detector in the fluorescence configuration.  [20 mdeg/0.05 dOD]: High sensitivity mode. Available when the FDCD range is within ±20 mdeg and the FDLD range is within ±0.05 dOD.	

	[200 mdeg/1.0 dOD]: Standard sensitivity mode. Available when the FDCD range is within ±200 mdeg and the FDLD range is within ±1.0 dOD.		
	[2000 mdeg/1.0 dOD]: Wide range mode. Available when the FDCD range is within ±2000 mdeg and the FDLD range is within ±1.0 dOD.		
	[10000 mdeg/1.0 dOD]:Maximum range mode. Available when the FDCD range is within ±10000 mdeg and the FDLD range is within ±1.0 dOD.		
[D.I.T.]	Selects the data acquisition time (integration time) per point.		
	J-1100: 5 msec to 8 sec		
	J-1500/1700: 0.1 msec to 30 sec		
[ <u>B</u> andwidth]	Selects the spectral bandwidth.		
	J-1100: 1 nm (fixed)		
	J-1500/1700: 0.01 nm to 16.00 nm		
[S <u>l</u> it width]	Specifies the slit width within the range from 1 to 4000 μm. Selecting		
	[Slit width] activates the text box for entering the slit width.		
[Wavelength]	Specifies the measurement start wavelength.		
	J-1100: 180 to 600 nm		
	J-1500: 163 to 1600 nm		
	J-1700: 163 to 2500 nm		
[Monitoring time]	Specifies the monitoring time when graph mode is selected.		
	Input range: 10 to 30000 sec		
[NIR D. I. T.]	Selects the data acquisition time (integration time) per point for NIR		
	region.		
	J-1700: 016 msec to 30 sec		
[NIR bandwidth]	Selects the spectral bandwidth for NIR region.		
	J-1700: 20 nm, 30 nm, 40 nm, 50 nm		
[NIR slit width]	Specifies the slit width within the range from 1 to 4000 µm. Selecting [Slit		
	width] activates the text box for entering the slit width. (Only J-1700)		

# 10. Appendix

## 10.1 Setting the Measurement Parameters

The parameters selected can seriously affect measurement results. The following summarizes how to select parameters.

#### 10.1.1 Measurement Wavelength Range

Most CD spectrum peaks appear in a specific wavelength region (short wavelength region as in the case of ultraviolet-visible absorption spectra for most organic compounds). If the optically active absorption band position for the sample is known, take measurements beginning at a wavelength of 50 to 100 nm before the leading edge of the spectrum and ending at the trailing edge of the spectrum where it converges at zero, although this method varies slightly depending on the width and shape of the spectrum.

#### 10.1.2 Data Acquisition Interval (Resolution)

#### 10.1.2.1 Spectra measurement

Usually, a value of about 0.2 nm is sufficient. However, if the scanning mode is set to [Step], approximately 1 nm is more appropriate. Make the resolution coarse if the spectrum peaks are broad and fine if they are sharp.

#### 10.1.2.2 Time-course measurement

Make the resolution fine if rapid changes with time are expected.

### 10.1.3 Scanning Speed

The scanning speed depends on the D. I. T. Under normal conditions, set the scanning speed at 20 to 100 nm/min and D. I. T. at 0.25 to 2 sec. Table 8.1 shows suggested D.I.T. values for different scanning speeds.

rable for Pinn values for amoronic scanning species			
Scanning speed (nm/min)	D.I.T. (recommended)	Upper limit	
10000	1.0 to 2.0 msec	32.0 msec	
5000	2.0 to 4.0 msec	64.0 msec	
2000	4.0 to 8.0 msec	0.25 sec	
1000	32.0 msec to 0.125 sec	0.5 sec	
500	64.0 msec to 0.25 sec	1.0 sec	
200	0.125 to 0.5 sec	2.0 sec	
100	0.25 to 1.0 sec	4.0 sec	
50	0.5 to 2.0 sec	8.0 sec	
20	1.0 to 2.0 sec	16.0 sec	
10	2.0 to 4.0 sec	16.0 sec	
5	2.0 to 8.0 sec	16.0 sec	
2	4.0 to 16.0 sec	16.0 sec	
1	8.0 to 16.0 sec	16.0 sec	

Table 10.1 D.I.T. values for different scanning speeds

#### 10.1.4 Number of Accumulations

The following relationship exists between the signal-to-noise ratio and the number of accumulations: S/N  $\propto \sqrt{(Number\ of\ accumulations)}$ .

Increasing the number of accumulations improves the signal-to-noise ratio for a spectrum. Determine the appropriate number of accumulations based on the spectrum (sample) condition and the overall measurement time (increasing the number of accumulations prolongs the measurement time).

If the sensitivity is lower than Standard, a single accumulation will suffice. Table 10.2 shows the suggested number of accumulations when a sample with an absorbance of 1 or less is measured with a D.I.T. of 2 sec.

Table 10.2 No. of accumulations and sensitivity (D.I.T. 2 sec)

Sensitivity	Number of accumulations
High	4 to 50
Standard, Low	1

Note: For time-course measurements, set the number of accumulations to 1. Cumulative measurement can be used in stopped flow measurement (see the instruction manual for the stopped flow unit).

#### 10.1.5 Response (D.I.T.)

#### 10.1.5.1 Spectra measurement

The following relationship exists between D.I.T. and the signal-to-noise ratio:

 $S/N \propto \sqrt{(Response)}$ .

The signal-to-noise ratio for a spectrum measured for 4 seconds is twice that for a spectrum measured for 1 second.

The spectral value at any given point in time is the average of values sampled before and after that time (D.I.T./2). Therefore, increasing D.I.T. leads to a greater effect of previous data on the current data. Do not increase D.I.T. excessively if scanning is carried out at high speed or if the resolution is low.

Table 10.3 shows suggested D.I.T. values for obtaining a spectrum with a high signal-to-noise ratio at a desired sensitivity. If the sensitivity is set at 10 mdeg and D. I. T. is set at 1 to 2 sec to improve the signal-to-noise ratio, increasing the number of accumulations is very effective because the spectrum is simultaneously averaged.

Table 10.3 D.I.T. values for obtaining high signal-to-noise ratio

CD scale (mdeg)	D.I.T. (sec)
10	0.5 to 16.0
200	0.125 to 0.5
2000	0.025 to 0.064

Note: A D.I.T. of 0.5 to 125 msec should be selected for high speed measurement using a stopped flow unit.

The above table also applies to a step scan. In this case, the measurement time is the sum of the wavelength stepping time and the data acquisition time at each step. If the D.I.T. is on the order of seconds, the number of accumulations will dominate the measurement time and the measurement time will be almost proportional to D.I.T. For a total wavelength measurement range of W (nm) and a data interval of Step (nm), the following relation holds between the total integration time and D.I.T.

Total Integration Time =  $(W/Step + 1) \times D.I.T.$ 

(W/Step + 1): Number of data points

#### 10.1.5.2 Time-course measurement

For time-course measurement, select a D.I.T. that is appropriate given the decay half-life of the CD signal due to a reaction. For normal reactions, set it to 1/10 of the decay half-life of the CD signal or smaller. For example, if the decay half-life is 20 msec, a D.I.T. of 0.5 to 2 msec is appropriate. If the decay is very slow, select a D.I.T. of 1 to 16 sec, taking into account the rate of change of the signal and the signal-to-noise ratio. When used as a monitor for HPLC, a D.I.T. of about 1 sec is suitable.

#### 10.1.6 Bandwidth and slit width

In most cases, set the measurement bandwidth to 1.0 nm. Decrease it when measuring a sharp spectrum such as a MCD (magnetic circular dichroism) spectrum, or increase when performing measurements using a micro cell, when the signal-to-noise ratio is low. When a longer wavelength detector (400 to 1100 nm) is used, increase the bandwidth and set the slit width to about 60  $\mu$ m to prevent the photomultiplier voltage (HT) from rising abnormally. However, ensure that the HT voltage does not become lower than 170 V.

- Note 1: If the slit width is increased until the HT voltage drops below 170 V, the photomultiplier may be damaged.
- Note 2: Most organic substances emit fluorescence. Therefore, measuring a sample having an absorbance of 2 or more at a bandwidth of 2 nm or more may distort the spectrum. Also, photolysis of a sample can occur in the ultraviolet region. If the sample is susceptible to photolysis, reduce the bandwidth to 0.5 nm or less.

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