

UV-Vis Analyst

Software for UV/Visible Spectrophotometer

User Manual

Contents

Functions	1
Main Functions	1
Spectrum Processing Function.....	2
System Check and Calibration Function	3
Starting.....	3
PC System Requirements	3
Install UV-Vis Analyst	4
Uninstall UV-Vis Analyst.....	6
Run UV-Vis Analyst.....	6
Setup Communication Port.....	7
Introduction	7
Main Interface	7
Menus Bar and Tools Bar.....	8
Operation	14
Single Wavelength Photometric Measurement.....	14
Fixed Points Measurement.....	15
Multi-wavelength Photometric Measurement	15
Concentration Measurement	17
Wavelength Scanning	22
Time Scanning (Kinetic Analysis)	38
DNA/Protein Measurement.....	41

Appendix.....	45
Methods of Quantitative Analysis	45

Functions

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

Main Functions

Single wavelength photometric measurement

- Go to a desired wavelength quickly and conveniently.
- Photometric value display mode can be changed (%T or Abs).

Fixed Points Measurement

Multi-wavelength Photometric Measurement

- Up to 20 wavelength points can be set up.
- Results will be grouped into a table format automatically.

Concentration Measurement

- 2 methods to set up the regression curve.
Up to 20 standards to set up the regression curve.
The UV-Vis Analyst will calculate the working curve using a linear equation that fits the data.
Enter factor values to generate regression curve.
- 3 methods for curve fit.
Linear fit, Quadratic fit and Cubic fit.

Wavelength Scanning

- Allow user to set scan step (0.1, 0.2, 0.5, 1.0 and 5.0nm).
- Spectrum display mode can be changed (Wavelength-%T or Wavelength-Abs).
- Peaks and valleys will be automatically detected after scanning (User can define the peak threshold).
- Powerful spectrum processing functions are provided.

Time Scanning

- Allow user to set scan Interval (0.5, 1.0, 2.0, 5.0, 10, 30 and 60s).
- Spectrum display mode can be changed (Time-%T or Time-Abs).
- Peaks and valleys will be automatically detected after scanning (User can define the peak threshold).
- Powerful spectrum processing functions are provided.

DNA/Protein Measurement

- 7 methods to measure DNA/Protein.
- Wavelength points and ratios can be set up.
- Results will be grouped into a table format automatically.

Spectrum Processing Function

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 through the "Display Setup" function.

Differentiation

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

Calculate Spectrum

You can calculate addition, subtraction, multiplication and division between two spectra with the resulting

data displayed on the screen.

System Check and Calibration Function

Instrument Validity Check

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.

Dark Current Check

You can resample the dark current of the instrument.

Spectrum Bandwidth Check

A special scan for checking spectrum bandwidth that will calculate the bandwidth value automatically.

Energy of Light Sources Check

It allows scan the energy of light sources with a fixed gain (0-7).

Reset Wavelength

It affords to relocate the 656.1nm.

Starting

This section introduces how to start to use the UV-Vis Analyst.

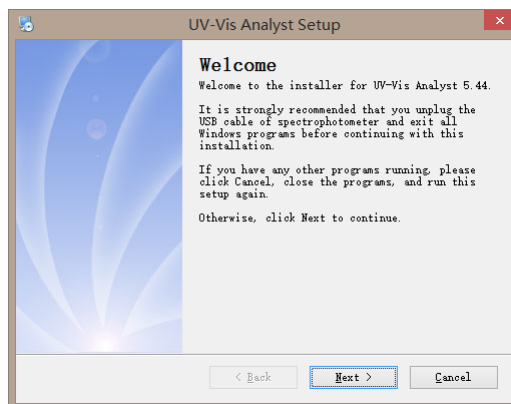
PC System Requirements

- Pentium or above PC;
- CD-ROM;
- USB Ports;
- 512MB Memory(1GB or Above is strongly recommended);
- 50MB or above hard disc Space;
- Microsoft Windows XP/Vista/7/8/10.

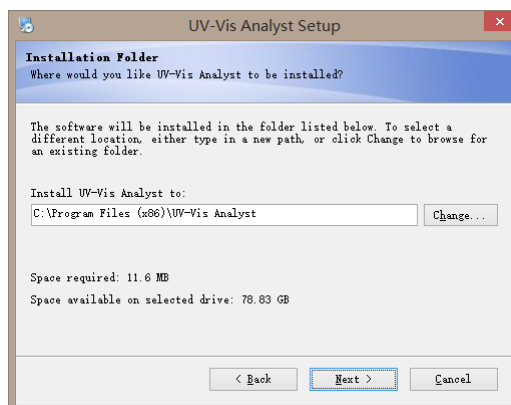
Install UV-Vis Analyst

Note: Please disconnect the USB Cable and unplug the USB Key before install the UV-Vis Analyst software.

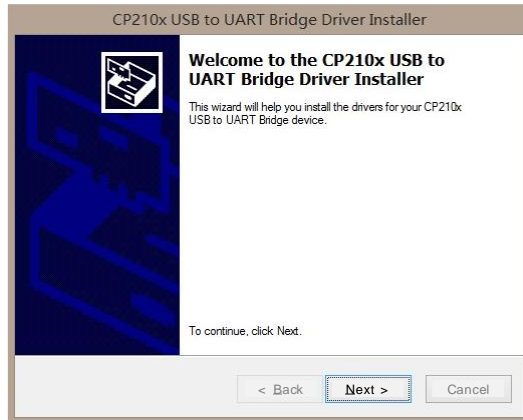
1. Put UV-Vis Analyst disc in the CD-ROM;
2. Double Click to open the CD-ROM, and then, double click **Setup.exe** which is under the root directory of CD to start installation, click **Next**;



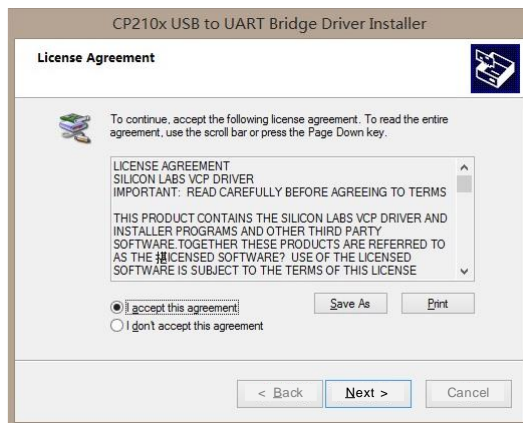
3. Choose install path, then click **Next** to copy files to PC;



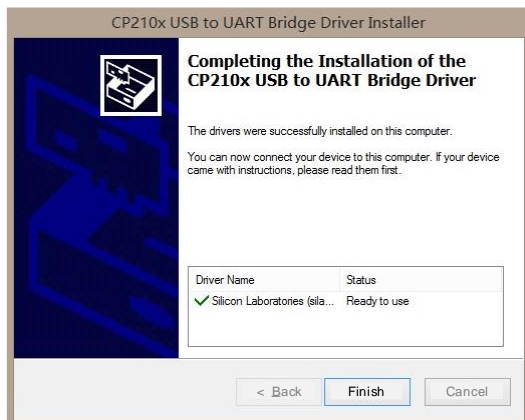
4. After finishing copy all files of UV-Vis Analyst, it will start install the USB Driver. Click **Next**;



5. Select "I accept this agreement". Click **Next** to copy files to PC;



6. Click **Finish** to finish install USB Driver;



7. Click **Finish** to finish all the setup.

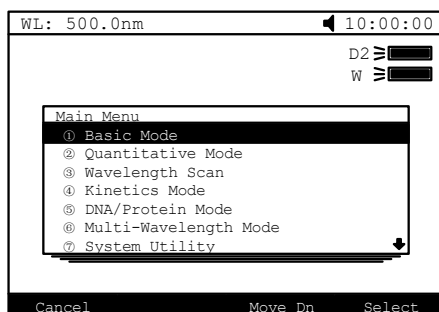
Uninstall UV-Vis Analyst

Start→All Programs →UV-Vis Analyst→Uninstall **UV-Vis Analyst** to remove.


Run UV-Vis Analyst

Note: Before you run UV-Vis Analyst, please check these things as follow:

- *Computer has connected to spectrophotometer by using the USB cable;*
- *Spectrophotometer is on main interface.*



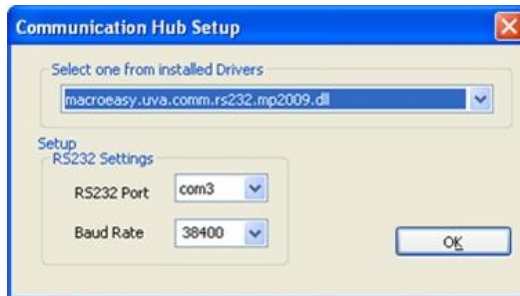
There are two ways to start the UV-Vis Analyst:

- Double-click shortcut icon  on the desktop.

- Start→All Programs→UV-Vis Analyst→**UV-Vis Analyst**.

Setup Communication Port

On the **UV-Photometer** menu, click **Comm. Hub Setup**, appears the following box, select the **RS232 Port** and **Baud Rate** (38400), click **OK**.

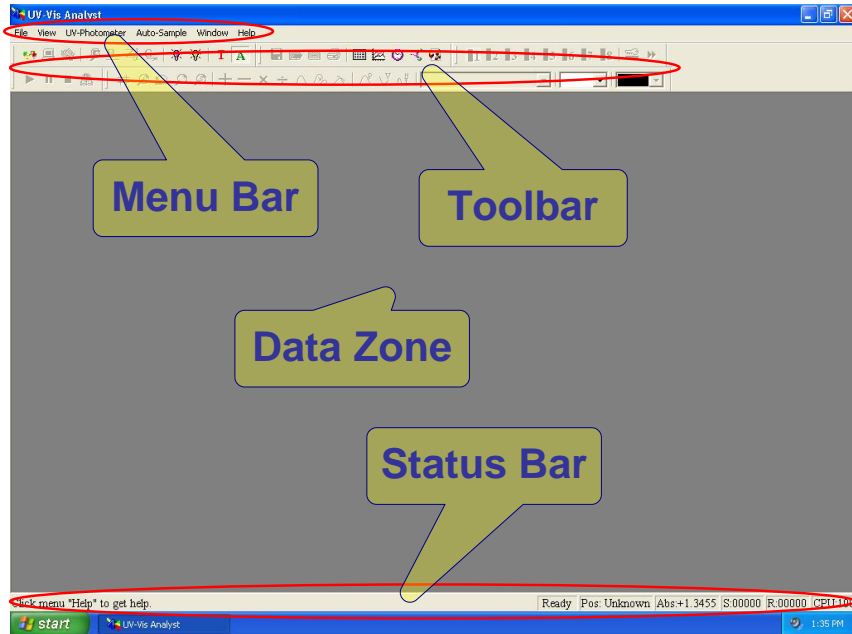


Introduction

We will introduce the UV-Vis Analyst in this chapter.

Main Interface




This is the main interface after start.






Menu Bar and Tools Bar




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.










Main Menu	Sub Menu	Icon	Function
File	New		New Fixed Points Measurement
			New Wavelength Scan Measurement
			New Time Scan Measurement

			New DNA/Protein Measurement
			New Instrument Validity
	Open...		Open a spectrum/data file
	Close		Close the current measurement
	Save		Save the current measurement
	Save As...		Save the current measurement as a new file name
	Open file from UV-Photometer		Open a file saved in instrument
	Export		Export data or method
	Print...		Print test report
	Print Setup...		Setup printer
	Exit		Exit UV-Vis Analyst
View	Status Bar		Display/Hide status bar
	Status of Spectrophotometer		Display status of spectrophotometer

	Status font		Setup font of status bar
	Customize		Define the info of display and print
	Peaks		Mark peak value
	Valleys		Mark valley value
	Magnify		Magnify the selected area
	Restore		Restore the default parameters for display
	Search		Search peak/valley one by one
UV- Photometer	Link Spectrophotometer		Connect to the Instrument
	Reset Spectrophotometer		Reset parameters of instrument
	Escape		Stop current measurement
	View dark Current		Retest the dark current
	Set Amplifier		Reset amplifier
	Locate 656.1nm		Relocate 656.1nm

	Calibrate System Baseline		Scan system baseline
	Automatic Blank Calibration		Do blank
	Slit Bandwidth *		Set slit bandwidth (0.5, 1.0, 2.0, 4.0)
	Set Unit		Set unit
	Turn on/off W lamp		Turn on/off W lamp
	Turn on/off D2 lamp		Turn on/off D2 lamp
	D2/W Switch Point		Set switch point of D2/W
	Comm. Port Setup		Setup comm. port
	Change Password		Set/Change login password
Auto-sample	Locate Cell **		Locate cell (1-8) to light path
	Setup Multicell **		Setup Multicell
	Autorun **		Measure multi samples automatically

Scan	Start		Start a measurement
	Stop		Stop a measurement
	Service		Measure spectrum and scan energy
Settings	Display Range		Setup scan display parameters
	Peak Height		Define peak/valley threshold
Compute	Add		Add two spectra
	Sub		Subtract one spectrum from another
	Multiply		Multiply two spectra
	Divide		Divide one spectrum from another
	Moving Window Averaging		Smooth a spectrum with the method Moving Window Averaging
	Savitzky-Golay Smoothing Filter		Smooth a spectrum with the method Savitzky-Golay Smoothing Filter
	Derivate		Derivative of a spectrum
	Resample		Resample a spectrum
	New Window		New measurement window as current


Window	Cascade		Multi windows display in a cascade
	Tile		Multi windows display in a tile
	Arrange Icons		Arrange all icons minimized
	Split		Split display area
Help	About UV-Vis Analyst		Display the information about the UV-Vis Analyst
			Setup measurement parameters
			Modify a measurement result
			Delete selected results
			Set and Goto one wavelength
			Display Instrument CPU information
			Delete current Spectrum
			Display result as mode %T
			Display result as mode Abs
			Undo Scale

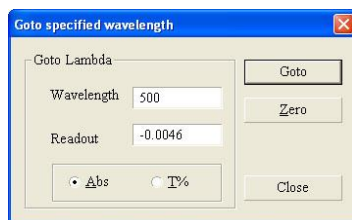
Operation

This chapter introduces how to use UV-Vis Analyst.

Single Wavelength Photometric Measurement

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

1. Click  on the toolbar, appears Goto specified wavelength.




2. Key in the desired wavelength value, click **Goto**. The minimum wavelength step is 0.1nm in a range from 190-1100nm.
3. Do blank.
 - **Single Beam:** Place the reference in the compartment, click **Zero**.
 - **Double Beam:** Skip to step 4.
4. Measure the Sample.
 - **Single Beam:** Place the sample in the sample compartment.
 - **Double Beam:** Place the reference in the reference compartment and place the sample in the sample compartment.

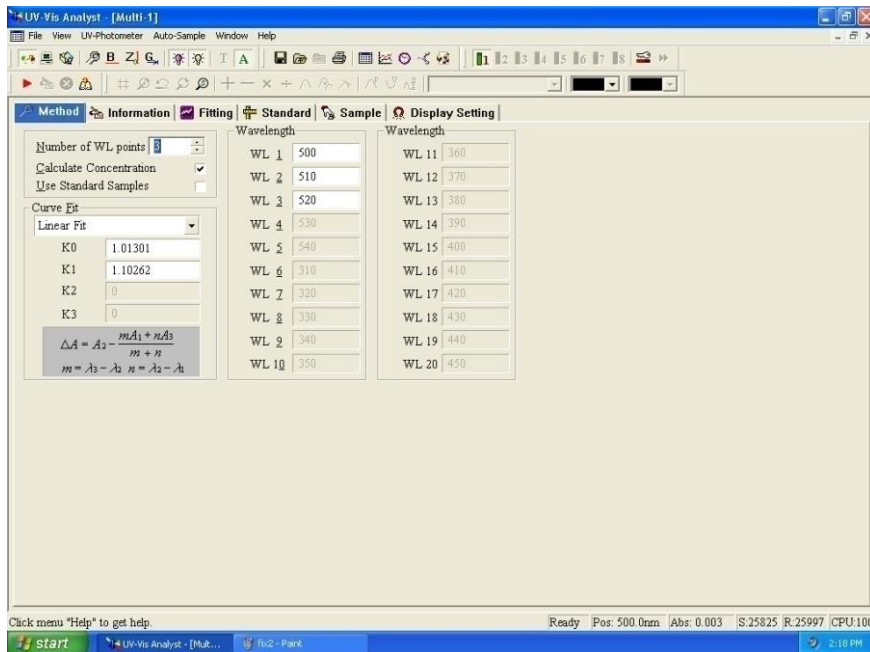
The photometric value will display in the Readout box.

Fixed Points Measurement

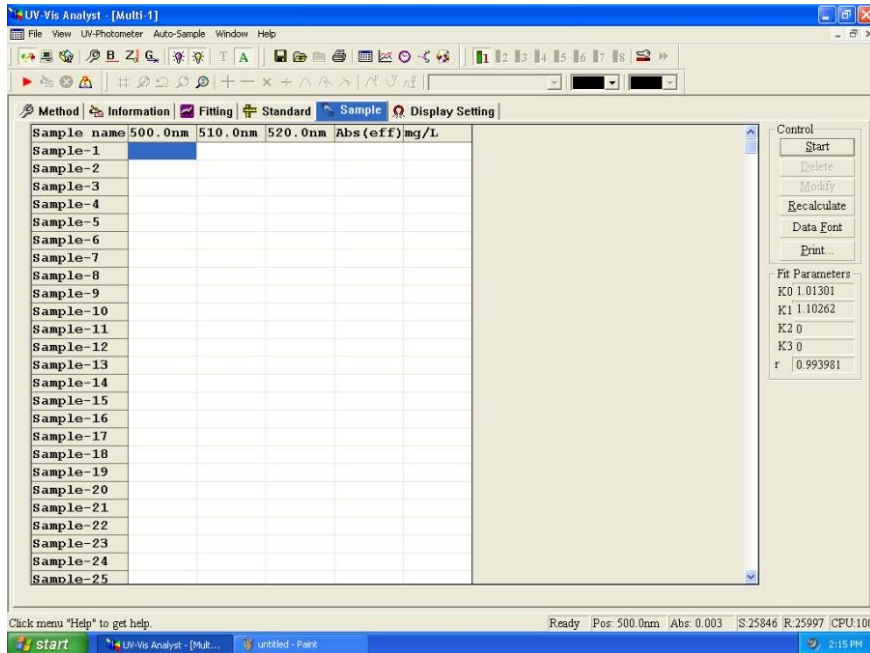
This software performs fixed wavelength measurement at 1-20 points. Allows to analyze unknown compounds against calibration standards.

Multi-wavelength Photometric Measurement

1. Click  on the toolbar, appears the following form.




2. Click the **Method** tab.
3. Type the number of wavelength points in the **Number of WL Points** box or click the up/down arrows next to the box. Leave the two boxes **Calculate Concentration** and **Use Standard Samples**.
4. Key in the wavelengths in the **Wavelength** boxes.
5. Click the **Sample** tab. It will display the following. The control menu contains six buttons: Start, Delete, Modify, Recalculate, Data Font and Print.



6. Do blank.


- **Single Beam:** Place the reference in the compartment,

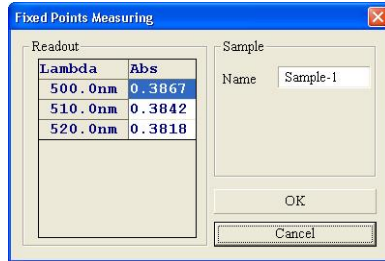
click .

- **Double Beam:** Skip to step 7.

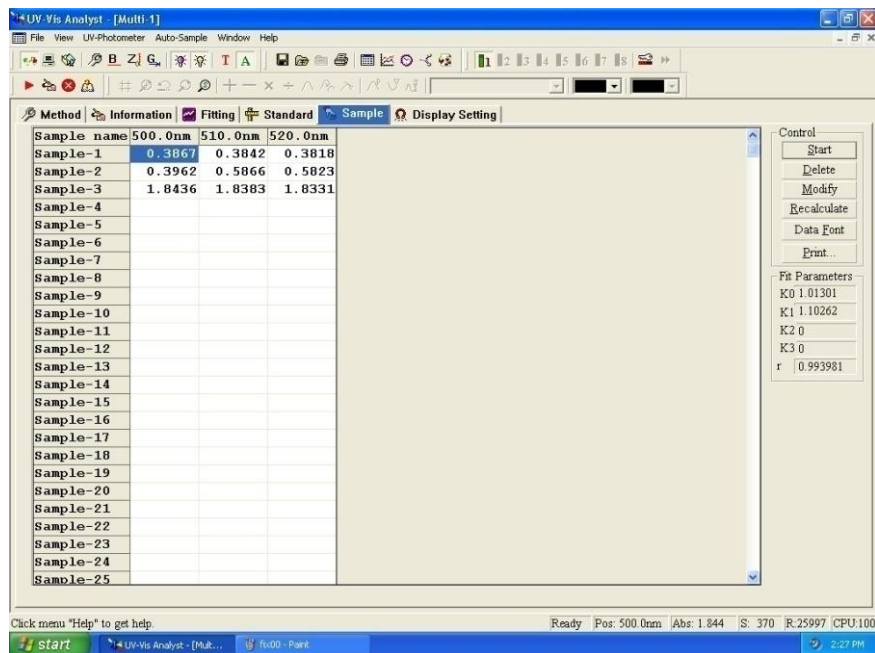
7. Measure the Sample.

- **Single Beam:** Place the sample in the sample compartment.
- **Double Beam:** Place the reference in the reference compartment and place the sample in the sample compartment.

Click  to run a new measurement. The display will change to the following. Key in the sample name in the **Name** box.



8. Click **OK**. The photometric data for sample will be listed in the Sample table.
9. Repeat steps 7-8 to measure all samples.



Concentration Measurement

Set Up Linear Regression Curve

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  on the toolbar.


2. Click the **Method** tab.
3. Enter the number of wavelength points in the **Number of WL Points** box.
4. Key in the wavelengths in the **Wavelength** boxes.
5. Tick the **Calculate Concentration** check box to activate concentration calculation.
6. Set up the linear regression curve.

Method 1: Set up the linear regression curve with prepared standards.

(1) Tick the **Use Standard Samples** check box.

(2) Click the **Standard** tab.

(3) Do blank.

- **Single Beam:** Place the reference in the compartment, click .

- **Double Beam:** Skip to step (4).

(4) Measure Standard Sample.

- **Single Beam:** Place the sample in the sample compartment.
- **Double Beam:** Place the reference in the reference compartment and place the sample (Standard 1) in the sample compartment.

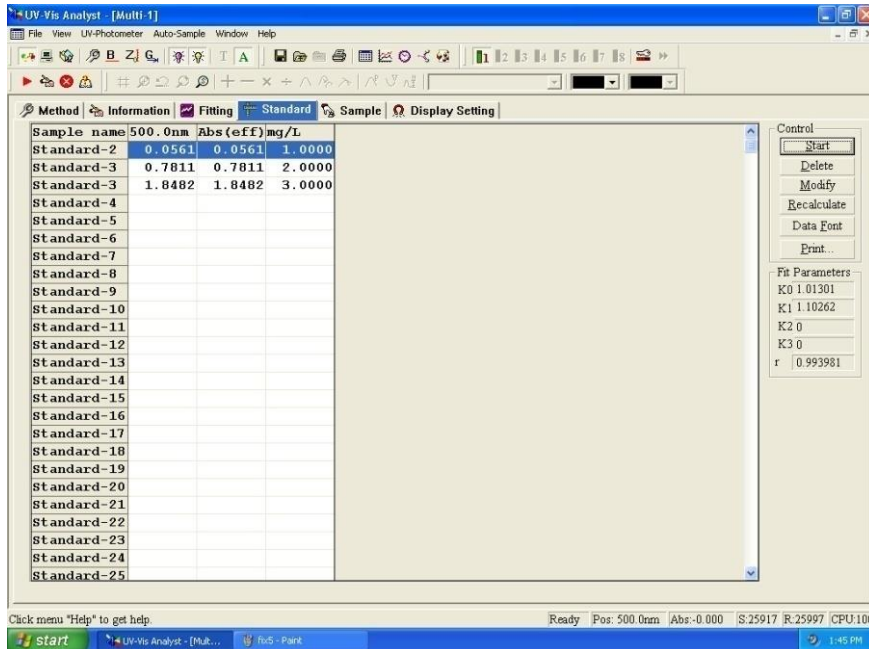
Click **Start** to run a measurement.

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

(6) Key in the sample name for the standard in the **Name** box.

(7) Click **OK**. The photometric data, ΔA and concentration will be shown in the standard table.

(8) Repeat steps 4-7 to measure all the prepared standards.



(9) Click down arrow in **Curve Fit** box to select curve fit method.

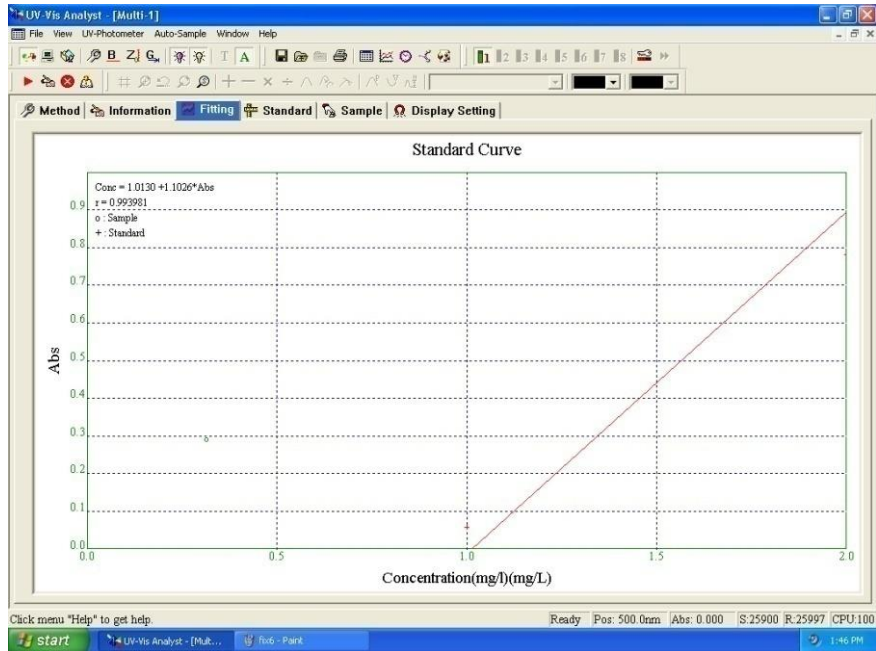
Method 2: Input the factor of the linear regression curve.

(1) Leave the **Use Standard Samples** check box.

(2) Click down arrow in **Curve Fit** box to select curve fit method.

(3) Input the factor of the linear regression curve.

7. Click **Fitting** tab to view the linear regression curve. Click **Display Setting** tab to set the display parameters and unit of concentration.



Method Information **Fitting** Standard Sample **Display Setting**

Display Range

Xmin 0 Xmax 2 Ymin 0 Ymax 1

Scales

Automatic Setting
 X Interval 20 Y Interval 0.2 Font
 Unit of Conc. mg/L




Display Content

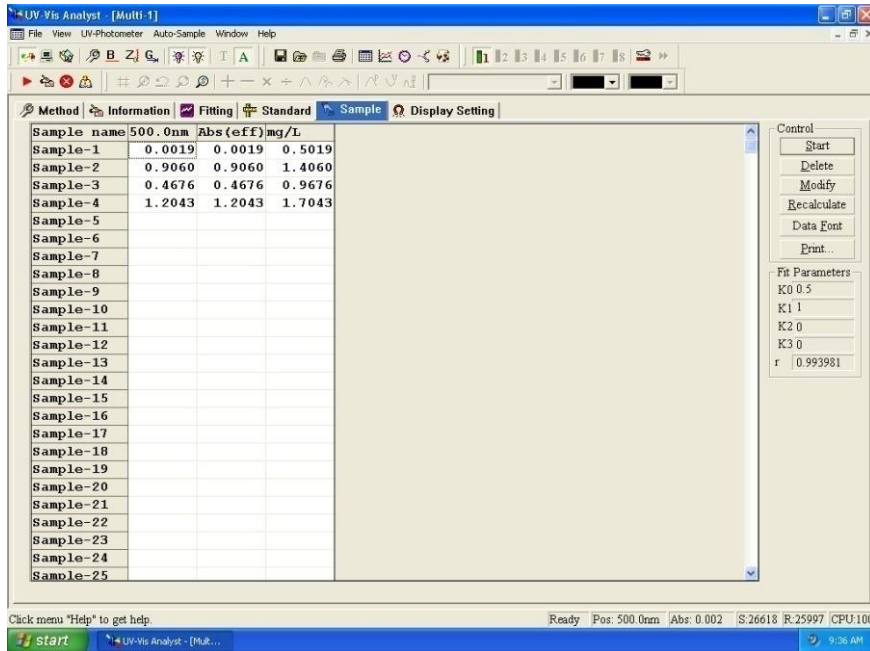
X-Axis Concentration(mg/l) Font Standard
 Y-Axis Abs Font Sample
 Title Standard Curve Font Fit Parameters Font

Click menu "Help" to get help. Ready Pos: 500.0nm Abs: 0.000 S:25911 R:25997 CPU:100

Measure Concentration by Using The Linear Regression Curve

The following procedure shows how to measure concentration of samples.


1. Set up linear regression curve or click  to open a file of linear regression curve (*.QUA).
 2. Click the **Sample** tab.
 3. Do blank.
 - **Single Beam:** Place the reference in the compartment, click .
 - **Double Beam:** Skip to step 4.
 4. Measure Sample.
 - **Single Beam:** Place the sample in the sample compartment.
 - **Double Beam:** Place the reference in the reference compartment and place the sample in the sample compartment.
- Click  to run a new measurement. Type the sample name in the **Name** box. The default name 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 4-5 to measure remaining samples.

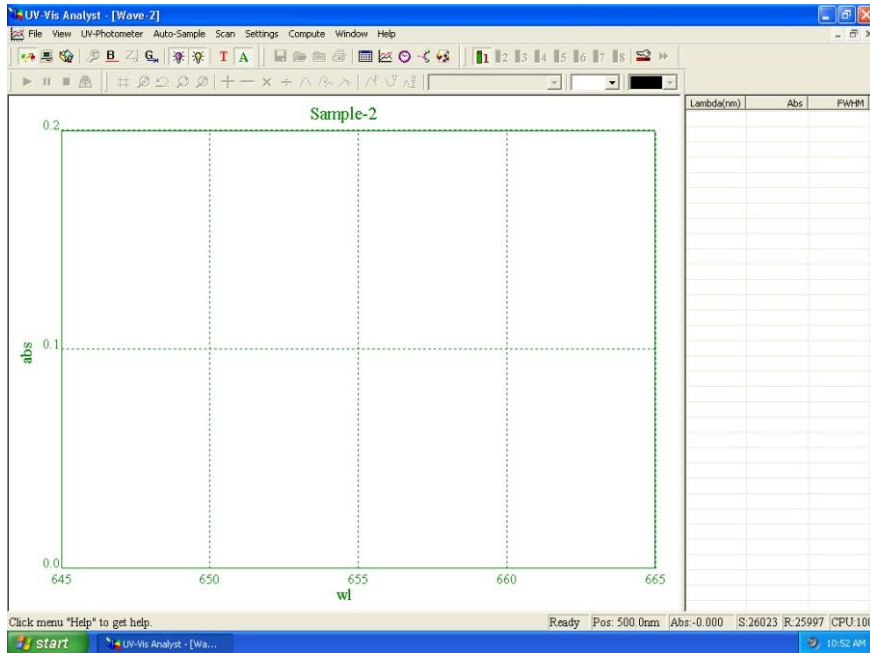



Wavelength Scanning


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


Sample Scan


1. Click  on the toolbar for a new sample scan measurement, appears the following form.

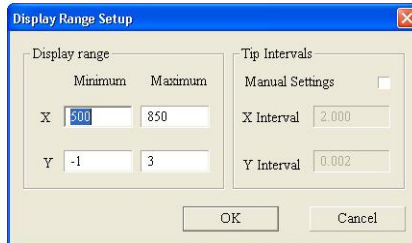



2. Click  on the toolbar, appears the following form. Input start wavelength in **From** box (range: 190-1100nm), end wavelength in **To** box (range: 190-1100nm), select scan interval (0.1, 0.2, 0.5, 1.0, 2.0 or 5.0nm) and Filter times (5, 10, 30 or 50), click **OK**.

3. Click  on the toolbar to select Transmittance


mode or click  to select Absorbance mode.

4. Click  on the toolbar to set display parameters.

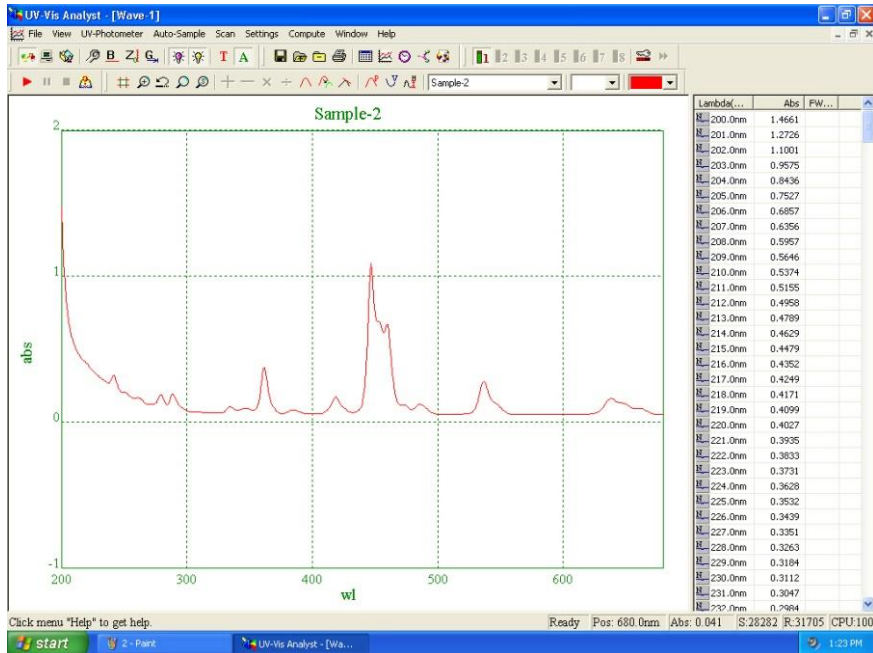


5. Baseline Scan.
- **Single Beam:** Place the reference in the compartment, click .
 - **Double Beam:** Skip to step 6.




6. Measure the Sample.
- **Single Beam:** Place the sample in the sample compartment.
 - **Double Beam:** Place the reference in the reference compartment and place the sample in the sample compartment.

Click  to scan sample, the real time spectrum

will be displayed. Click  to cancel while scanning.

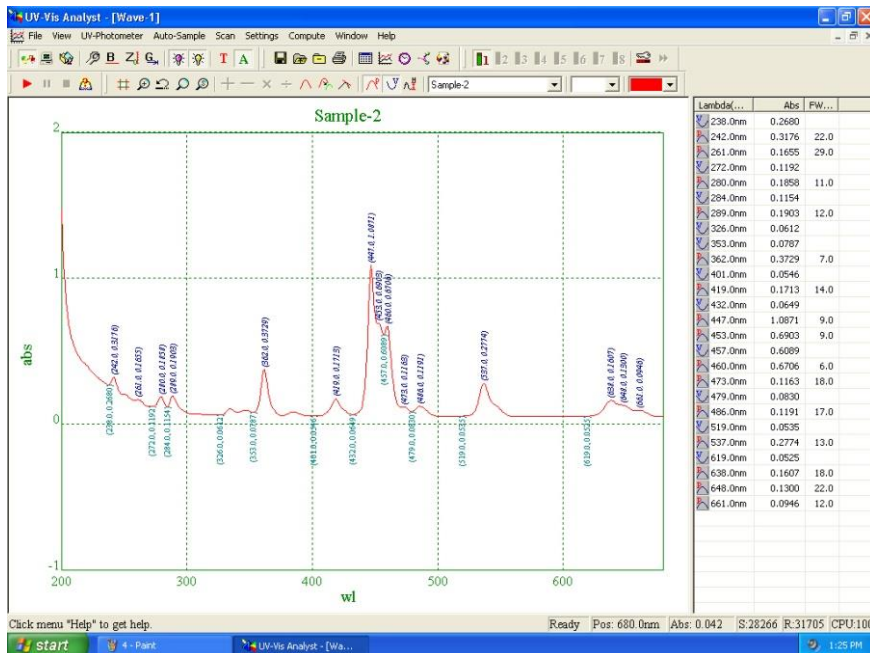


Auto List Peaks and Valleys

Click  on the toolbar to set the peak/valley threshold (range: 0 to 1.000, step: 0.001), Input the threshold value, click OK. Click  to list peaks and click  to list valleys.


Setup peak/valley threshold

Please key in the threshold(Abs)




Rescale



Click  on the toolbar to set the new parameters for display.


Original Scales





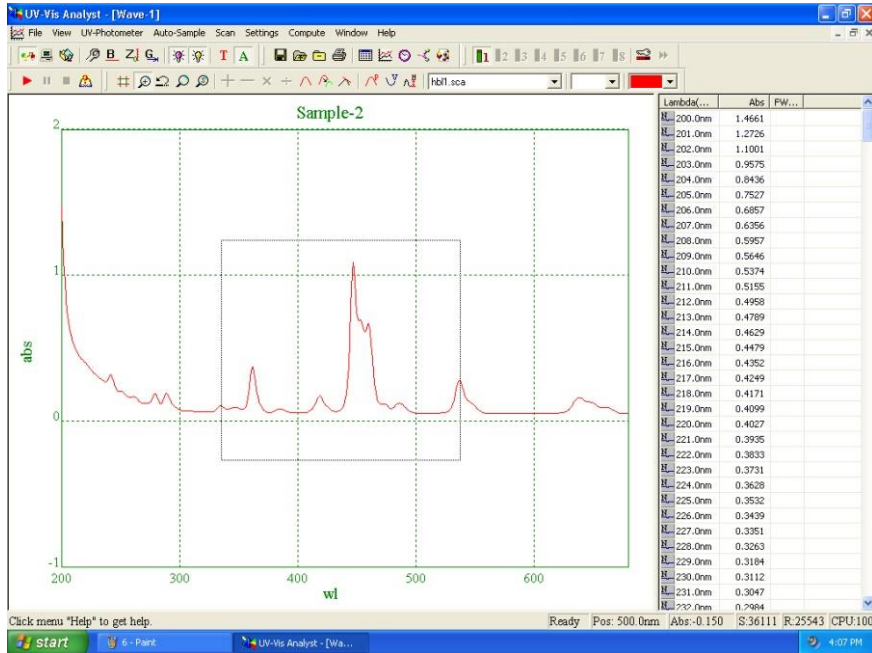
Click  on the toolbar to restore the default display settings.

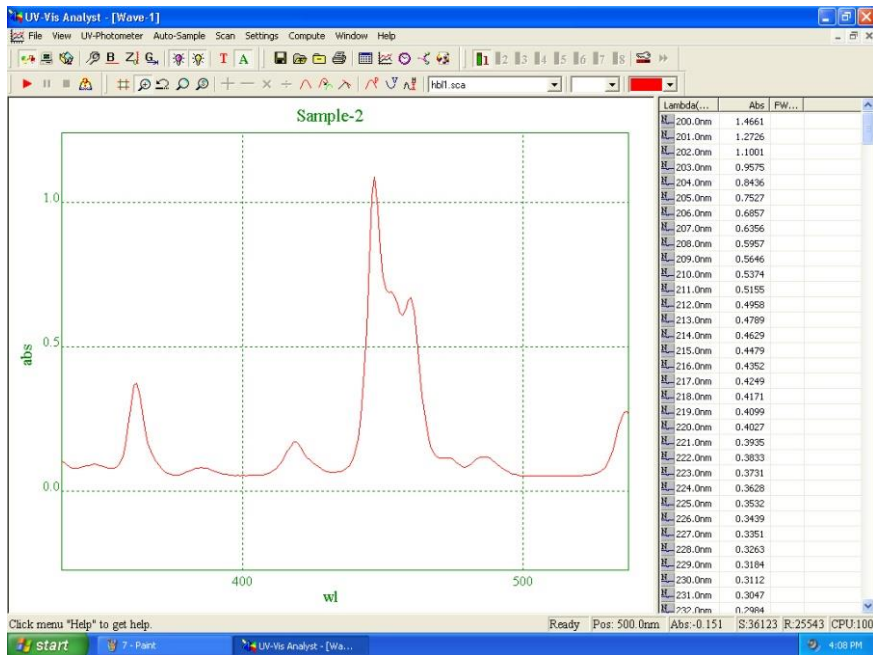
Zoom Selected Area




Click  on the toolbar to activate zoom function. Position the cursor in the upper-left corner of the area you want to select. Hold the left mouse button to drag the cursor to outline the spectrum area you want to enlarge. Release the mouse button. The part of the spectrum which is displayed within the outlined area

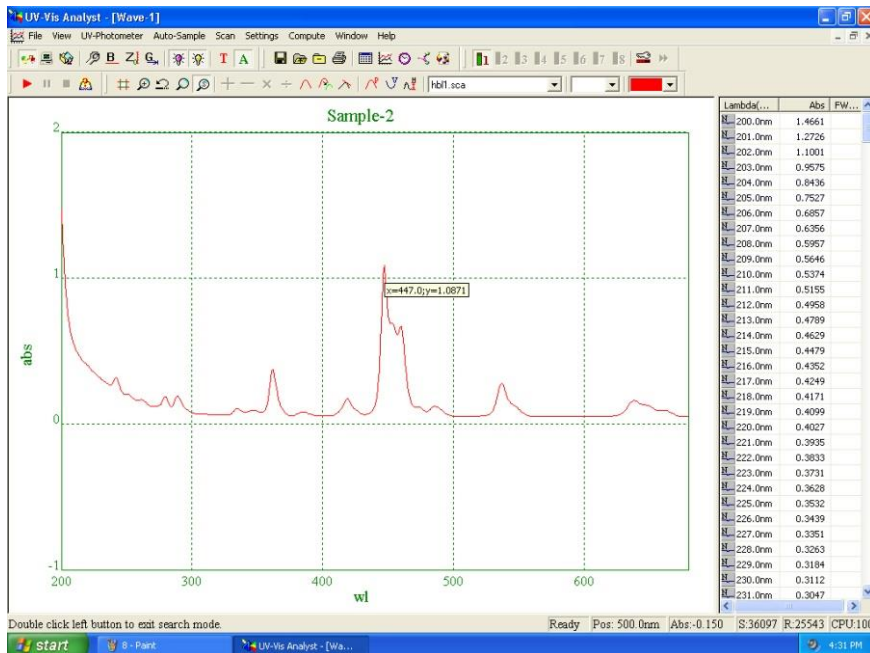
will be enlarged. Click  to undo scale. To cancel zoom to click  again.





Trace a Spectrum

Click  on the toolbar, a crosshair cursor appears, move the cursor on the spectrum. Move the crosshair cursor left or right on the spectrum. The data in the cursor window indicate the X-axis and Y-axis values for the current cursor location. Click key "ESC" to release the crosshair cursor.




Select a Spectrum as Current

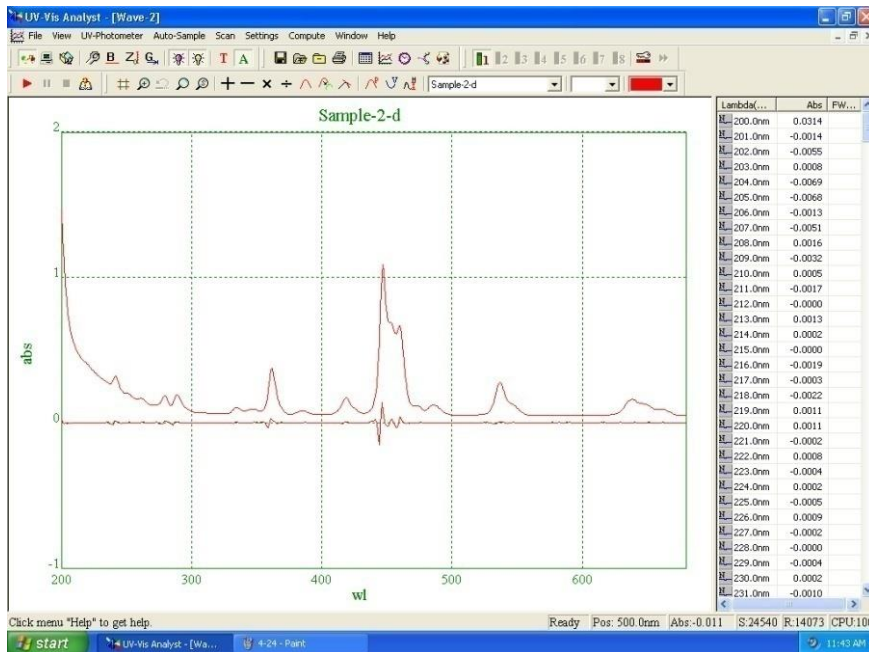
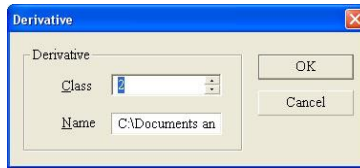
As UV-Vis Application Software can display several spectrum overlaid on the screen, you should specify the spectrum you wish to process. Click the **down** arrow on the toolbar. All spectrums will be listed in the pull-down menu. Click the spectrum you want to select. Its name will be listed in the **Name** Box and it will be referred to as Current Spectrum.




Derivative

Click  on the toolbar. The following dialogue box appears. 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

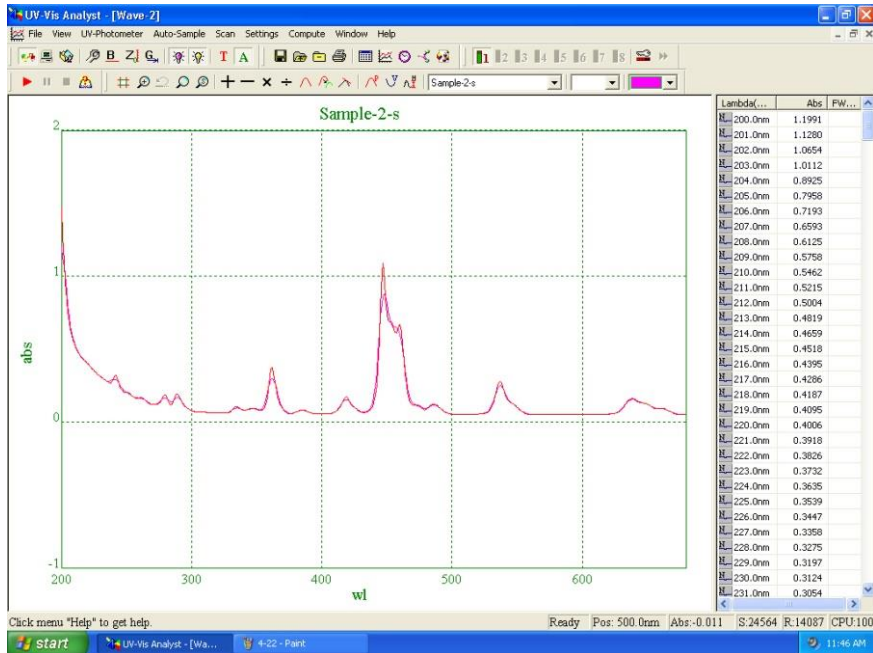
overlaid with the original one.



Moving Window Averaging

Click  on the toolbar. Appears following form. Click **up/down** arrow of the **Range** box to select range value, key a file name in the **Name** box, click **OK**. The result spectrum will be displayed overlaid with the original one.

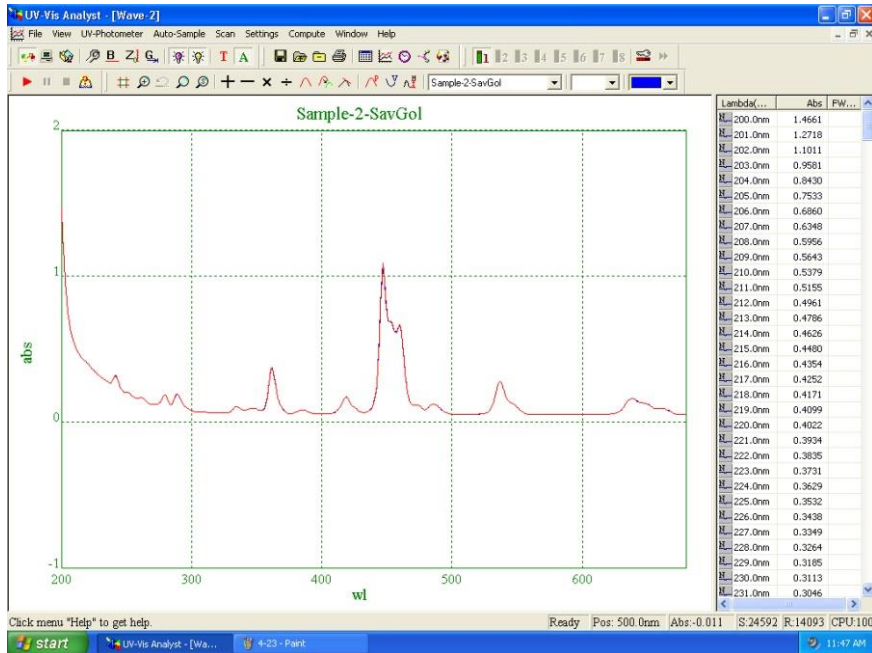




Savitzky-Golay Smoothing Filter


On the **Computer** menu, click **Savitzky-Golay Smoothing Filter**. Appears following form. Click **up/down** arrow to select the parameters, key a file name in the **Name** box, click **OK**. The result spectrum will be displayed overlaid with the original one.

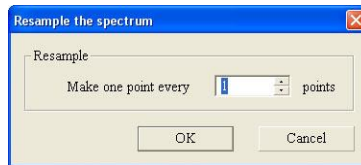
The 'Smooth the spectrum' dialog box is shown. It has a title bar with a close button. Inside, there is a 'Smooth' label, a 'Range' input field with a dropdown arrow, and a 'Name' input field containing the text 'Sample-2-s'. There are 'OK' and 'Cancel' buttons on the right side.

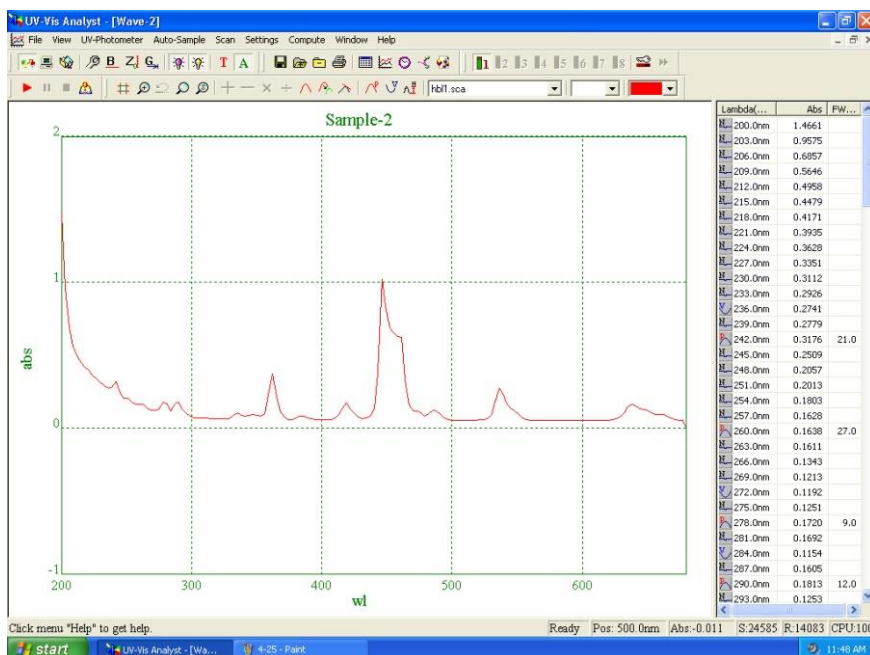


Resample




Click  on the toolbar. The following dialogue box will be displayed. Click **Up/Down** arrow to select Sample times. Click **OK**. The new spectrum displays.



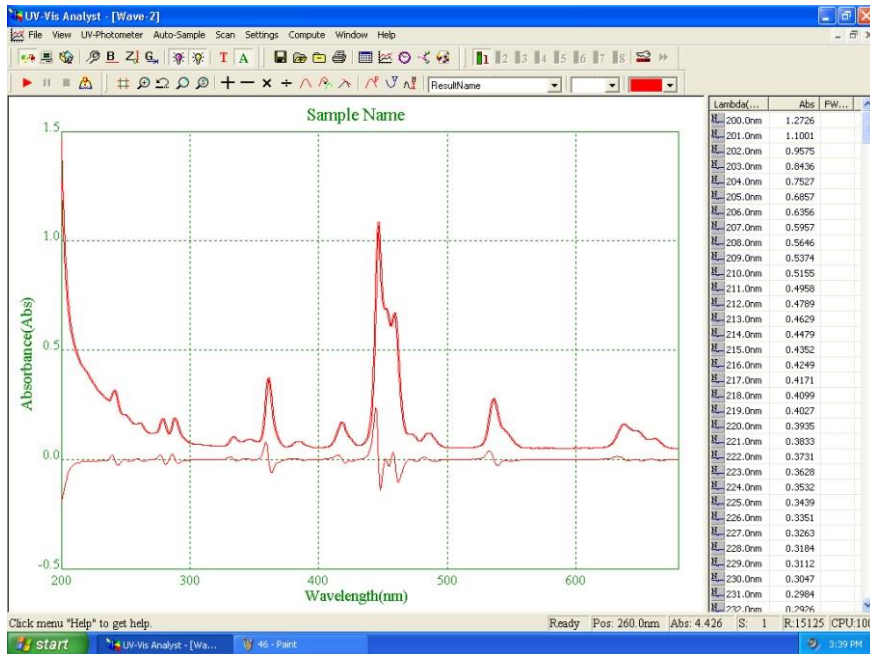
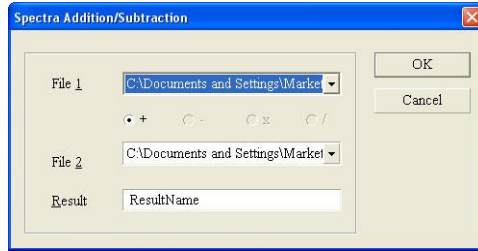


Spectrum Addition

Spectrum addition can assist in the development of artificial spectrum in multi-component mixtures.


Click  on the toolbar. The following dialogue box will be displayed. Click the **down** arrow next to **File 1** to select a spectrum and define it as source 1. Select a spectrum for **File 2** in the same way. It will not allow you to select the same spectrum twice. Key in a name for the result spectrum and click **OK**. The result spectrum will be displayed on the screen.

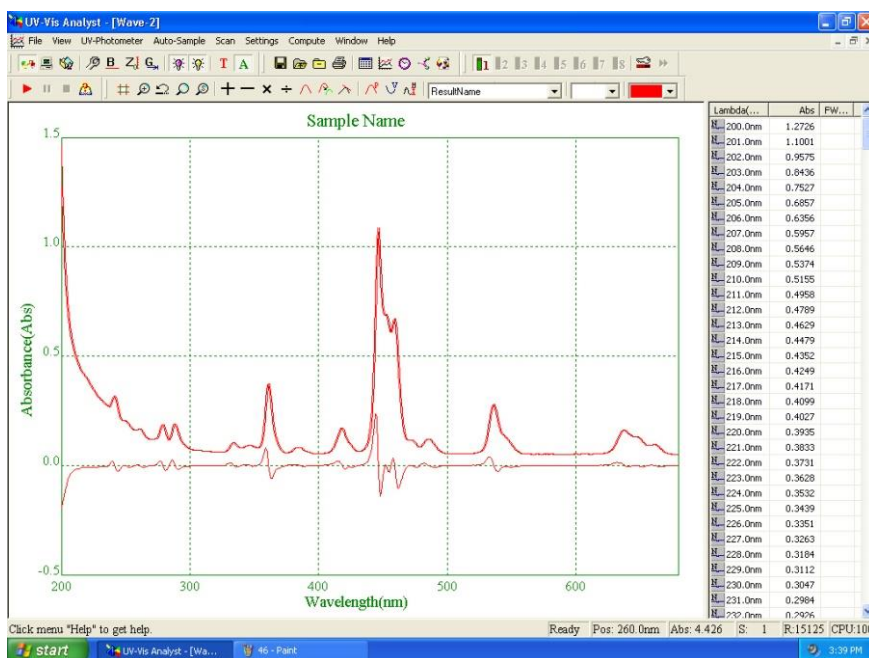
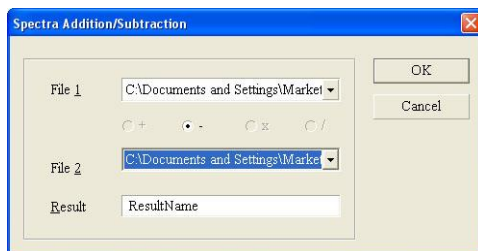
Note: UV-Vis Analyst will only add, subtract, multiply and divide two spectrums that are already displayed on the screen. Before arithmetic processing, load or collect two spectrums from memory.



Spectrum Subtraction


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

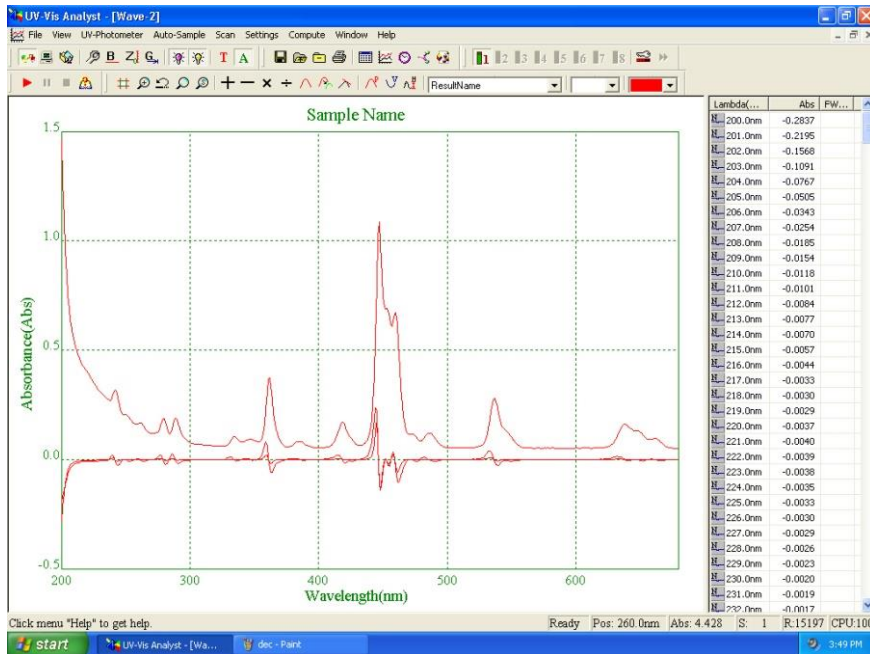
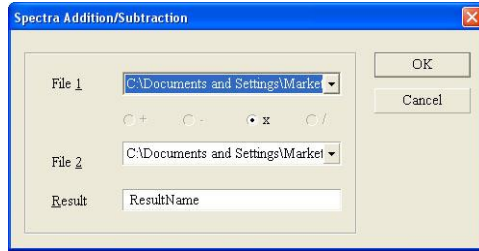
Click  on the toolbar. The following dialogue box will be displayed. Click the **down** arrow next to **File 1** to select a spectrum and define it as source 1. Select a spectrum for **File 2** in the same way. It will not allow you to select the same spectrum twice. Key in a name for the **Result** spectrum and click **OK**. The result spectrum will be displayed on the screen.



Spectrum Multiplication

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


Click  on the toolbar. The following dialogue box will be displayed. Click the **down** arrow next to **File 1** to select a spectrum and define it as source 1. Select a spectrum for **File 2** in the same way. It will not allow you to select the same spectrum twice. Key in a name for the **Result** spectrum and click **OK**. The result spectrum will be displayed on the screen.

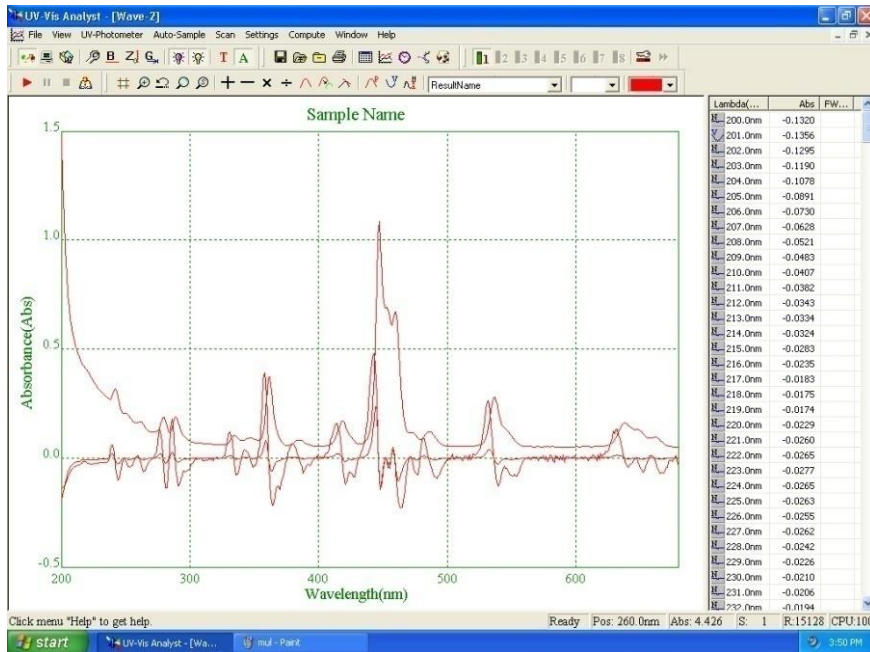


Spectrum Division

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




Click  on the toolbar. The following dialogue box will be displayed. Click the **down** arrow next to **File 1** to select a spectrum and define it as source 1. Select a spectrum for **File 2** in the same way. It will not allow you to select the same spectrum twice. Key in a name for the **Result** spectrum and click **OK**. The result spectrum will be displayed on the screen.




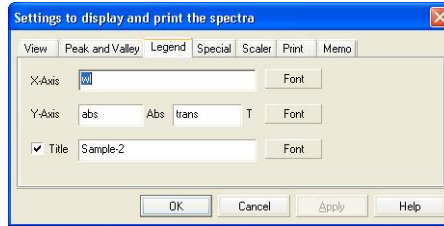
Unload a Spectrum

Select the spectrum you want to unload as the **Current**

Spectrum, click  on the toolbar to remove the spectrum from the display.


Define Display Information

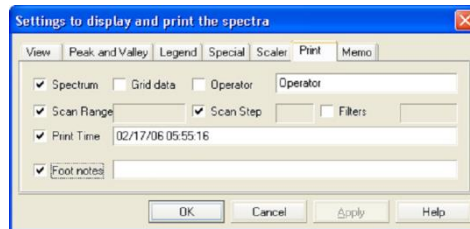
Click  on the toolbar, appears the **Settings to display and print the spectra** form, click the **Legend** tab, type the information for display.



Edit Print Information



Click  on the toolbar, appears the **Settings to display and print the spectra** form, click the **Print** tab, type the information for print out.




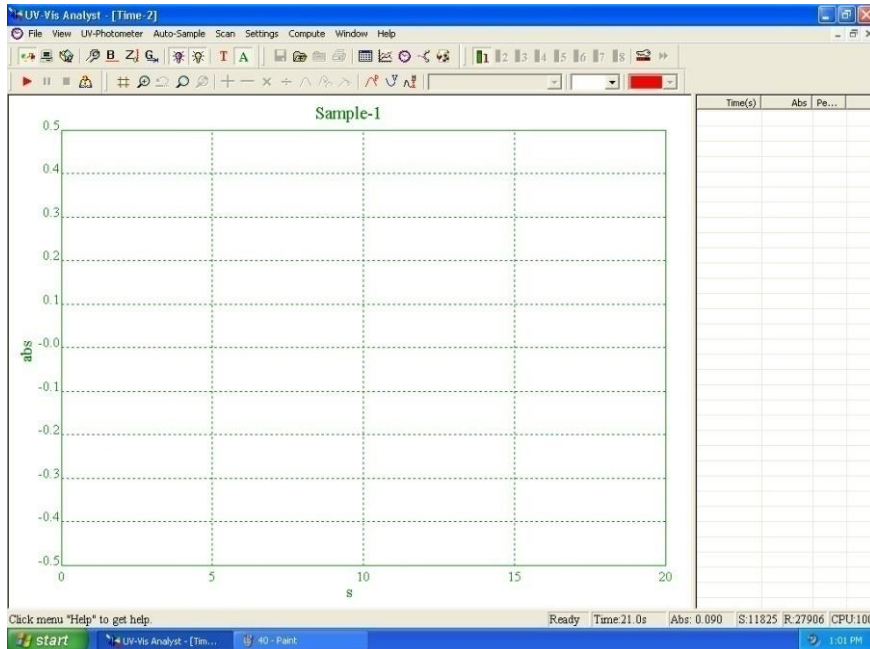
Time Scanning (Kinetic Analysis)




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

Sample Scan




1. Click  on the toolbar, the following dialog box will appear.



2. Click  on the toolbar to select the transmittance mode or click  to select the absorbance mode.
3. Click  on the toolbar. A dialogue box will be displayed. 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 100000 seconds. Seven scan intervals can be selected from 0.5S, 1S, 2S, 5S, 10S, 30S and 60S. Click **OK**.


4. Do blank.
 - **Single Beam:** Place the reference in the


compartment, click .

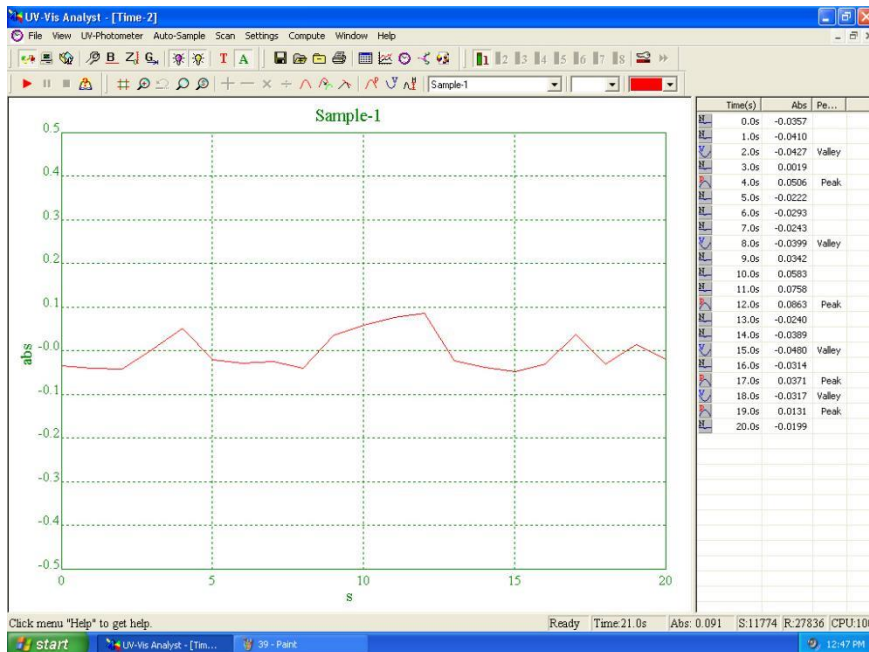
- **Double Beam:** Skip to step 5.

5. Measure Sample.


- **Single Beam:** Place the sample in the sample compartment.
- **Double Beam:** Place the reference in the reference compartment and place the sample in the sample compartment.

Click  on the toolbar. The instrument will start scanning automatically. The graph will be displayed on the screen during time scanning. You can stop scanning

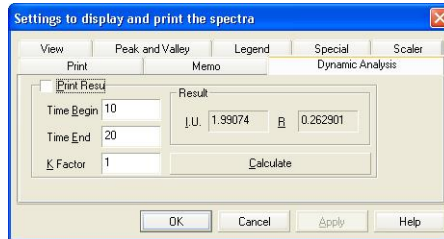
by clicking .




Calculate Rate

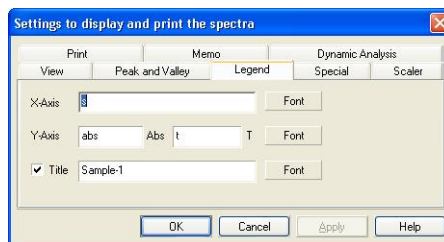
Click  on the toolbar, appears the **Settings to display and print the spectra** form, click the **Dynamic Analysis** tab, type the begin time in **Time Begin** box,

type the end time in **Time End** box, and type the K factor in **K Factor** box, click **Calculate**, the result will be displayed.




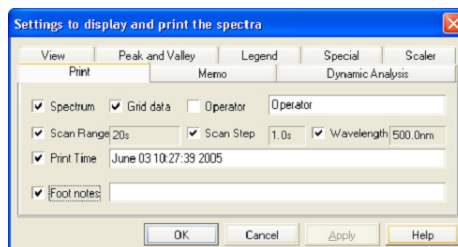
Define Display Information

Click  on the toolbar, appears the **Settings to display and print the spectra** form, click the **Legend** tab, type the information for display.



Edit Print Information

Click  on the toolbar, appears the **Settings to display and print the spectra** form, click the **Print** tab, type the information for display.




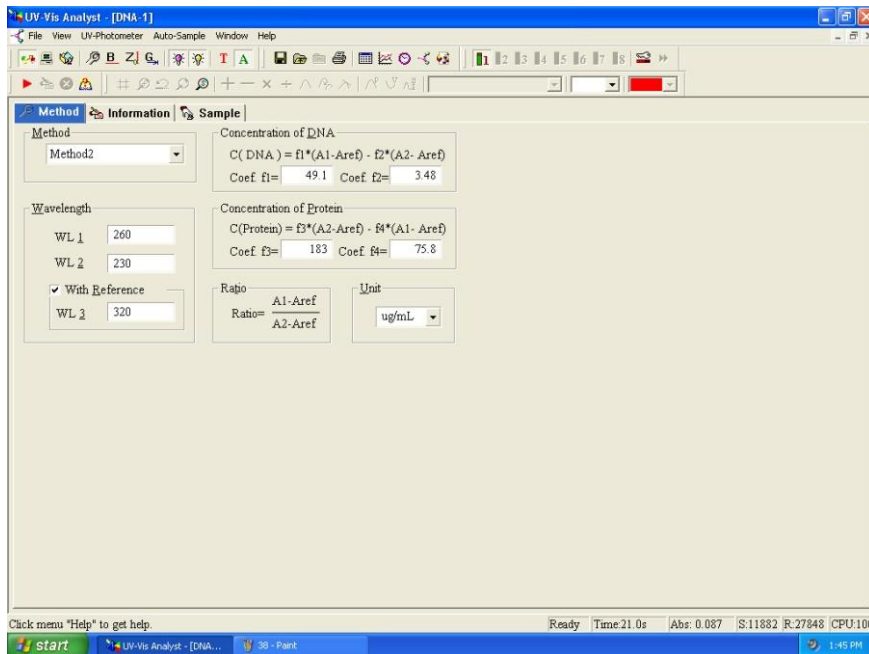
DNA/Protein Measurement

This chapter describes how to perform DNA/Protein

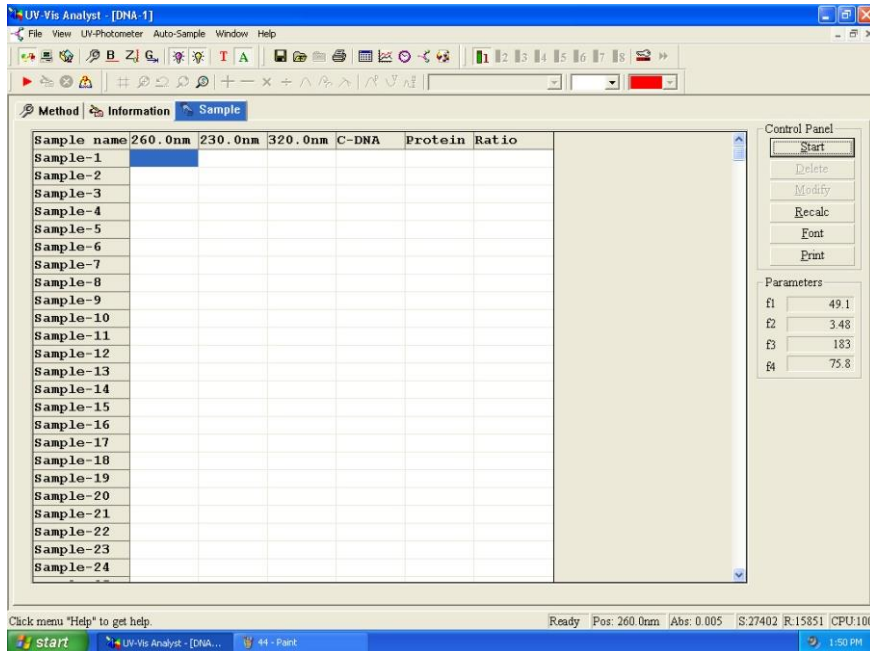
measurement.

DNA/Protein Measurement


1. Click  on the toolbar, the following dialog box will appear.



2. Click the **down** arrow of the **method** to select the **test method**. Key in the wavelength position in the **Wavelength** box. Key in the value of **DNA/Protein Conc.**
3. Click the **Sample** tab. It will display the following. The control menu contains six buttons: **Start**, **Delete**, **Modify**, **Recalculate**, **Font** and **Print**.




4. Do blank.

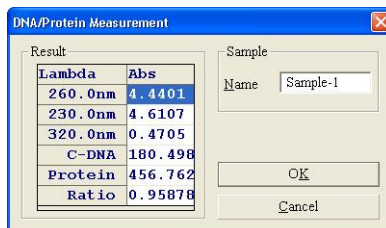
- **Single Beam:** Place the reference in the compartment, click .

- **Double Beam:** Skip to step 5.

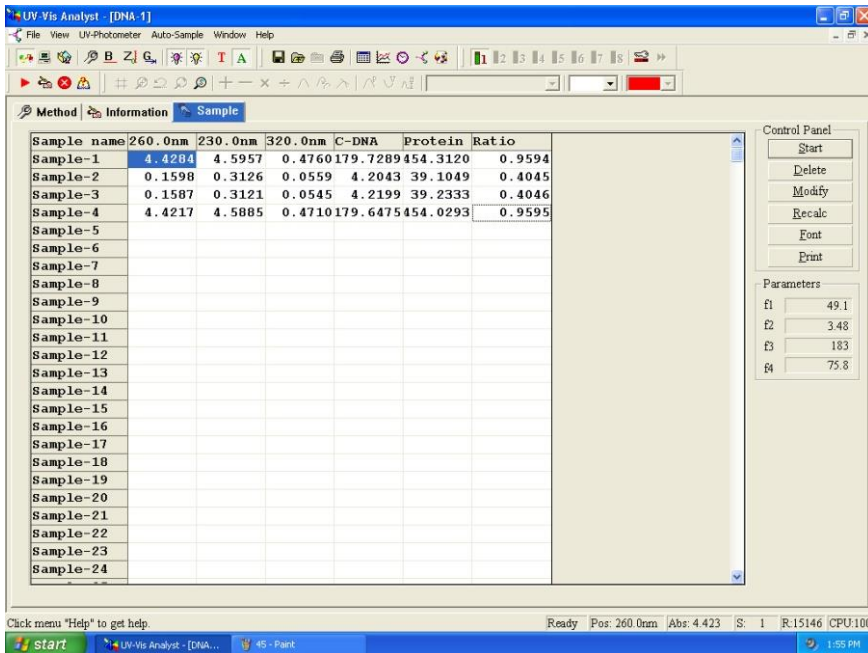
5. Measure Sample.

- **Single Beam:** Place the sample in the sample compartment.
- **Double Beam:** Place the reference in the reference compartment and place the sample in the sample compartment.

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



6. 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. Click **OK** after the measurement is complete. The photometric data for **Sample 1** will be listed in the sample table.
7. Repeat steps 5-6 to test all samples.



Appendix

Methods of Quantitative Analysis

Single Wavelength Method: $Abs. = A_1$

Double Wavelengths Method: $Abs. = m \cdot A_1 - n \cdot A_2$

Three Wavelengths Method: $Abs. = A_1 - (WL_1 - WL_2) \cdot (A_2 - A_3) / (WL_2 - WL_3) - A_3$

UV-VIS ANALYST SOFTWARE FOR SPECTROPHOTOMETER