SpectroQuest™

SPECTROPHOTOMETER APPLICATION SOFTWARE

VERSION 5.3

MANUAL

United Products & Instruments, Inc.
182 Ridge Road, Suite E
Dayton, New Jersey 08810, USA
Tel: 732-274-1155 Fax: 732-274-1151
E-mail:info@unicosci.com

TABLE OF CONTENTS

Functions

Main Functions

This section introduces the main functions of the UV-Vis Analyst software.

Fixed Points Measurement

Single Wavelength Photometric Measurement

Photometric value (%Transmittance or Absorbance) can be read at a single wavelength quickly and conveniently.

Multiwavelength Photometric Measurement

Up to 20 wavelength points can be set up in the multi-wavelength photometric measurement mode. Results will be grouped into a table format automatically. Results can be saved on hard drive or floppy diskettes for later use.

Concentration Measurement

The UV-Vis Analyst provides the following capabilities in concentration measurement;

- You can use up to 20 wavelength measurements to generate the regression curve.
- You can use up to 20 standards to set up the regression curve. UV-Vis Analyst will calculate the working curve using a linear equation that fits the data.
- Abnormal reading for standard and samples can be deleted and modified after measurement.
- You can enter factor values to generate regression curves.
- Analytical results can be sent to a printer. Method and results can be saved on hard drive.

Wavelength Scanning

Features:

- You can acquire wavelength spectra accurately and conveniently with selection of steps of 0.1, 0.2, 0.5, 1.0 and 5.0 nm which correspond to speed ranges from 10 nm/min to1000 nm/min.
- Light source switching position can be user defined from 339 nm to 1000 nm. Light sources and filters are automatically changed during scanning.

- Peaks and valleys will be automatically detected after scanning. User can define the peak threshold.

- Powerful spectrum processing functions are provided. (See Chapter 5).

- Spectra can be printed out on a printer. Analytical results can also be saved on the hard drive or floppy diskettes for later use.

Time Scanning

The UV-Vis Analyst allows you to record the absorbance or transmittance value of a sample as a function of time at a specified wavelength:

- On-line display of absorbance or transmittance with time graduations on the abscissa.

- Graphs can be output to a printer. Analytical results can also be saved on hard drive or floppy diskettes for later use.

- Photometric values at specified intervals can be printed in table format. Data can also be exported to EXCEL® software for statistical calculations.

DNA/Protein Measurement

Wavelength points and ratios can be set up in the DNA/Protein measurement mode. Results will be grouped into a table format automatically. Results can be saved on hard drive or floppy diskettes for later use.

Instrument Validity

Up to 10 wavelength points can be set up in the instrument validity mode. Two methods can be selected (Photometric Validity measurement and Wavelength Validity measurement) and tolerance can be entered. Results will be grouped into a table format automatically. Results can be saved on hard drive or floppy diskettes for later use.

Spectra Processing Function

Spectra processing functions include:

- Trace a Spectrum
  The cursor can be moved to a desired point in the spectrum displayed on the screen and the photometric data at this point is displayed.

- Automatic Peak Detection
  After a scanning is complete, peaks and valleys can be automatically detected and listed in a table format. They will also be labeled on the spectrum.

- Scale Expansion
  Simultaneous expansion of the X and Y axes are provided with the “Zoom” function. Display range can also be changed though the “Display Setup” functions.

- Differentiation
  You can calculate and display the first through to the fourth derivative spectra for a given spectrum. Derivative spectra are useful for enhancing spectral data that are not readily apparent in an absorbance spectrum.

- Calculations Between Spectra
  You can calculate addition, subtraction, multiplication and division between two spectra with the resulting data displayed on the screen.

Automatic System Initialization Function

The UV-Analyze performs the following calibration and self-diagnosis functions automatically:

- Memory Check

- Lamp Ignition Check

- Wavelength Drive Mechanism Check

- Automatic Wavelength Calibration

Basic Operation

Introduction:
This chapter provides information for basic operation of the UV-Vis spectrophotometer Application Software.

Main Menu

After entering the software, the Main Menu appears on the display. Click on File then New. Five main functions are listed on the dialog box. They are **Fixed Points Measurement, Wavelength Scan Measurement, Time Scan Measurement**, **DNA/Protein Measurement** and **Instrument Validity**. The **Fixed Points Measurement** function includes *multi-wavelength photometric measurement* and *concentration measurement*.

Menu bar and **Toolbar** are both provided in the software offering you two ways to select a desired function.

- On the menu bar, use your keypad or mouse to select the desired function.

- Almost all the functions listed in the menu bar can be reached by clicking a corresponding button in the toolbar.

*** Note:** These buttons only available when 6 x 1 (or 8 x 1) Auto cell holder is fitted.

Icon	Function	Icon	Function
	Connect/ disconnect to the instrument		CPU load
	Load a file saved in instrument		Method setup
	Zero calibration		Background calibration
	Turn on/off W lamp		Go to Lambda (nm)
	Transmittance mode		Turn on/off D2 lamp
	Save to file		Absorbance mode
	Unload a spectrum		Load a spectrum/data file
	Fixed points measurement		Print
	Time scan measurement		Wavelength scan measurement
	Instrument Validity		DNA/Protein measurement
	Cell 2*		Cell 1*
	Cell 4*		Cell 3*
	Cell 6*		Cell 5*
	Auto run*		Setup multicell*
	Modify a sample		Start a measurement
	Delete a sample		Stop a measurement
	Display range setup		Display and print setting
	Original scales		Activate ZOOM function
	Add two spectra		Trace cursor
	Multiply two spectra		Subtract one spectrum from another
	Smooth a spectrum		Divide one spectrum from another
	Derivative of a spectrum		Resample a spectrum
	List valleys of a spectrum		List peaks of a spectrum
	Undo Scale		Define peak/valley threshold

Setup

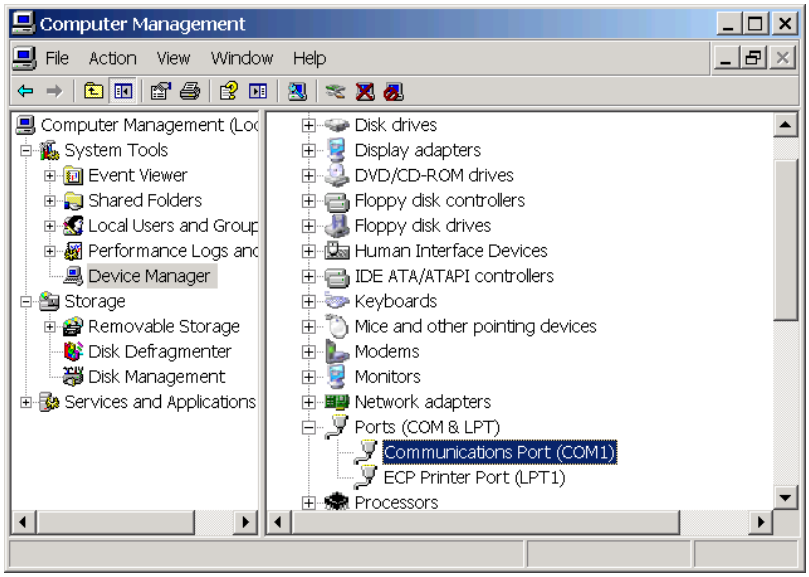
The UV-Vis Analyst cannot control the Instrument before setting the Comm. Port and plug the dongle (Passkey).

Communication Ports and USB Driver

Use RS232 Port for RS232 printer and for Internal Software(Firmware) Upgrade:

When RS232 connection is used set the RS232/USB seleletion switch to the right (upgrade: for internal software upgrade and RS232 printer). The communication port is usally COM1. It may vary. So check the port assignment on your computer following the steps below:

- At your computer main screen right-click on “My Computer”.
- Select and click on“Manage”;
- then select and click on “Device Management”;
- then click on “ Ports(COM &LPT)” the port assignment information is displayed as shown below:



Use USB Port for PC Connection:

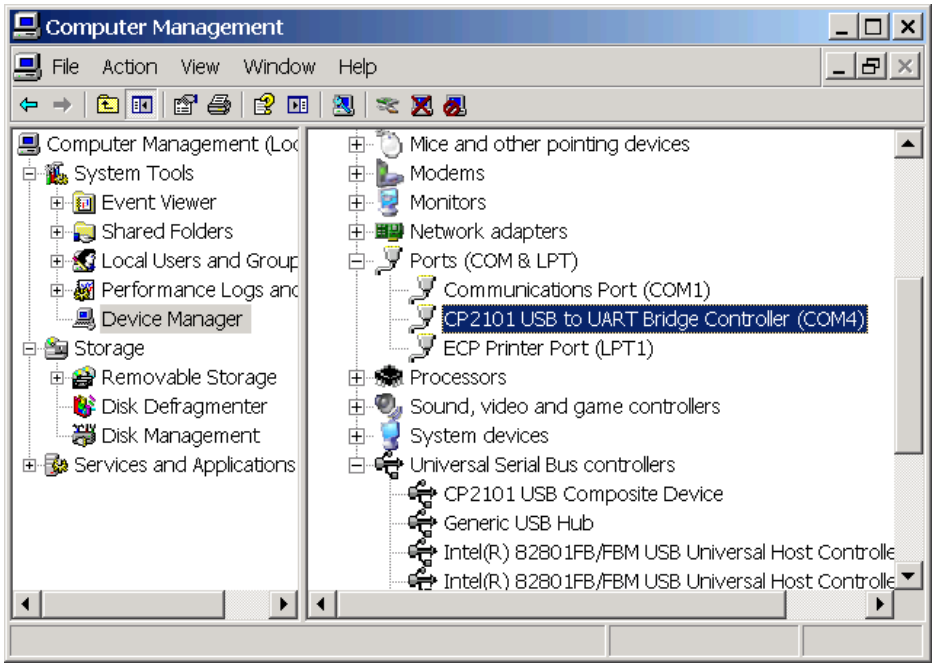
USB Port is designed for PC computer connection for use with PC application software (not for firmware upgrade). To use USB port: 1) set the RS232/USB selection switch to the left (normal). 2) USB driver CP2101 (USB to UART Bridge Controller) must be installed in your computer.

A copy of USB driver CP2101x is supplied in the CD. You may download a latest version of CP2101x from Internet.

To install USB driver CP2101 onto your computer connect your computer to the spectrophotometer USB port (make sure the RS232/USB selection switch is set on the left normal position). Turn on the spectrophotometer. Your computer finds the new hardware and starts to search for hardware driver. Direct it to CD drive or other location where the USB driver CP2101 is saved.

A communication port will be assigned for CP2101 in your computer. The port assignment may vary depend the specific computer configuration. To check the port assignment follow the steps below:

- At your computer main screen right-click on “My Computer”.
- Select and click on“Manage”;
- then select and click on “Device Management”;
- then click on “ Ports(COM &LPT)” the port assignment information is displayed as shown below. COM4 is assigned in this case. Select the same port (COM4) when connecting PC to the spectrophotometer.



Set Comm. Port

On the **UV-Photometer** menu, click **Comm Port Setup** appears the following box, select the Comm. Port and set Baud Rate = 38400, Click **OK**.

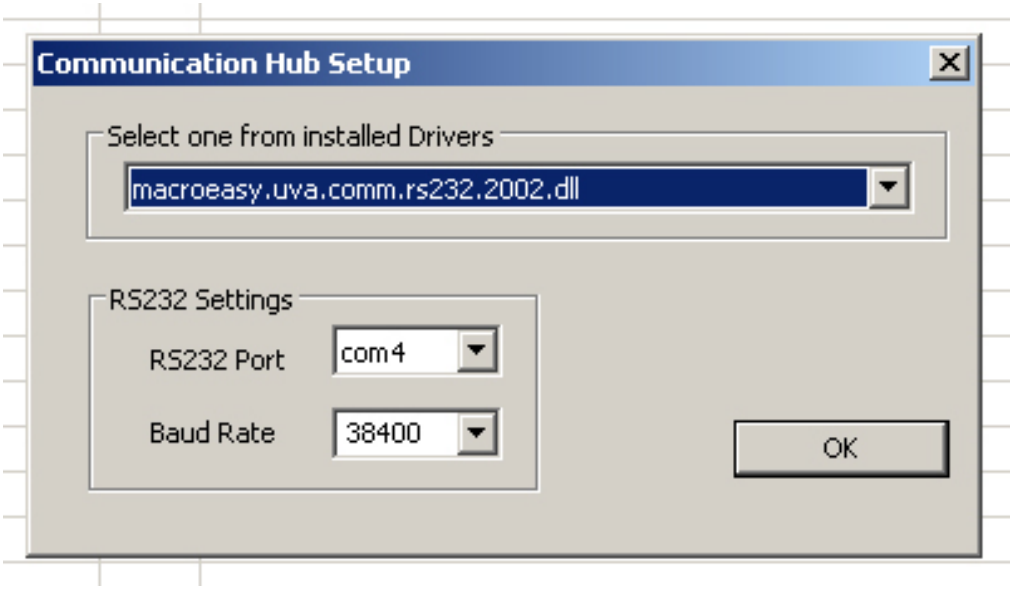


Fig. 3-1

Plug Dongle (Passkey)

Please plug the attached dongle into any USB port of the computer before you turn on the instrument. See Fig 3-3 and Fig 3-4. And DO NOT unplug it during you operate the instrument with the application software.

Note: Please keep the dongle carefully, Contact us at sales@unicosci.com if it is lost and the cost will be charged.

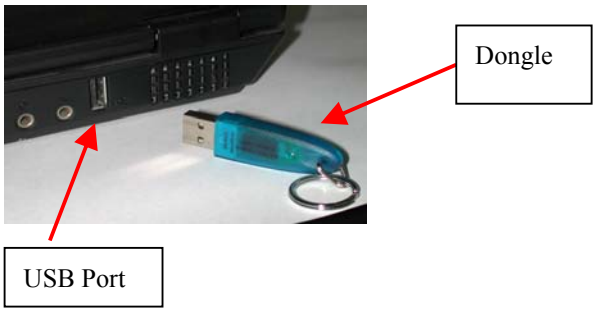


Fig 3-3

Fig 3-4

Single Wavelength Measurement

The UV-Vis Analyst provides a convenient method to measure photometric value at a fixed wavelength.

1. Click  on the toolbar.

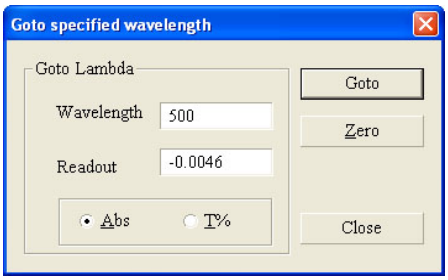


Fig. 4-1

2. Key in the desired wavelength position and click **Goto**. The minimum wavelength step is 0.1nm in a range from 190-1100nm.

3. Place a reference in the sample compartment and click **Zero**.

4. Place a sample in the sample compartment. The wavelength position and photometric value will be displayed in the **Readout** box.

Fixed Point Measurement

This chapter describes how to perform fixed wavelength measurements at 1-20 points and how to analyze unknown compounds against calibration standards.

This section shows how to set up fixed point measurement

1. On the **File** menu, click **New**, the following dialog box will appear. Select **Fixed Points Measurement** and click **OK**.

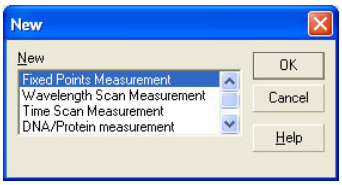


Fig. 5-1

or click  on the toolbar

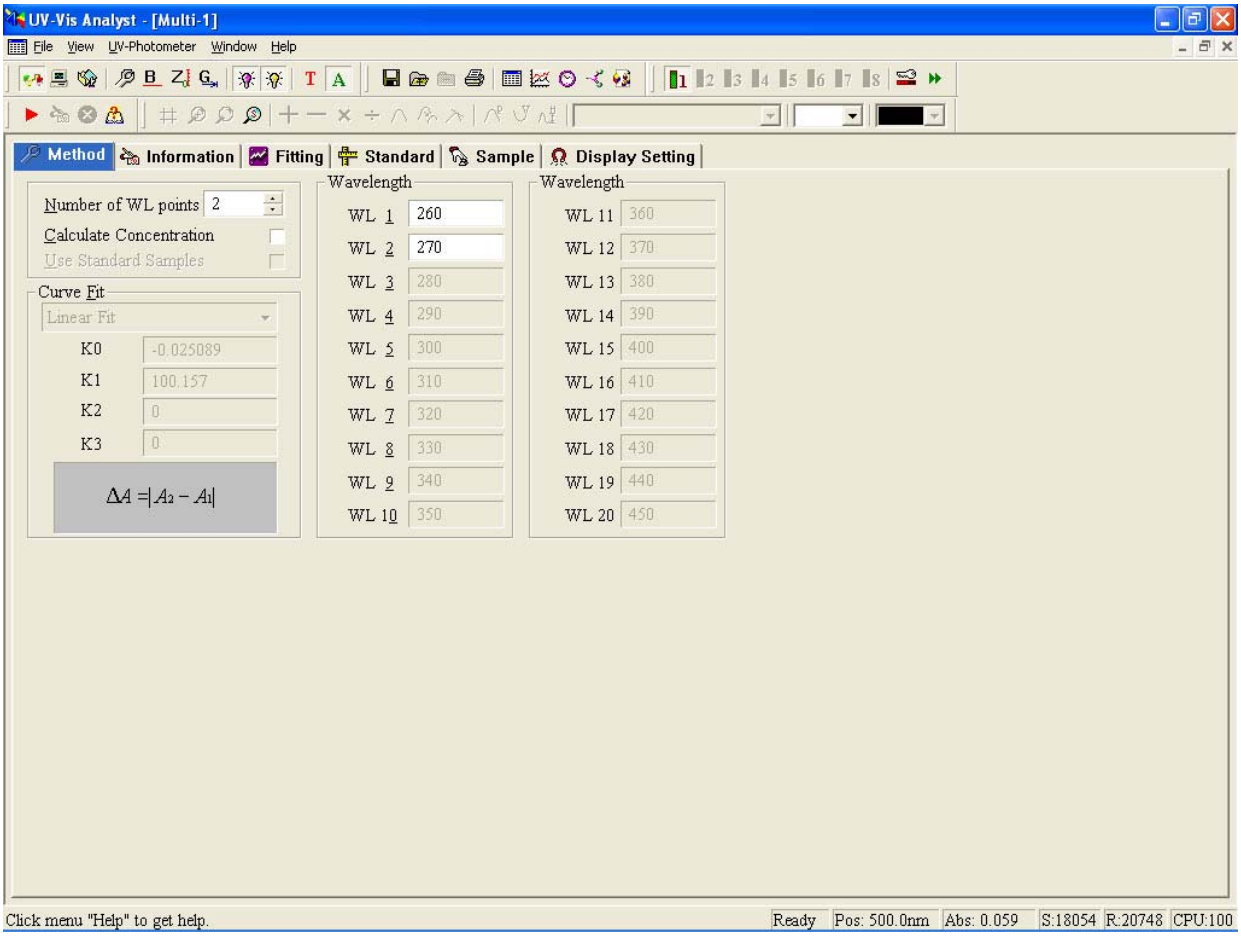


Fig. 5-2

2. Type the number of wavelength points in the **Number of Points** box, or click the **up/down** arrows next to the box set the wavelength points. Leave the two boxes **Calculate Concentration** and **Use Standard Samples** blank.

3. Key in the wavelengths in the **Wavelength** box.

4. Click the **Sample** tab. It will display the following. The control menu contains six buttons: **Start**, **Delete**, **Modify**, **Recalculate**, **Data Font** and **Print**.

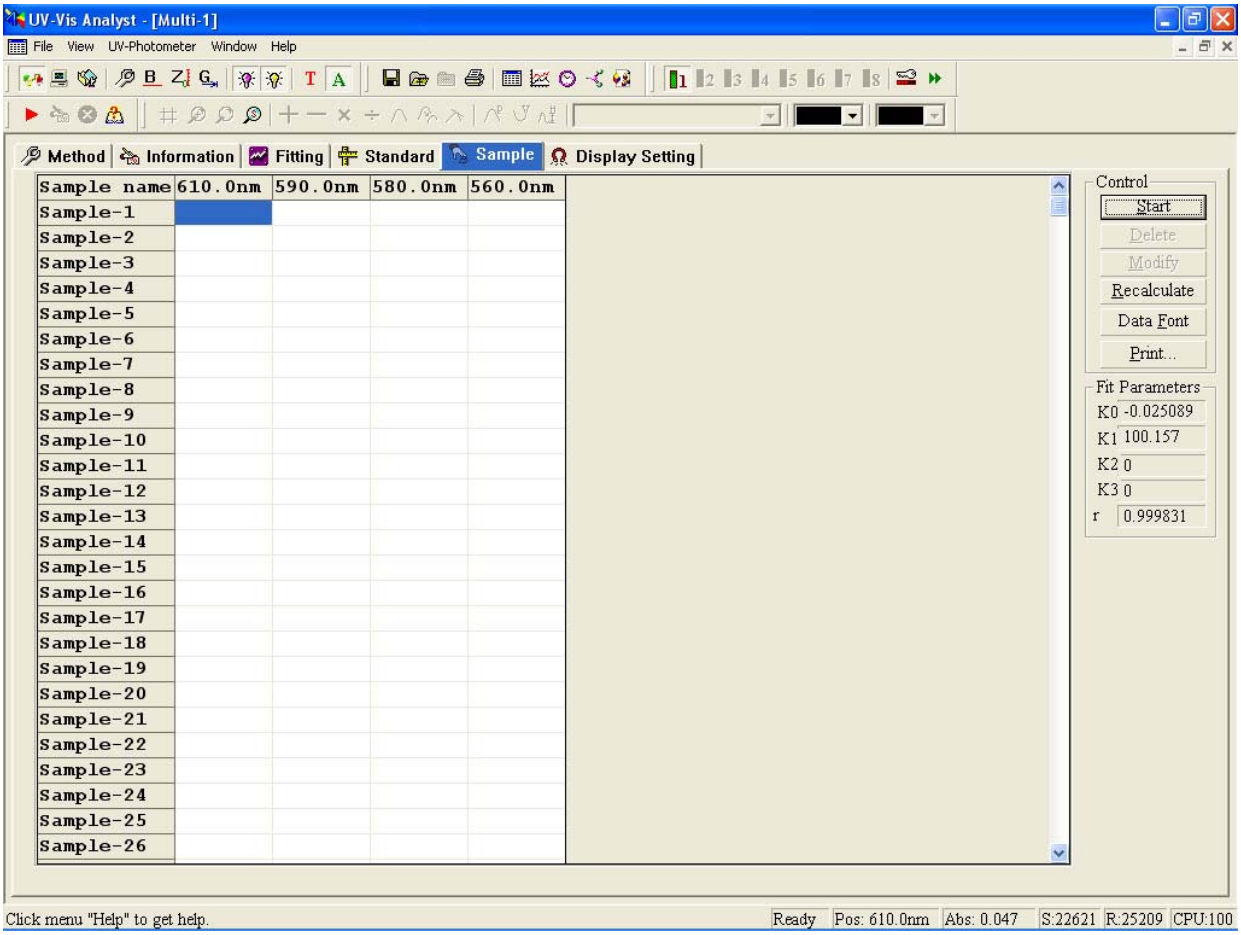


Fig. 5-3

5. Place a blank in the sample compartment.

6. Click  to zero the instrument.

7. Place a sample in the sample compartment.

8. Click **Start** or  to run a new measurement. The display will change to the following.

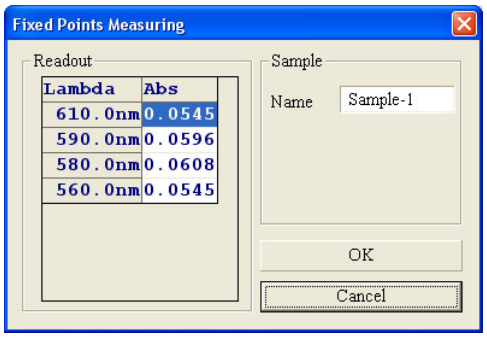


Fig. 5-4

9. The UV-Vis Analyst will read the photometric value of sample 1 at the fixed wavelength automatically. Key in the sample name in the Name box.

10. Click **OK** after the measurement is complete. The photometric data for sample 1 will be listed in the sample table.

11. Repeat steps 7-10 to measure all samples.

12. Click **Print** to print out the table displayed.

Linear Regression Analysis

Method Setup

There are two methods available to set up the linear regression curve. You can use standards to set up the regression curve or just key in the parameters manually. Use the following steps to select the method you wish to use.

1. Click the **Method** tab.

2. Enter the number of wavelength points in the **Number of Points** box, or click the **up/down** arrow next to this box. With 2 wavelengths, the absorbance at the second reference wavelength is subtracted from the first to correct for background absorbance. With 3 wavelengths, the baseline between the first and third wavelengths is calculated and its value at the second wavelength is subtracted from the absorbance at the second wavelength to give the peak height.

3. Key in the wavelengths in the **Wavelength** boxes.

4. Tick the **Calculate Concentration** check box to activate concentration calculation. If you leave this check box blank, you will only get results in absorbance or in % transmittance.

5. Tick the Use Standard Samples check box if you wish to set up the regression curve with prepared standards. Leave this check box blank if you want to use the existing standard curve parameters.

6. Select the curve fit required. Choices available are: Linear fit, Quadratic fit or Cubic fit. At least three standards are required for a Quadratic fit, and four are required for a Cubic fit.

Using Standards for Calibration Curve Setup

This section shows you the procedure of using standards to setup the calibration curve. In the following example, we use two wavelength points which are 260.0 nm and 280.0 nm to set up the regression curve.

1. Click the **Standard** tab.

2. If a blank is prepared, place the cuvette which contains the blank solution in the sample holder. Click  for blank correction.

3. Place Standard 1 in the sample compartment.

4. Click **Start** to run a measurement.

5. Key in the concentration value of Standard 1 in the Conc. box.

6. You can define a new name for the standard in the Name box. Otherwise it will default to **Standard-1**.

7. After the UV-Vis Application Software completes the measurement of Standard 1, click **OK**. The photometric data, △A and concentration will be shown in the standard table. Repeat steps 3-6 to measure all the prepared standards.

8. Incorrect results can be modified or deleted. To do this, click the standard name in the sample column, then click **Delete** (or click ). The following dialog box will be shown on the display.

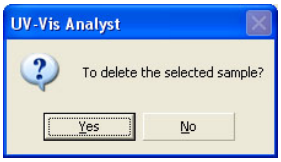


Fig. 5-5

Click **Yes** to delete the standard reading.

9. Click on **Fitting** to see the calibration curve. Note that unless sufficient standards have been used, the previous calibration parameters will not have been updated.

10. Click **Display Setting** tab. This allows you to change the display range and set scale intervals. Annotation can also be added on this page.

After you have changed the display parameters, click **Fitting**, and the display will change to reflect your new settings.

Note: The unit of concentration you set in the above dialog box should be the same as that set in your standards.

Sample Test

The following procedure shows how to read samples

1. Click the **Sample** tab. The screen display will change to this

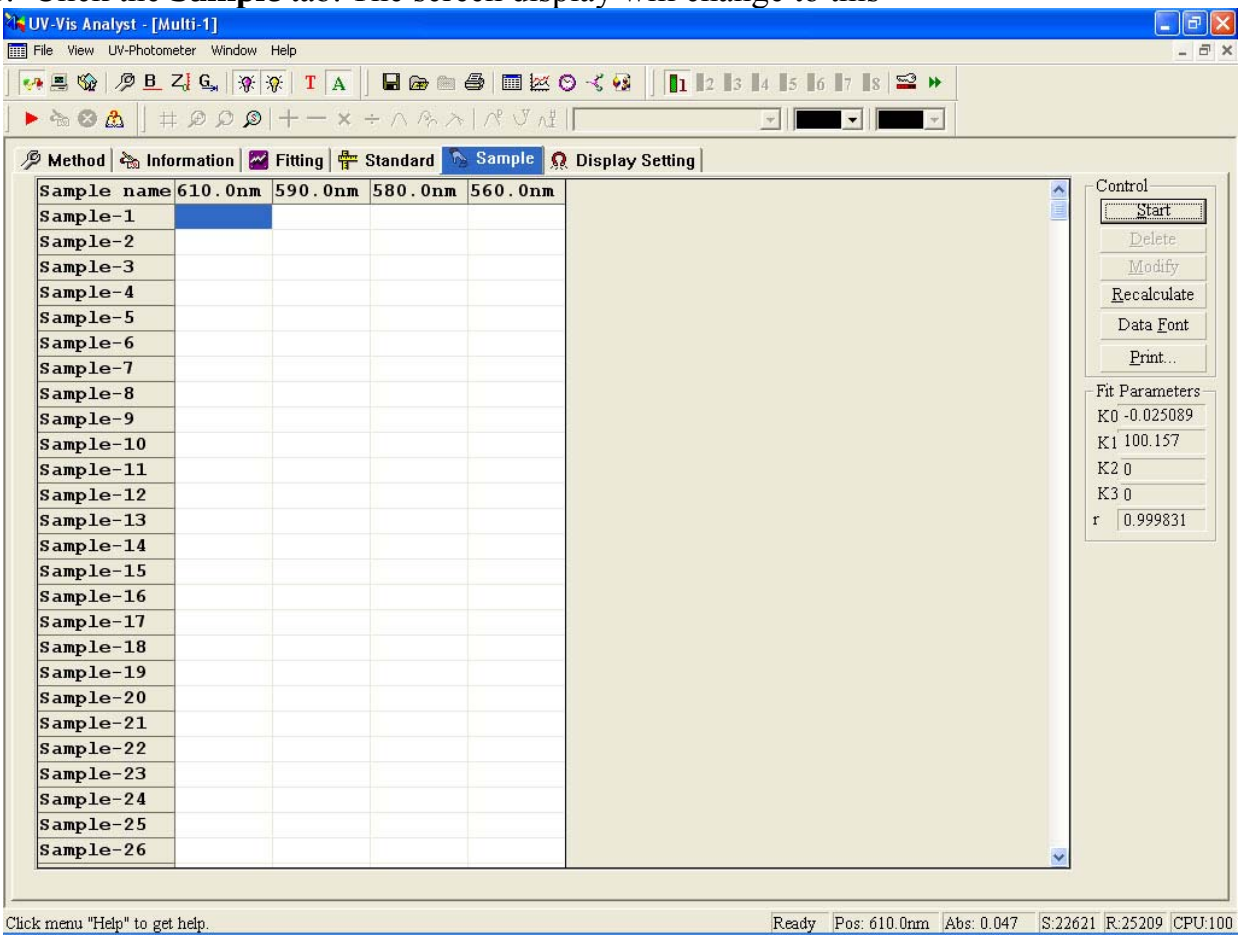


Fig. 5-6

2. Place Sample 1 in the sample cuvette holder.

3. Click **Start** to run a measurement.

4. UV-Vis Application Software will display the photometric value of Sample 1 at the fixed wavelength positions automatically. Type the sample name in the **Name** box. The default is **Sample-1**.

5. Click **OK**. The photometric result for Sample-1 will be listed in the sample data. Delta Abs. and concentration value of Sample-1 will also be displayed in columns 3 and 4.

6. Repeat steps 2-5 to test remaining samples.

7. Click **Print** to print out the table displayed.

Save Files

1. On the File menu, click Save or click the icon on the toolbar. A new dialog box will be displayed.

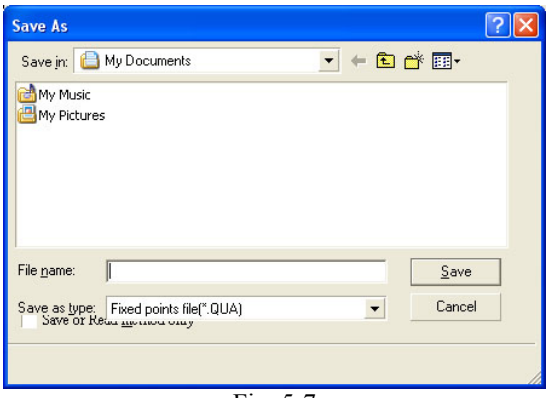


Fig. 5-7

2. Select a folder and key in a file name in the File name box. The file type for fixed points measurement defaults to *.QUA.

3. Click **Save**.

Load Files

1. On the File menu, click Open or click the icon on the toolbar. The display will change to the following.

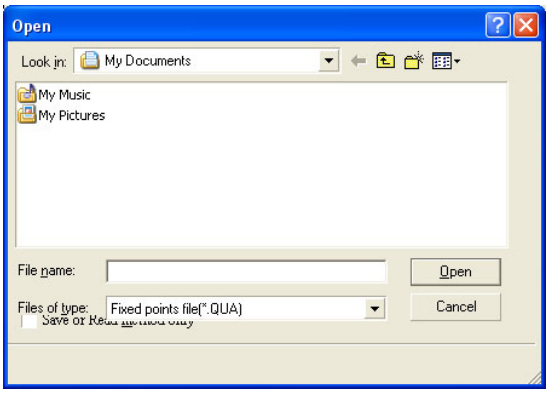


Fig. 5-8

2. Select a folder and filename.

3. Click **OK** to open the selected file.

Wavelength Scanning

This chapter describes how to collect a spectrum while using **Wavelength Scan** function.

Selecting Wavelength Scan Mode

On the **File** menu, click **New**, the following dialog box will appear. Select **Wavelength Scan Measurement** and click **OK**

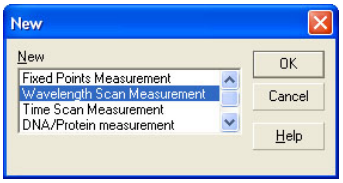


Fig. 6-1

or click  on the toolbar

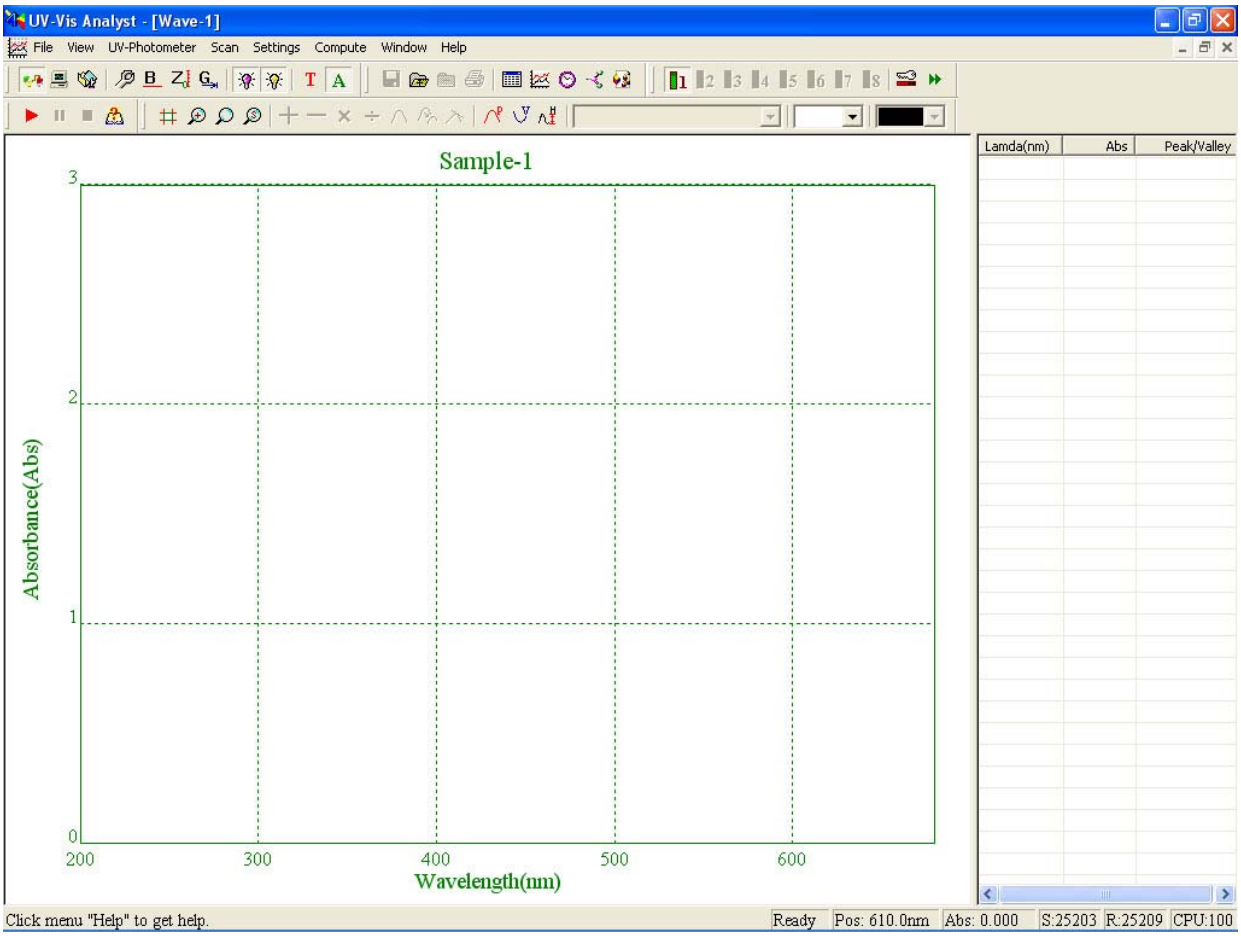


Fig. 6-2

Setting the Lamp Switching Wavelength Position

You can set a new switching point to replace the current one through the following steps:

1. On the **UV-Photometer**, then click **D2/W Switch Point(s)**. The display will change to the following.

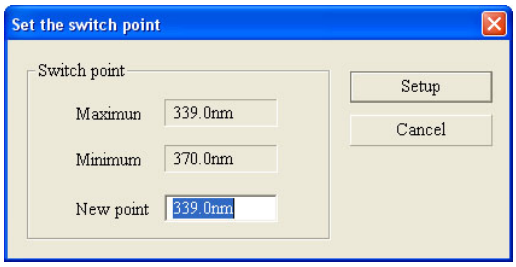


Fig. 6-3

2. Key in the lamp switching wavelength position in the **New point** box. It should be within the range 339 nm to 370 nm.

3. Click **Setup** return to the wavelength scan sub-menu.

Note: If the switching point of the lamps is changed, a new baseline correction must be performed using the **B** icon.

Step by Step Operation

This section describes how to operate the UV-Vis Application Software in the Wavelength Scan Mode.

Selecting Data Acquisition Mode

Use the following steps to select the Data Acquisition mode (%T, Abs) that you wish to use in the wavelength scanning measurement.

Click  on the toolbar to select % transmittance mode or click  to select absorbance mode.

Entering Wavelength Scan Setup Variables

You can use the following steps to set up the variables for wavelength scan.

1. Click  on the toolbar. The display will change.

2. Key in the lower limit of scan range in the **From** box. Acceptable entries range from 190 nm to 1100 nm.

3. Key in the upper limit of scan range in the **To** box. Acceptable entries range from 190 nm to 1100 nm.

4. Click the arrow next to **Step**, and select a scan interval. Six scan intervals can be selected from 0.1nm, 0.2 nm, 0.5 nm, 1.0nm, 2.0nm and 5.0 nm.

5. Select a smoothing filter value.

6. Click **OK** return to the wavelength scan sub-menu.

Collecting a Spectrum in Wavelength Scan

Once you have set up the operation conditions for wavelength scanning you are ready to collect a spectrum.

The following procedure shows you how to collect a spectrum.

1. Place a blank in the sample cuvette holder. Close the cover of the sample compartment.

2. Click  to scan the baseline.

3. Place a sample in the sample cuvette holder. Close the cover of the sample compartment.

4. Click  on the toolbar. The instrument will start scanning automatically.

5. If you wish to stop scanning for any reason, click  on the toolbar.

6. The real time spectrum will be displayed on the screen during scanning.

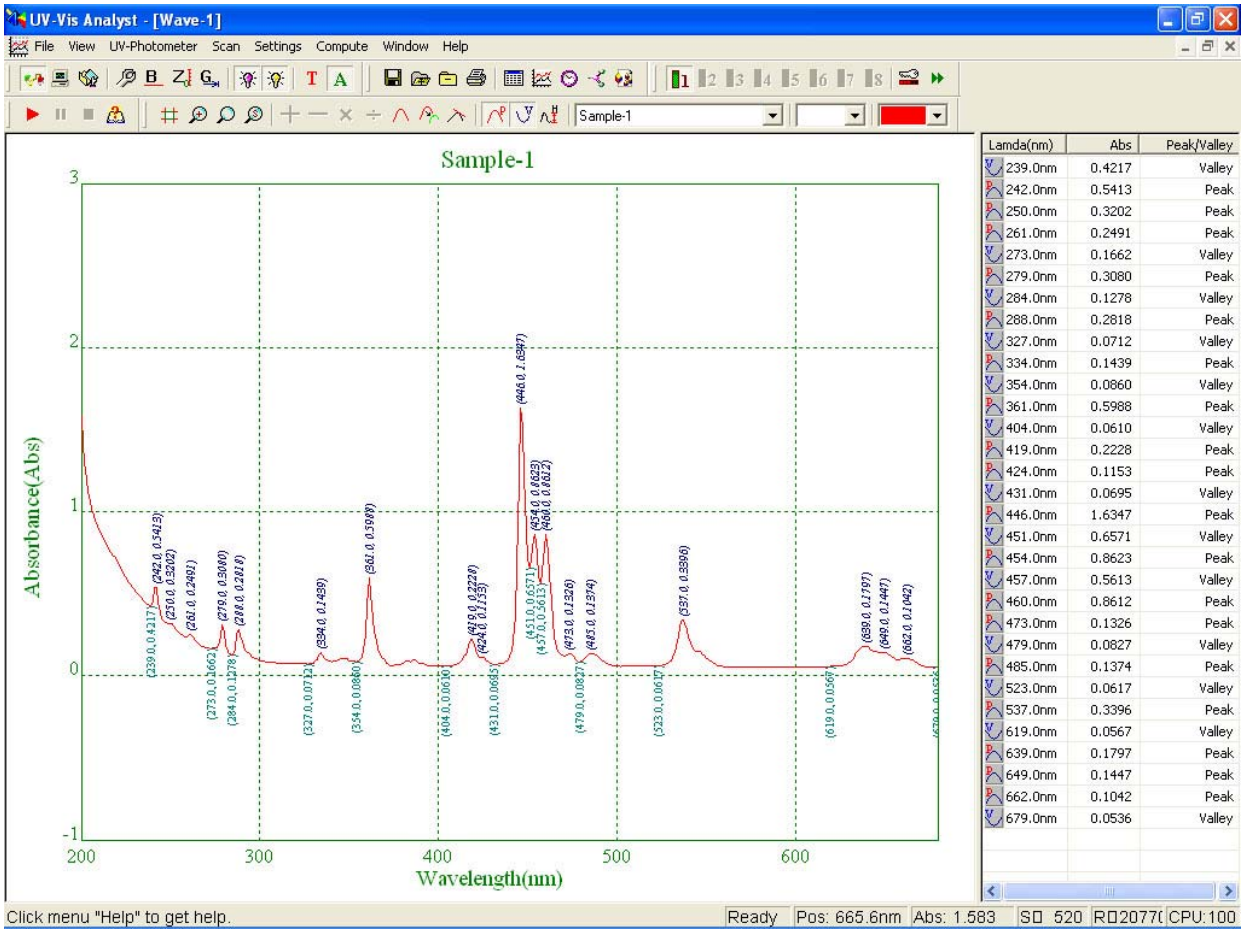


Fig. 6-4

If you click the right mouse button on this screen, various functions will be displayed on a drop-down menu.

File—this will allow you to:

- Load
- Save as
- Remove
- Open file from UV-Spectrophotometer
- Print
- Print setup

View—this will allow you to view:

- Toolbar
- Status Bar
- Status of Spectrophotometer
- Status Font

UV-Spectrometer—this will allow you to:

- Link Spectrophotometer
- Escape
- Background
- Auto zero
- Spectral slitwidth—allows you to perform slitwidth test
- W lamp—turn tungsten lamp ON/OFF
- D_2 lamp—turn D_2 lamp ON/OFF

Scan—this allows you to:

- Start
- Stop
- D_2 Spectral Slitwidth or Energy Scan

Customize—contains sub-pages that allow you to:

- **View**—Set the minimum and maximum (Abs or %T) axes you require to view your scan. The minimum and maximum wavelength axes can also be set.
- **Peak and Valley**—Label any peaks and valleys in your spectrum and allows you to choose the font, colour (for colour printers) and size of the labels. Note—see page 41 on setting threshold for these peaks.
- **Legend**—Change the X/Y axis font and sample name and font (if required). The colour of this text can also be changed (for colour printers).
- **Special**—Choose color required for a scan (for use with a plotter)
- **Scalar**—Manually set the interval range of both the X and Y axes. Also gives you the choice of grid lines ON/OFF as well as changing the color of the grid lines (for colour printers). Text font, size and colour (for colour printers) may be set at the X and Y axis increments.
- **Print**—Add a footnote to the scan. The text font, size and colour (for colour printers) can also be selected.
- **Memo**—Define memory information for printout.

Baseline

During scanning, the unit will use the system baseline which was checked during system initialization. For particular experiments where the background matrix is a strong absorber, we suggest you run the baseline again using these steps.

1. Place a sample cuvette which contains a reference or blank solution in the sample cuvette holder.

2. On the **UV-Photometer** menu, click **Autozero**, or click  on the toolbar.

The unit will begin the collection of a baseline automatically. The new baseline will be

stored in the baseline memory and will be used in all subsequent experiments until you run a new baseline.

Spectrum Processing

Introduction:

Once you have acquired and displayed a spectrum, the following options are available.

1. RESCALE
2. ZOOM
3. PEAKS & VALLEYS
4. TRACE
5. ARITHMETIC PROCESS
6. FILES

The following table shows you the general functions of spectrum processing.

Option	Variable	Range	Function
RESCALE	X-Axis Y-Axis	190 to 1100nm -1 to 3	Reset the display scale of a spectrum
ZOOM	X-Axis Y-Axis	190 to 1100 nm -1 to 3	Expands either or both axes for more detailed viewing
PEAKS AND VALLEYS	TABLE THRESHOLD	ABS=0.001 to 1.000 in 0.001 increments. % T=0.1 to 100.0 in 0.1 increments	List the peaks and Valleys of a spectrum List the Y-Axis values over which the instrument detects a peak or valley
TRACE			Permits reading of values from the on-screen spectrum using the cursor
ARITHMETIC PROCESS	A+B A-B A*B A/B DERIV		Sum of two spectra Subtracts one spectrum from another Product of two spectra Divide one spectrum by another Displays a 1st through 4th order derivative
FILES	SAVE LOAD UNLOAD		Save the current processing spectrum Load a previously saved spectrum Remove a spectrum from display

Select a Current Spectrum

As UV-Vis Application Software can display several spectra overlaid on the screen, you should specify the spectrum you wish to process.

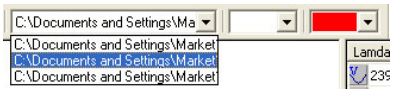


Fig. 6-5

1. Click the **down** arrow. All spectra will be listed in the pull-down menu.

2. Click the spectrum you want to select. Its name will be listed in the Name Box and will be referred to as **Current Spectrum**.

Rescale

The following steps show you how to change the display range of a spectrum.

1. On the **Settings** menu, click **Display Range**. or click  on the toolbar (or click the right mouse button when over the scan window. The screen will change as follows.

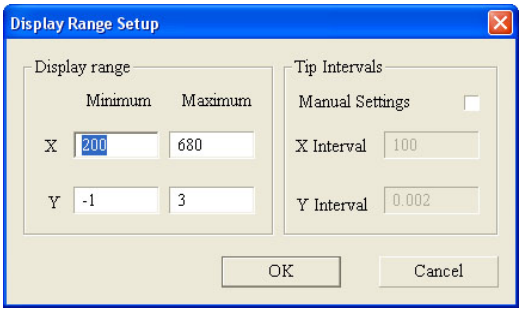


Fig. 6-6

2. Key in the display range variables for x-axis and y-axis. The maximum range for X-axis is from 190 to 1100 and the maximum range for Y-axis is from -1 to 3.

3. You can also set display intervals on both X and Y axes. To do this, first tick the box of Manual Settings and then key in the intervals.

4. Click **OK**.

Note: Click  on the toolbar to restore the default display settings.

Zoom

Using a mouse, you can easily zoom in to part of the spectrum.

1. Click  on the toolbar.

2. Position the cursor in the upper-left corner of the area you want to select.

3. Hold the left mouse button to drag the cursor to outline the spectrum area you want to enlarge.

4. Release the mouse button. The part of the spectrum which is displayed within the outlined area will be enlarged. Click  to undo scale. To zoom again, click twice  (once to cancel and once to re-activate).

The following is an example of this function.

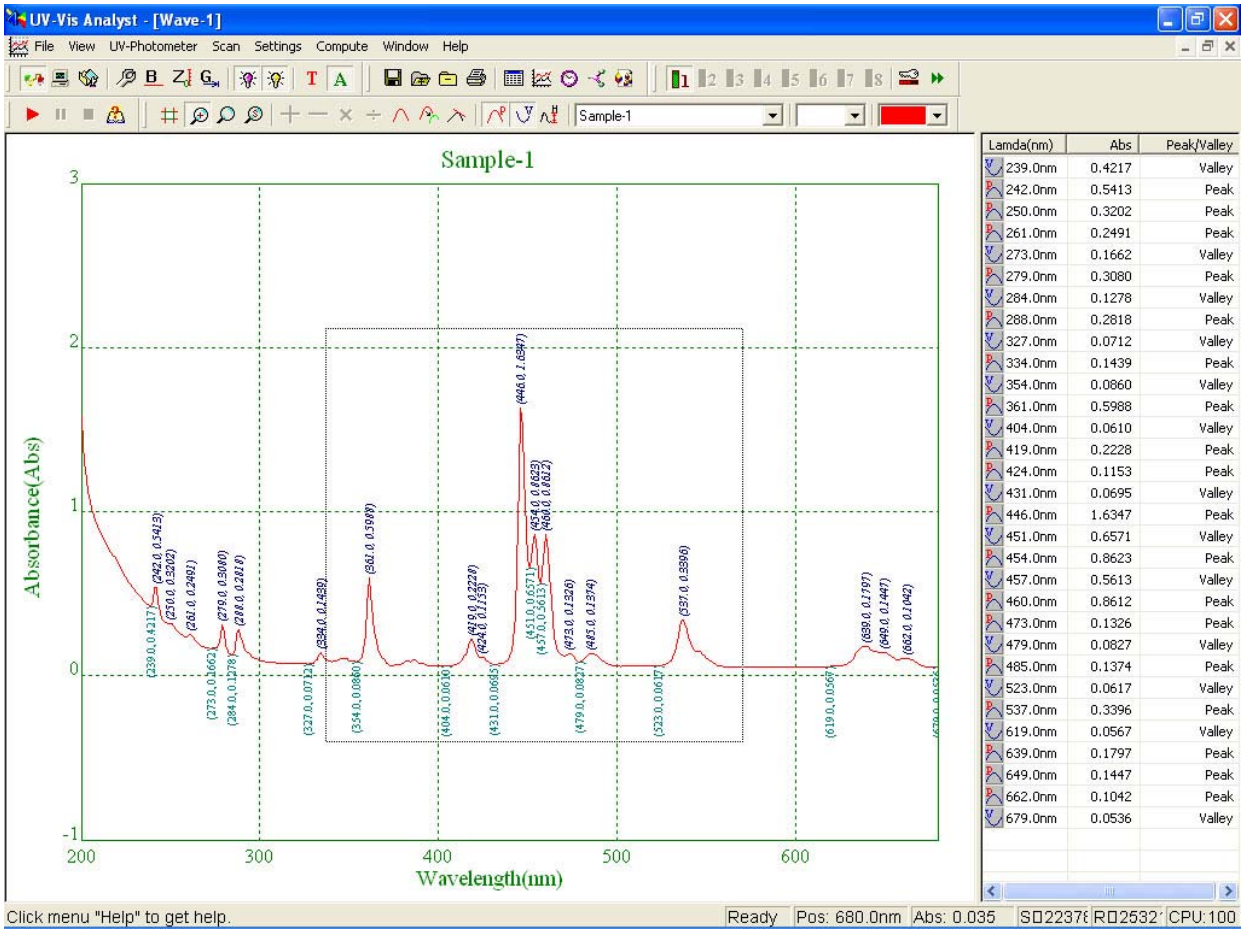


Fig. 6-7

Peaks & Valleys

List the Peaks and Valleys of a spectrum

Once a spectrum is displayed on the screen and is selected as the Current Spectrum:

1. On the **View** menu, click **Peaks**, or click  on the toolbar, All peaks detected will

be listed in a table format beside the spectrum.

2. On the **View** menu, click **Valleys,** or click  on the Toolbar. Valleys of the spectrum displayed will be listed. Following is an example of this function.

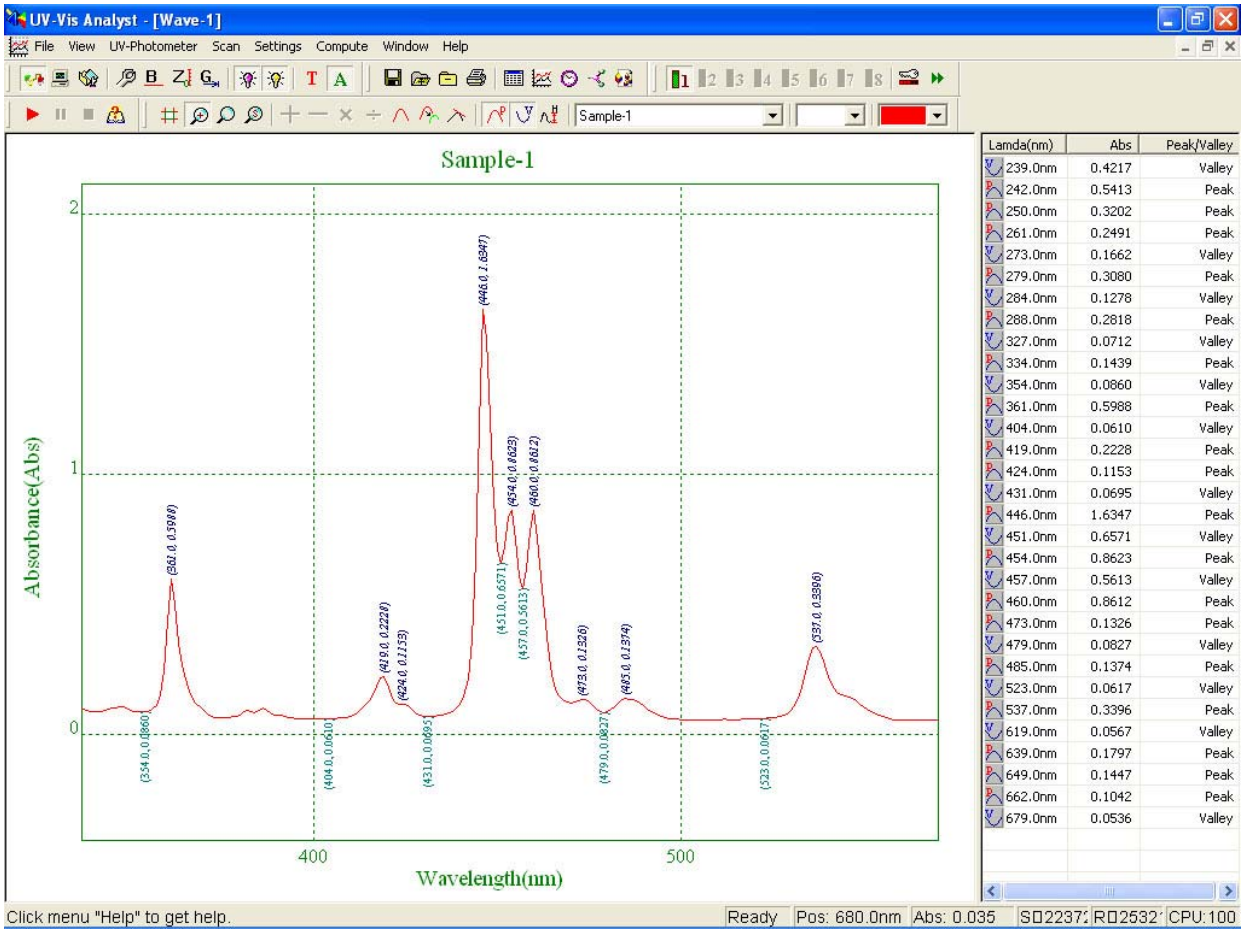


Fig. 6-8

Peaks are listed above the spectrum, while valleys are listed below it.

Threshold

The threshold value measures the absorbance from a valley to peak. If the value is greater than the one you choose for Threshold, the instrument will detect smaller peaks and even background noise if you lower the value far enough.

The UV-Vis Application Software allows you to change the threshold value used in peak and valley detection. On the **Settings** menu, click **Peak Height**, or click  , the following dialog box will be displayed.

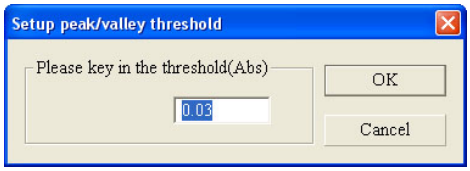


Fig. 6-9

Type the threshold value in the box and click **OK**. UV-Vis Application Software will then use the new threshold to detect peaks and valleys.

Note: A setting of 0 will basically label every data point. The larger the value, the more data points, and only the larger peaks will be labeled.

Trace

1. Once a spectrum is displayed on the screen and it is selected as the Current Spectrum, go to the **View** menu, click **Search**, or click  on the toolbar. The display will change to.

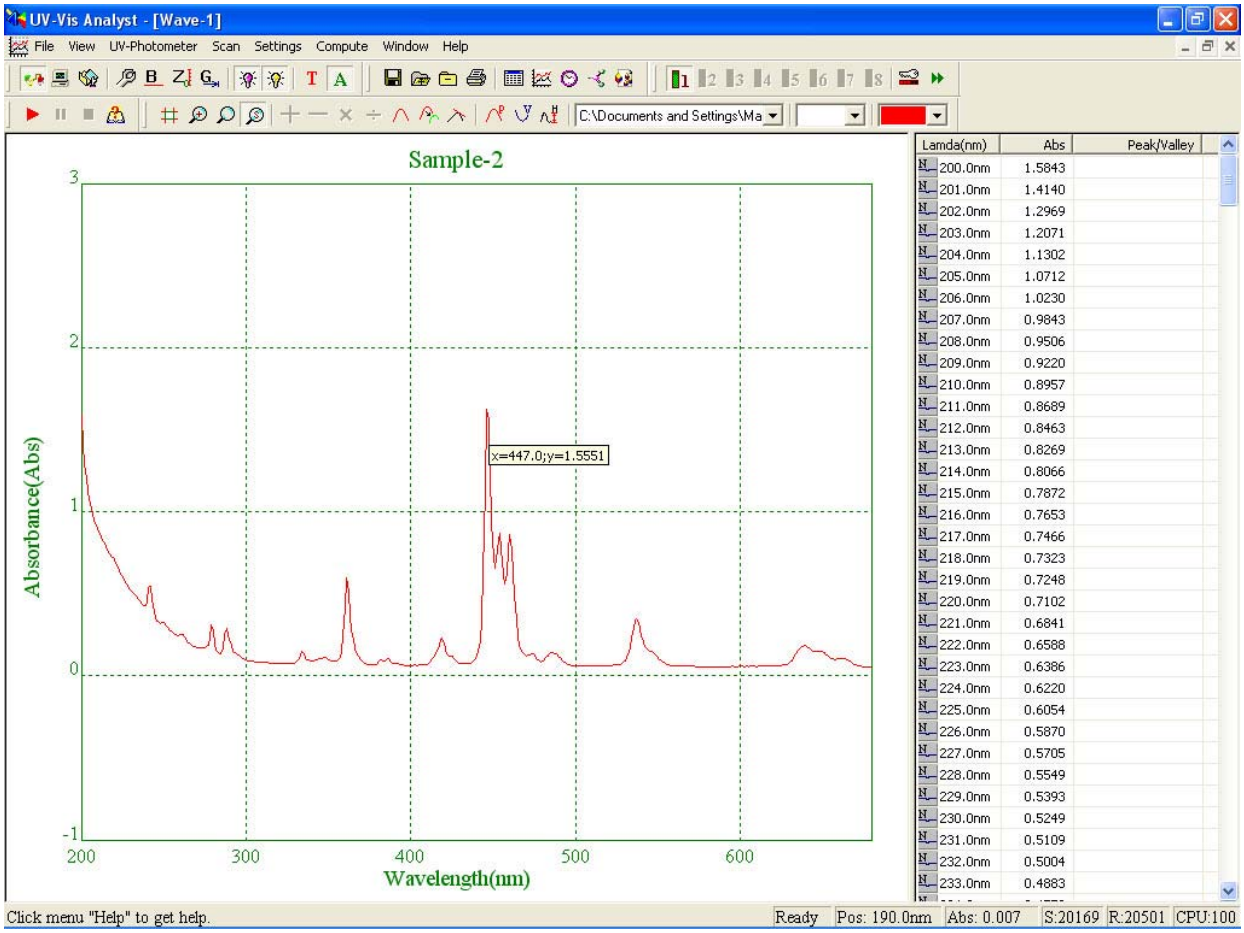


Fig. 6-10

2. A crosshair cursor will appear with x and y axes values displayed.

3. Move the crosshair cursor left or right on the spectrum.

4. The data in the cursor window indicate the X-axis and Y-axis values for the current cursor location.

5. Double click the left mouse button to release the crosshair cursor.

Note: To accurately set the crosshair, you can use the ←, → buttons.

Derivative

1. Once a spectrum is displayed on the screen and it is selected as the Current Spectrum, then on the **Compute** menu, click **Derivative**, or click  on the toolbar. The following dialogue box will be displayed.

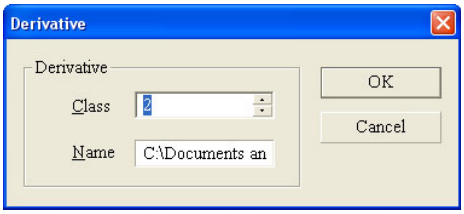


Fig. 6-11

2. Key in the class of derivative (1-10, depending on whether 1st, 2nd, … 10th derivative is required) and type a name for the result spectrum, then click **OK**. The result spectrum will be displayed overlaid with the original one.

Smooth

Once a spectrum is displayed on the screen and it is selected as the Current Spectrum, then on the **Compute** menu, click **Smooth**, or click  on the toolbar.

Resample

1. Once a spectrum is displayed on the screen and it is selected as the Current Spectrum, then on the **Compute** menu, click **Resample**, or click  on the toolbar. The following dialogue box will be displayed.

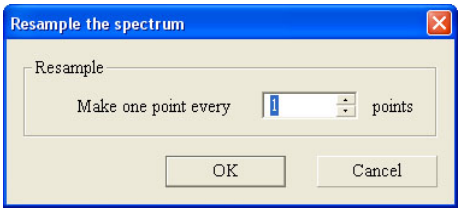


Fig. 6-12

2. Click **Up/Down** arrow to select Sample times.

3. Click **OK**.

Adding Spectra

Adding spectra can assist in the development of artificial spectra in multi-component mixtures.

UV-Vis Application Software will only add two spectra that are already displayed on the screen. Before arithmetic processing, load two spectra from memory. In the following example, we have two spectra saved in directory "C:\Documents and settings\Market", which are "Sample1.sca" and "Sample2.sca".

1. On the **Compute** menu, click **Add**, or click  on the toolbar. The following dialogue box will be displayed.

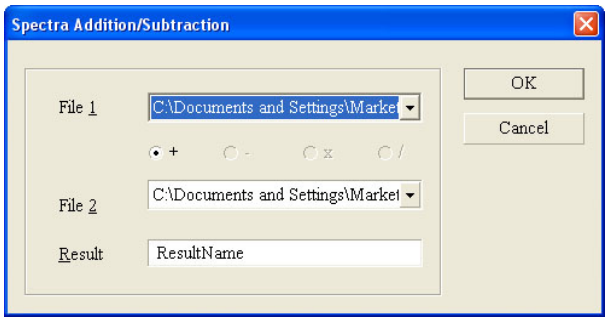


Fig. 6-13

2. Click the **down** arrow next to **Source 1** to select a spectrum and define it as source 1. Select a spectrum for **Source 2** in the same way. UV-Vis Application Software will not allow you to select a spectrum not displayed on the screen or select the same spectrum twice.

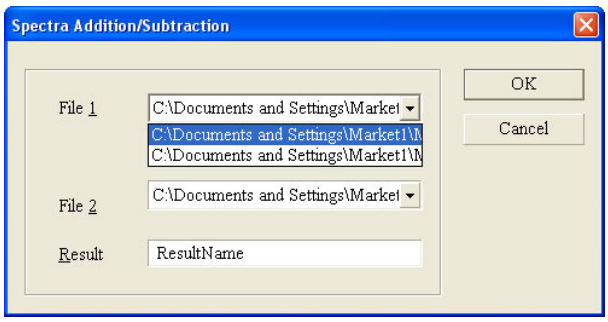


Fig. 6-14

3. Key in a name for the **Result** spectrum and click **OK**. The unit will start processing with the result displayed on the screen.

Spectral Subtraction

Subtracting one spectrum from another has been a classical technique to offset spectral interference from the spectrum of interest.

UV-Vis Application Software will only process the subtraction of two spectra that are already displayed on the screen. Before arithmetic processing, load two spectra from memory. In the following example, we have two spectra saved in directory "C:\Documents and settings\Market", they are "Sample1.sca" and "Sample2.sca".

1. On the **Compute** menu, click **Sub**, or click  on the toolbar. The following dialogue box will be displayed.

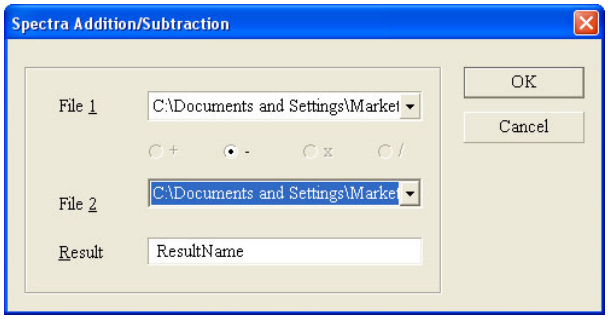


Fig. 6-15

2. Click the **down** arrow next to **Source 1** to select a spectrum and define it as source 1. Select a spectrum for **Source 2** in the same way. UV-Vis Application Software will not allow you to select a spectrum not displayed on the screen or select the same spectrum twice.

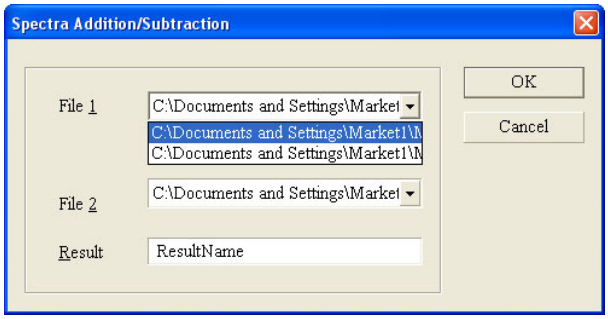


Fig. 6-16

3. Key in a name for the Result spectrum and click **OK**. The UV-Vis Application Software will start processing with the result displayed on the screen.

Spectral multiplication

Multiplying spectra can assist in the development of artificial structure of spectra in multi-component mixtures.

UV-Vis Application Software will only multiply two spectra that are already displayed on the screen. Before arithmetic processing, load two spectra from memory. In the following example, we have two spectra saved in directory “C:\Documents and settings\Market”, they are “Sample1.sca” and “Sample2.sca”.

1. On the **Compute** menu, click **Multiply**, or click  on the toolbar. The following dialogue box will be displayed.

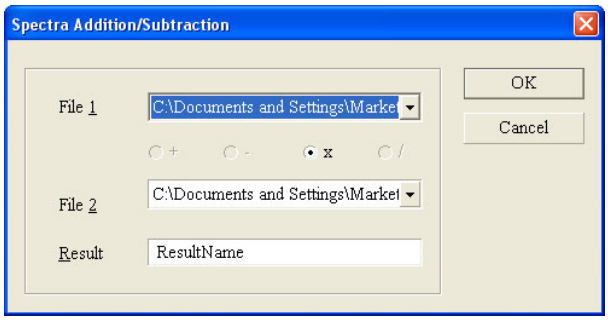


Fig. 6-17

2. Click the **down** arrow next to **Source 1** to select a spectrum and define it as source 1. Select a spectrum for **Source 2** in the same way. UV-Vis Application Software will not allow you to select a spectrum not displayed on the screen or select the same spectrum twice.

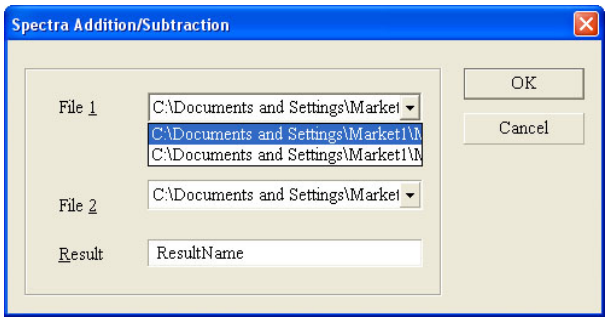


Fig. 6-18

3. Key in a name for the Result spectrum and click **OK**. The UV-Vis Application Software will start processing with the result displayed on the screen.

Spectral division

Dividing one spectrum from another has been a classical technique to offset spectral interference from the spectrum of interest.

UV-Vis Application Software will only process the division of two spectra that are already displayed on the screen. Before arithmetic processing, load two spectra from memory. In the following example, we have two spectra saved in directory “C:\Documents and settings\Market”, they are “Sample1.sca” and “Sample2.sca”.

1. On the **Compute** menu, click **Divide**, or click  on the toolbar. The following dialogue box will be displayed.

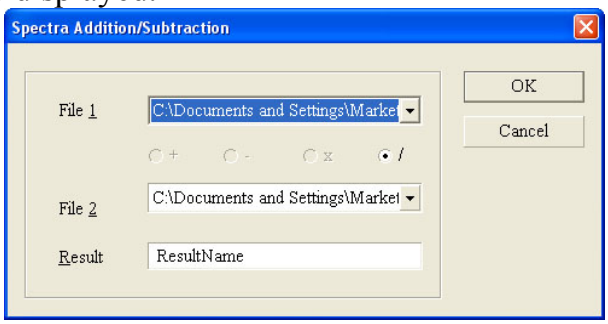


Fig. 6-19

2. Click the **down** arrow next to **Source 1** to select a spectrum and define it as source 1. Select a spectrum for **Source 2** in the same way. UV-Vis Application Software will not allow you to select a spectrum not displayed on the screen or select the same spectrum twice.

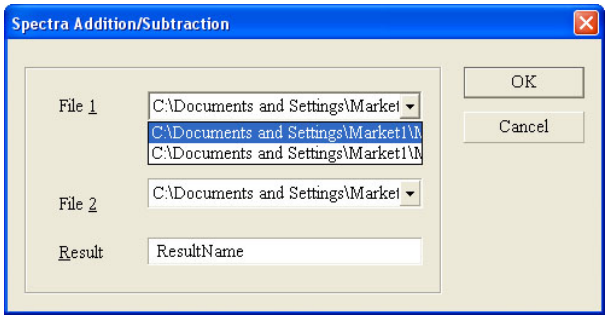


Fig. 6-20

3. Key in a name for the Result spectrum and click **OK**. The UV-Vis Application Software will start processing with the result displayed on the screen.

Save a Spectrum

1. On the **File** menu, click **Save**, or click  on the toolbar. The screen will display the following.

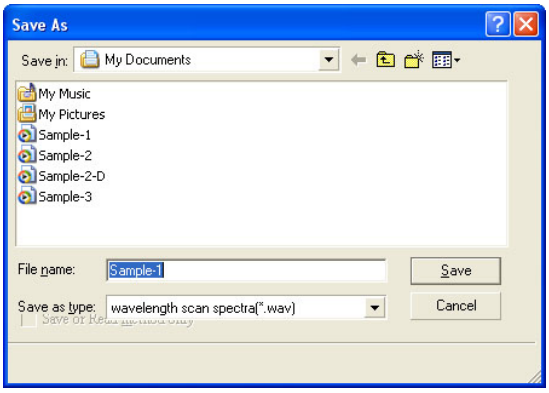


Fig. 6-21

2. Select a folder and key in a file name in the **File name** box. The default file type for wavelength scanning is *. sca.

3. Click **Save**.

Load a Spectrum

1. Click  on the toolbar. The screen will display the following.

2. Select the directory, then select the file name.

3. Click **Open**.

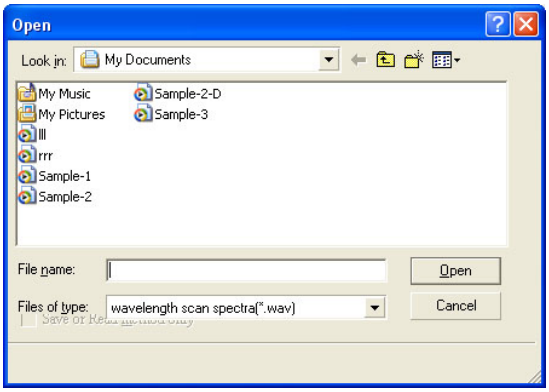


Fig. 6-22

Delete a Spectrum

You can delete a spectrum if you do not want it displayed on the screen.
For example, two spectra are displayed on the screen. They are Sample1.sca and Sample2.sca and we want to remove Sample2.sca from the screen.

1. Click the **down** arrow. All spectra displayed will be listed in the pull-down menu.

2. Click **Sample2.sca** and select it as the **Current Spectrum**.

3. Click  on the toolbar, **Sample2.sca** will be removed from the display. This will not remove the spectrum from memory.

Time Scanning (Kinetic Analysis)

Introduction:

This chapter tells you how to obtain the absorbance or transmittance value for a sample as a function of time at a given wavelength.

Selecting Time Scan Mode

On the **File** menu, click **New**, the following dialog box will appear.

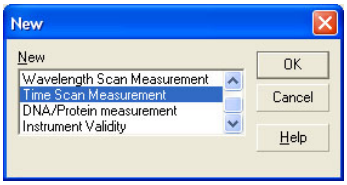


Fig. 7-1

or click  on the toolbar.

The screen will display the time scan interface as shown below.

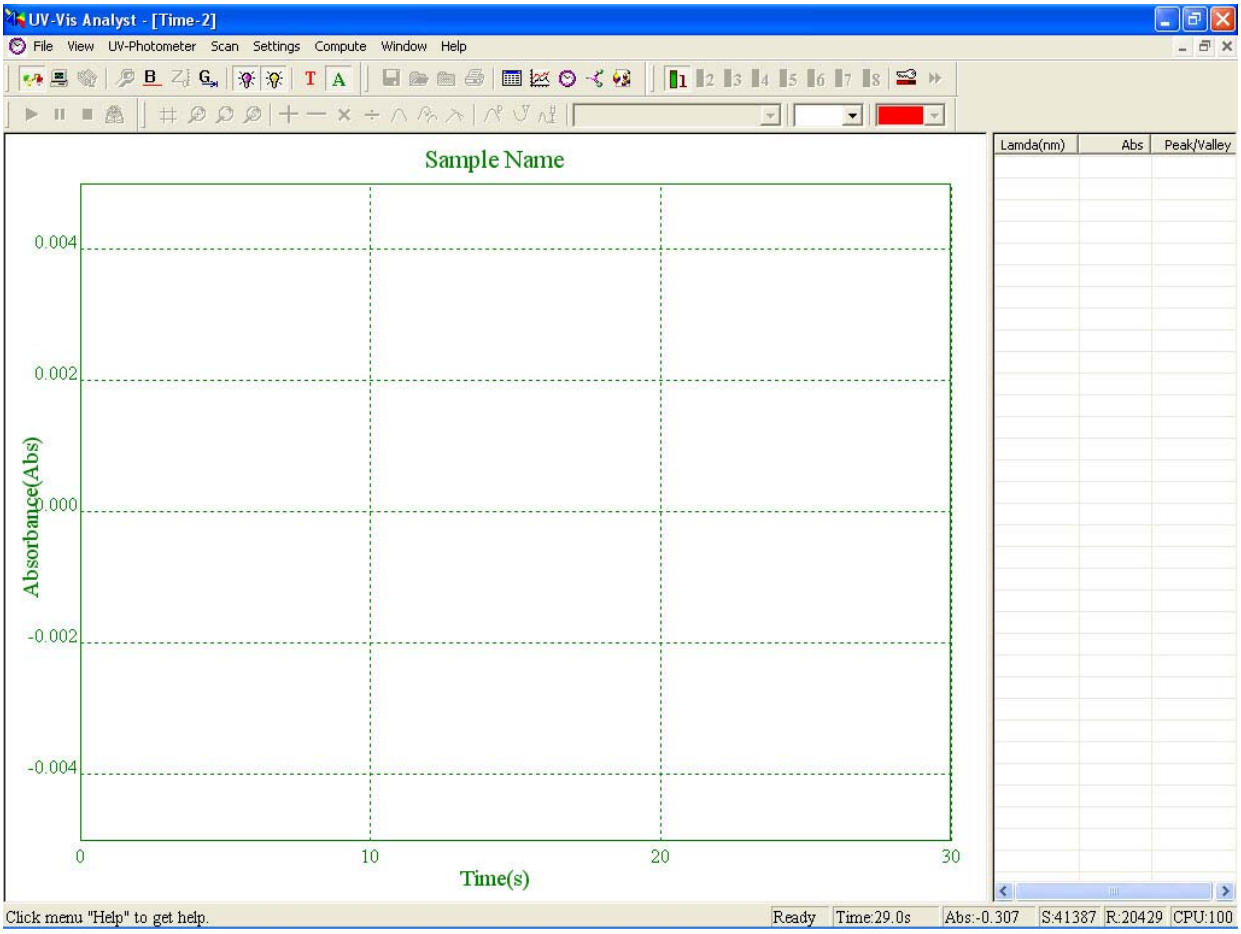


Fig. 7-2

Step by Step Operation

This section describes how to operate the UV-Vis Application Software in the Time Scan Mode.

Selecting Data Acquisition Mode

Click  on the toolbar to select the % transmittance mode
Or

Click  to select the absorbance mode.

Entering Time Scan Setup Variables

You can use the following steps to set up the variables for time scan.

1. Click  on the toolbar. A dialogue box will be displayed.

2. Key in the wavelength, total time (in seconds) and scan step in the above dialog box. The wavelength range should be within 190 to 1100 nm. The upper limit for total time is 100,000 seconds. Seven scan intervals can be selected from 0.5S, 1S, 2S, 5S, 10S, 30S and 60S.

3. Click **OK**, the screen will return to the Time Scan sub-menu.

Collecting a Time Scan Graph

Once the operation conditions have been set up, you are ready to collect a time scan.
To collect a time scan, follow this procedure:

1. Place a blank solution in the sample cuvette holder. On the **UV-Photometer** menu, click **Autozero**, or click  on the toolbar.

2. Take out the blank in the sample holder, place a sample in it and close the cover.

3. Click  on the toolbar. The instrument will start scanning automatically.
4. You can stop scanning by clicking  .

5. The graph will be displayed on the screen during time scanning.

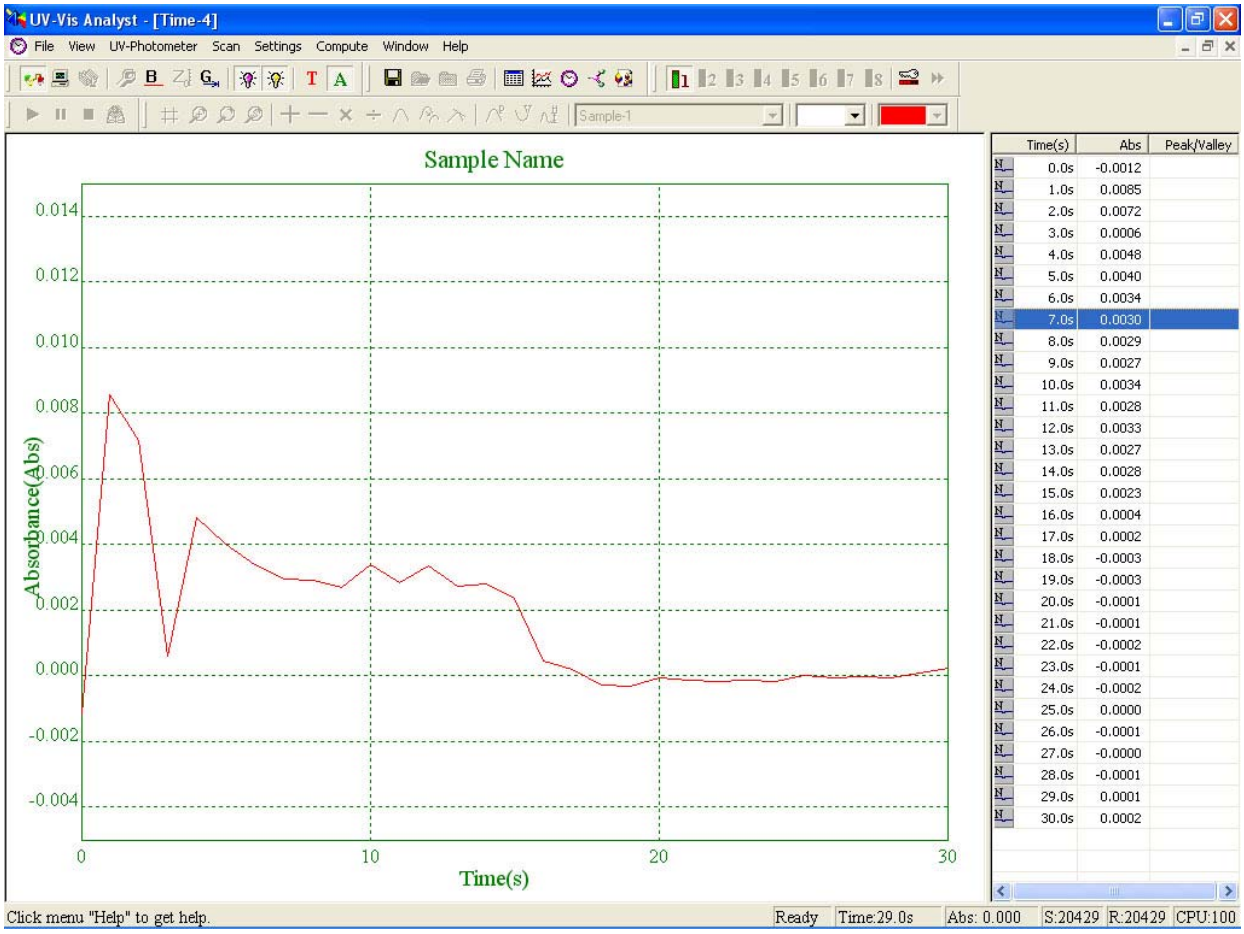


Fig. 7-4

For rate measurement, right click to produce dialog box. Click on **Customize**. Select Dynamic Analysis.

Enter Begin and End Times and Factor to calculate the rate in International Units.

Graph Processing

Introduction:

After you have acquired and displayed a timescan, the following options are available (**For operation, refer to the same chapter of the Wavelength scan**):

1. RESCALE
2. PEAKS & VALLEYS
3. TRACE
4. ARITHMETIC PROCESS
5. FILES

The following table shows you the general functions of graph processing.

Option	Variable	Range	Function
RESCALE	X-Axis Y-Axis	0 to 100000(seconds) -1 to 3	Expands either or both axes for more detailed viewing
PEAKS AND VALLEYS	TABLE THRESHOLD	ABS=0.001-1.000 in 0.01 increments %T=0.1-100.0 in 0.1 increments	List out the peaks and valleys of a spectrum List the Y-Axis values over which the instrument detects a peak or valley
TRACE			Permits reading of values from the on-screen spectrum using the cursor
PROCESS	DERIV		Displays a 1st through 4th order derivative spectrum
FILES	SAVE LOAD UNLOAD		Save the current processing spectrum load a previously Saved spectrum Remove a spectrum from display

DNA/Protein Measurement

This chapter describes how to perform DNA/Protein measurement.

Selecting DNA/Protein Measurement

On the **File** menu, click **New**, the following dialog box will appear. Select **DNA/Protein Measurement** and click **OK**.

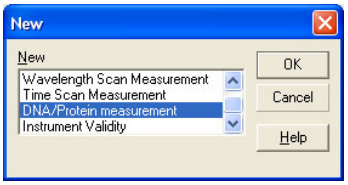


Fig. 8-1

or click  on the toolbar

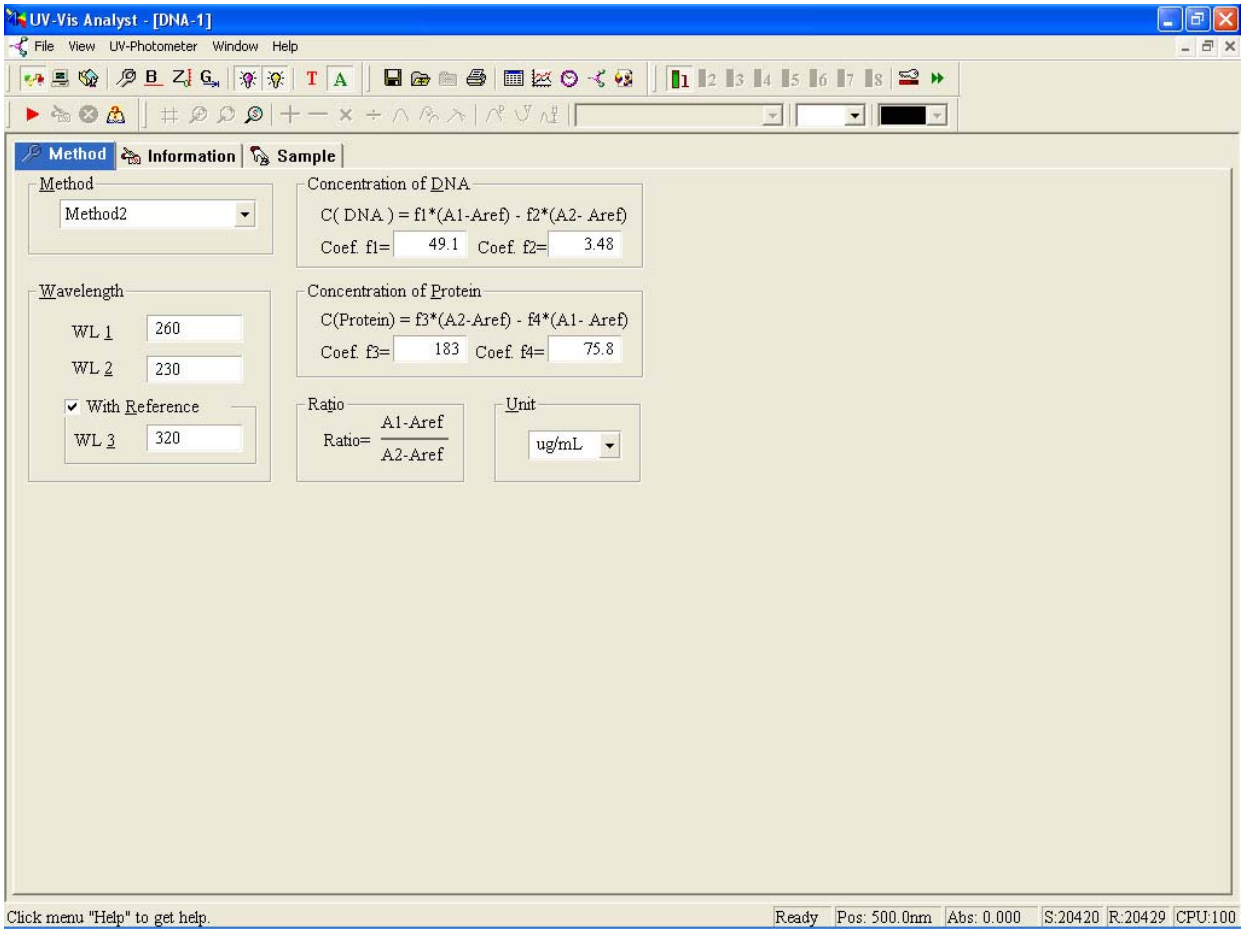


Fig. 8-2

Step by Step Operation

1. Click the **down** arrows of the **method** to select the **test method**.

2. Key in the wavelength position in the **Wavelength** box.

3. Key in the value of **DNA/Protein Conc**.

4. Click the **Sample** tab. It will display the following. The control menu contains six buttons: **Start**, **Delete**, **Modify**, **Recalculate**, **Font** and **Print**.

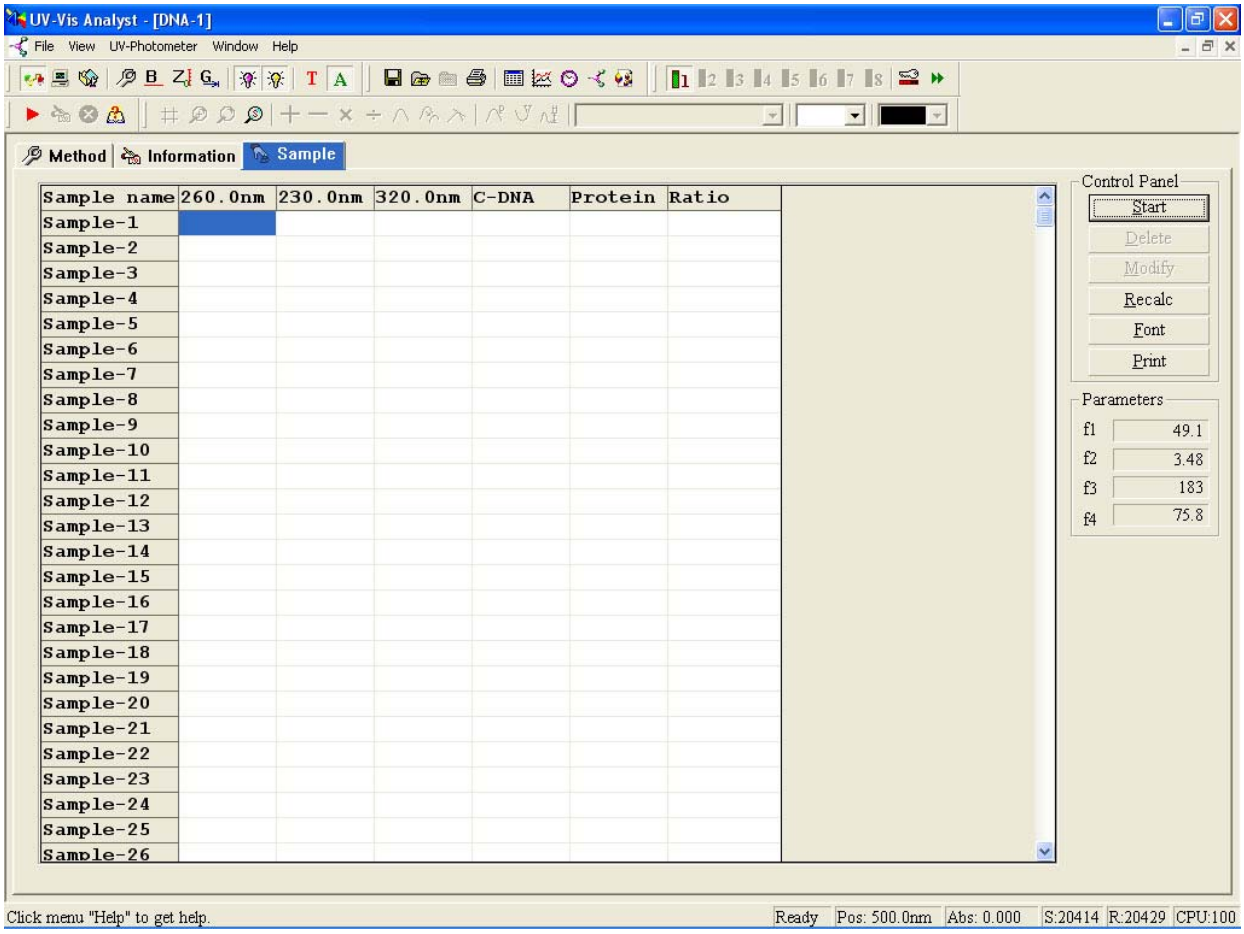


Fig. 8-3

5. Place a blank in the sample compartment.

6. Click  to zero the readings.

7. Place a sample in the sample compartment.

8. Click **Start** or  to run a new measurement. The display will change to the following.

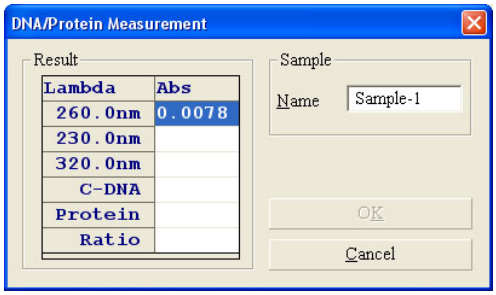


Fig. 8-4

9. The UV-Vis Application Software will read the photometric value of sample 1 at the fixed wavelength automatically. Key in the sample name in the Name box.

10. Click **OK** after the measurement is complete. The photometric data for sample 1 will be listed in the sample table.

11. Repeat steps 7-10 to test all samples.

12. Click **Print** to print out the table displayed.

Save Files

1. On the File menu, click Save or click the icon on the toolbar. A new dialog box will be displayed.

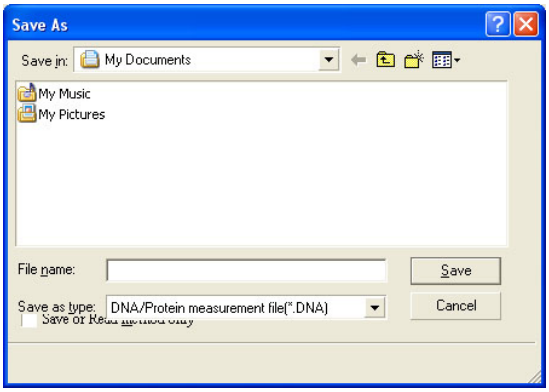


Fig. 8-5

2. Select a folder and key in a file name in the File name box. The file type for fixed points measurement defaults to *.dna.

3. Click **Save**.

Load Files

1. On the File menu, click Open or click the icon on the toolbar. The display will change to the following.

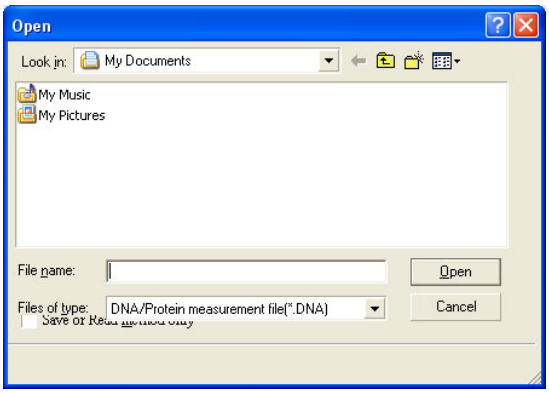


Fig. 8-6

2. Select a folder and file name.

3. Click **OK** to open the selected file.

Instrument Validity

This chapter describes how to perform Instrument Validity.

Selecting Instrument Validity

On the **File** menu, click **New**, the following dialog box will appear. Select **Instrument Validity** and click **OK**.

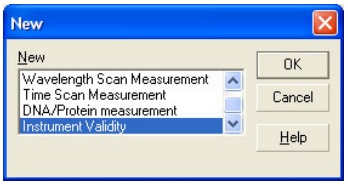


Fig. 9-1

or click  on the toolbar

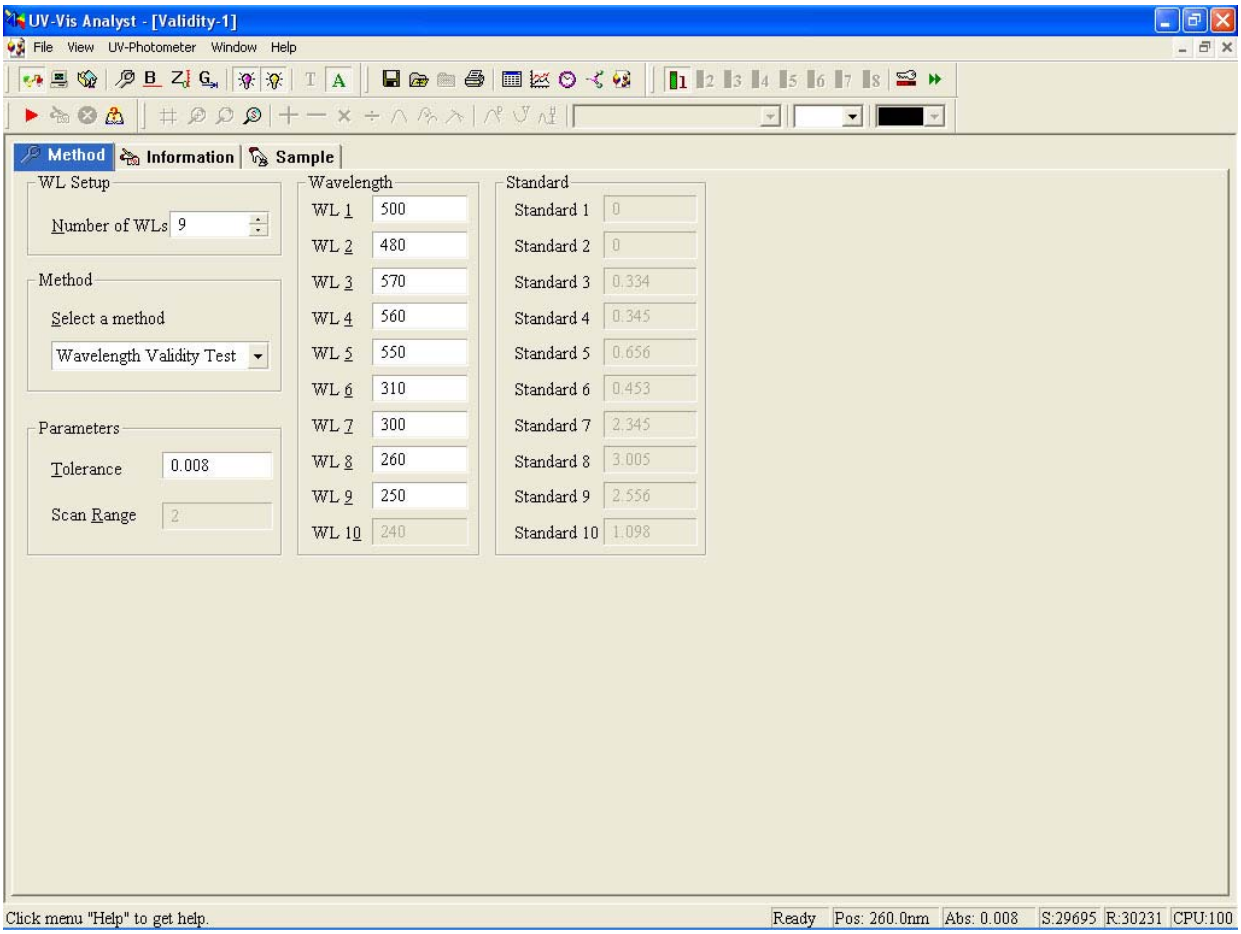


Fig. 9-2

Step by Step Operation

1. Click the **down** arrows of the **method** to select the **test method**.

2. Type the number of wavelength points in the **Number of Points** box, or click the **up/down** arrows next to the box set the wavelength points.

3. Key in the wavelength position in the **Wavelength** box.

4. Key in the tolerance in the **Parameters** box.

5. Click the **Sample** tab. It will display the following. The control menu contains six buttons: **Start**, **Delete**, **Modify**, **Recalculate**, **Data Font** and **Print**.

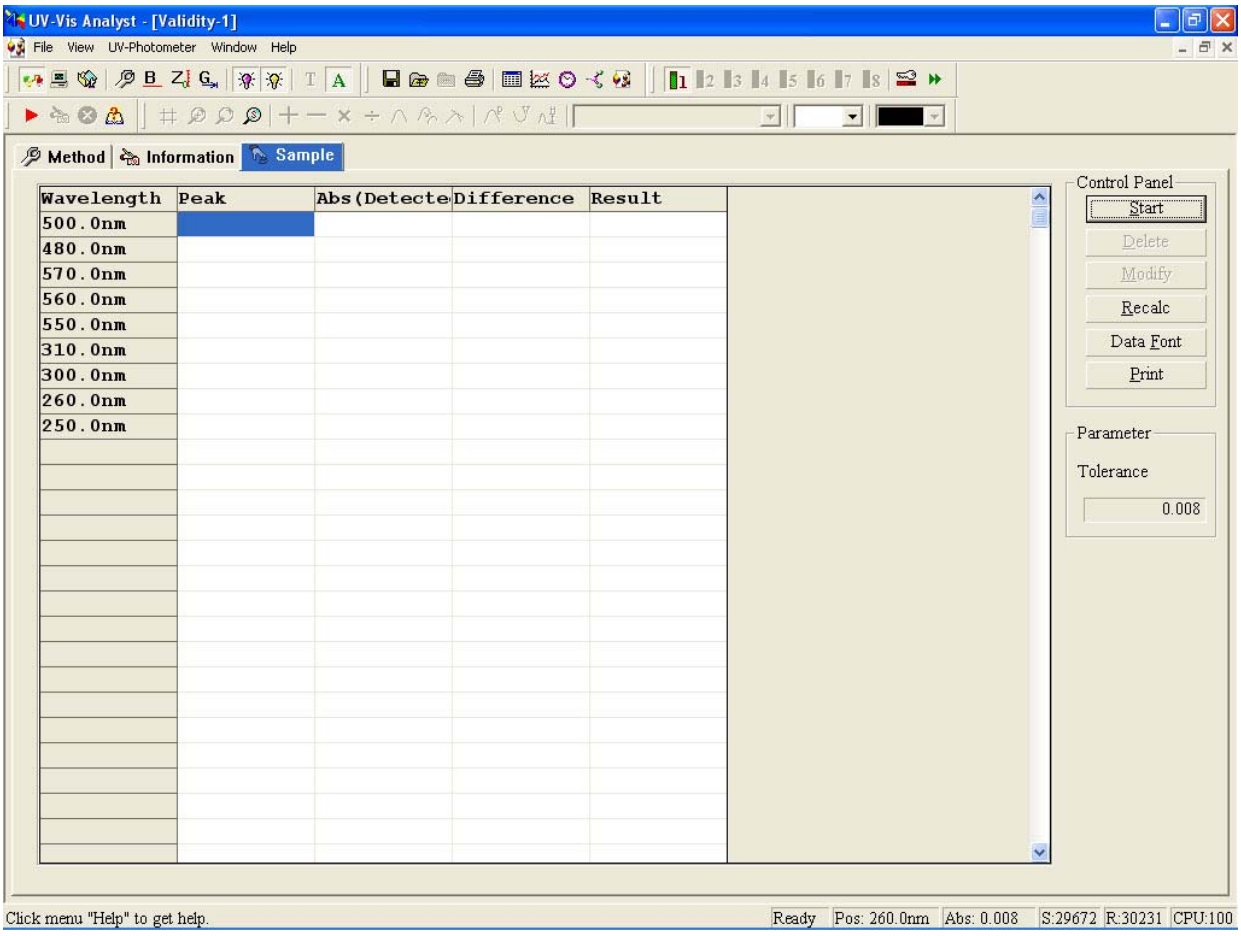


Fig. 9-3

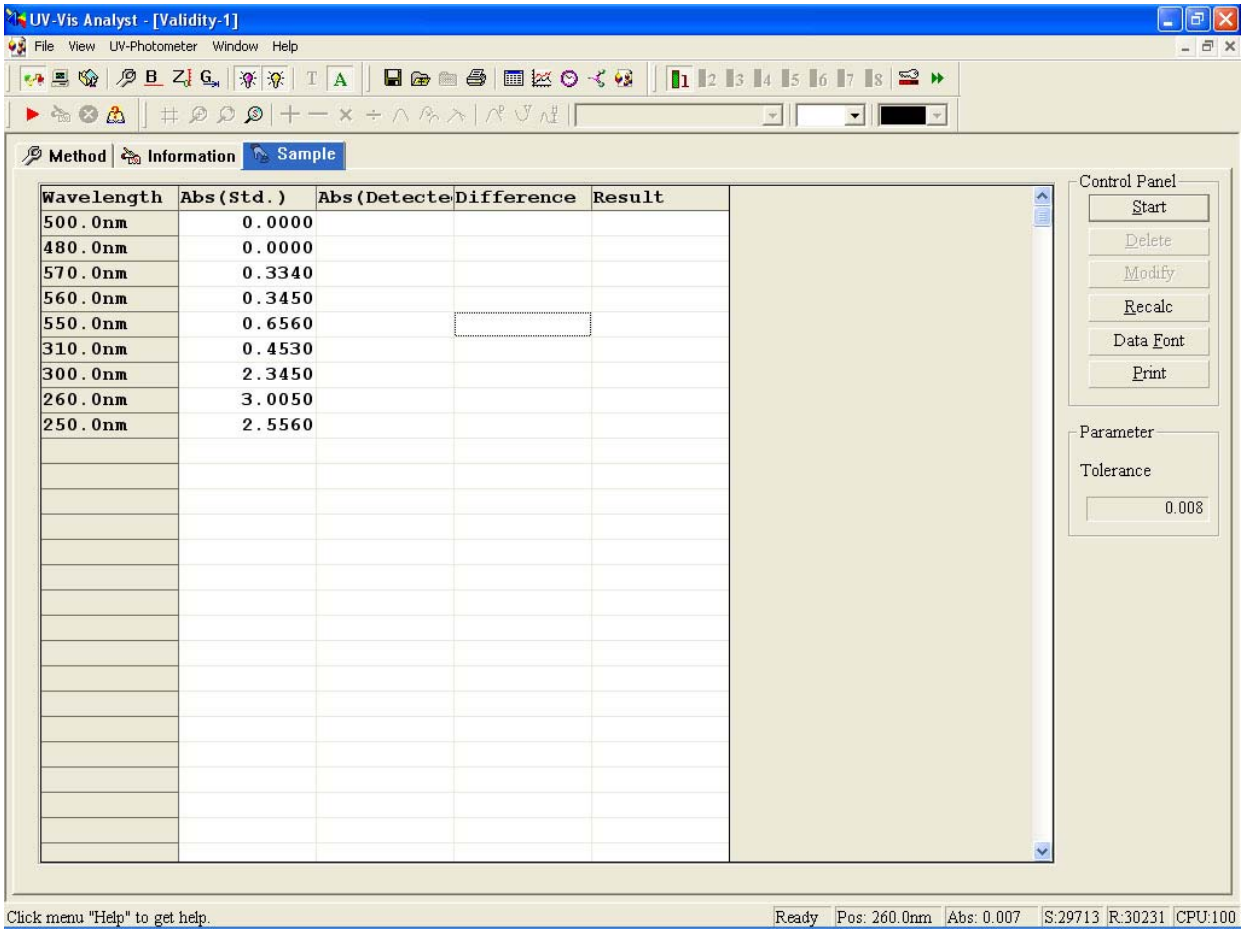


Fig. 9-4

6. With a blank or air in the sample compartment, press **Z** to zero the instrument.

7. Place a standard in the sample compartment.

8. Click **Start** or  to run a new measurement. The display will change.

9. The UV-Vis Application Software will read the peaks of sample 1. Key in the sample name in the Name box.

10. Click **OK** after the measurement is complete. The wavelengths and photometric values for sample 1 will be listed in the sample table.

11. Click **Print** to print out the table displayed.

Save Files

1. On the File menu, click Save or click the icon on the toolbar. A new dialog box will be displayed.

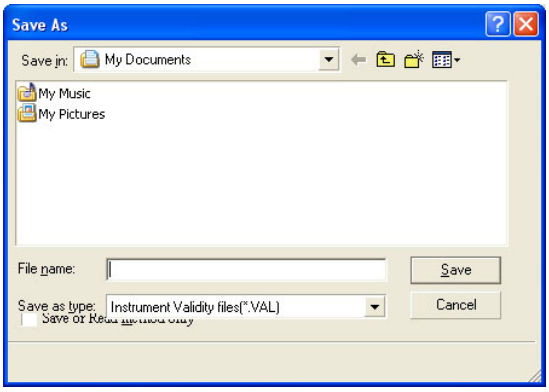


Fig. 9-6

2. Select a folder and key in a file name in the File name box. The file type for fixed points measurement defaults to *.VAL.

3. Click **Save**.

Load Files

1. On the File menu, click Open or click the icon on the toolbar. The display will change to the following.

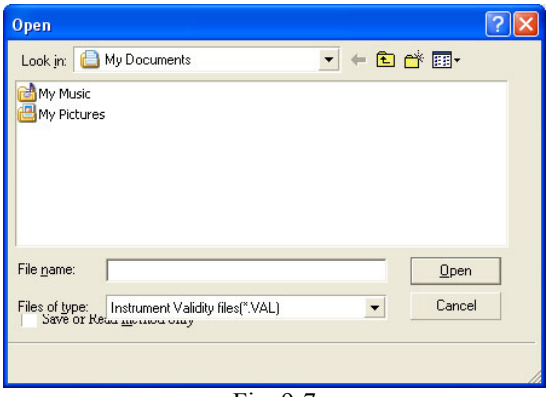


Fig. 9-7

2. Select a folder and filename.
3. Click **OK** to open the selected file.

Assistant Function

Password Protection

Setting a Password

You can set a password if you require the instrument to be used;

To set the password:

1. Click on **UV-Photometer** in the top menu.

2. Click on **Change Password**. The following prompt appears.

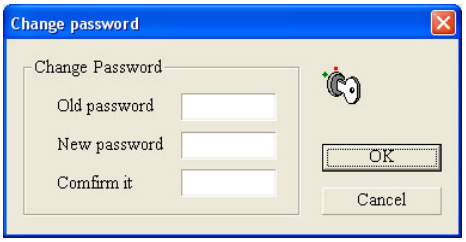


Fig. 10-1

3. Enter up to 8 characters in the New Password field.

4. Re-enter exactly the same characters in the Confirm it field.

Note: Any characters can be used, but the password is case-sensitive. Ensure you use the same case when entering characters in both fields. If exactly the same characters are not entered in both fields, you will be prompted to try again. If you wish to abort setting a password, clear both fields by deleting all characters therein. Once a password is selected, the next time you start the UV-Vis Application Software, the following prompt will appear.

Fig. 10-2

Input your password and click **Login.**

Note: Use a password that is easily remembered without being obvious to others. It is a good idea to write the password down (in case you do forget it) and secure it in a safe place.

Changing a Password

Once a password has been set, the **New Password** and **Confirm it** fields are grayed out although the **Change Password** field is active.

To change the current password:

1. Type the current password in the **Old Password** field

2. Only if the old password is correct will the **New Password** and **Confirm it** fields become active

3. Proceed as per"Setting a New Password" and enter the new password in both the **New Password** and **Confirm it** fields.

Auto sampling (Needs 8-Cell Automatic Cell Changer)

This chapter describes how to perform measurement by Autorun.

1. Click  on the toolbar, the following prompt will appear

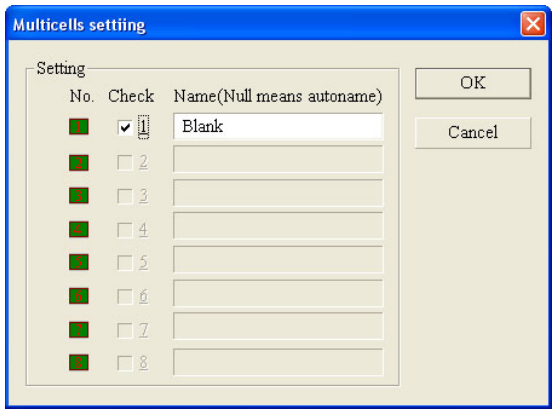


Fig. 10-3

Tick the numbers of the cells and key the name in the **Name** box.

2. Click **OK**.

3. Click  on the toolbar, it will complete measuring automatically.

Open a file saved in instrument

This chapter describes how to open a file saved in the ram of instrument.

1. Click on **File** in the top menu**,** then click **Open file from Photometer**

or

Click  on the toolbar. The following prompt will appear

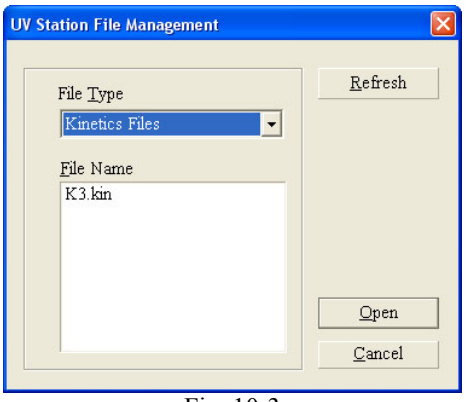


Fig. 10-3

2. Click **File Type** to select the type of the file, the file name will list in the **File Name** box.

3. Select the file name and click **Open** to load the file.