User Manual

DRAWELL
Artist of Science

Please read the manual before installation and operation.

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Special Statement

Please read this manual carefully before installation or operation. The company will not take responsible for any trouble or damage due to unproper use.

The company has the final interpretation of this manual. Modifications of the manual due to improvements of the instrument will not be announced.

The company will conduct 12 months free repair from the date of delivery if the instrument is in strict accordance with the instructions and the transport safety specification. (Vulnerability and consumable parts as light source, cuvettes, sample cups are not included)

Please use our original packaging when returning the instrument for service with accessories and the warranty card.

Any chapteror images of this manual are not allowed to borrow, copy and translate to other languages without permission of the company.

Notice

1.The instrument is suitable for analysis in laboratory. If the instrument is needed outside the lab, please make the field work environment meets the environmental requirements of the laboratory.

2.Pleaseuse the original package when moving the instrument.

3.Pleasewait 30 minutes after turning on the instrument to make it stable.

4.When the instrument is on, the temperature of the vents on top left corner is high. Please keep the air circulating and away from the vents surface.

5. When the instrument is on, the temperature of the vents on top left corner is high. Please keep the air circulating and away from the vents surface.

6. Please make sure the fans on the left side and top left corner operate normally. If the fans are not functioning, please turn off the instrument for repairs.

7.When an error occurred by wrong operation or other machine or instrument error, shut down the instrument immediately. When the software is not operating properly, Start TaskManager to end the "Prolab.exe" process, then restart the software and the instrument.

8.DO NOT loose the screws in the monochromator. Keep the environment clean.

9.Cut the power before opening the instrument. Pay attention to the high-voltage electrical components on the left rear of the instrument.

10.Cover the instrument with dust proof if the instrument is not used for a long time.

MENU

1 Instrument Overview

1.1 Theory

The near-infrared spectroscopy does not require dilution of the sample, does not require a special short path, and does not disperse the sample with a non-absorbent matrix like traditional spectral analysis techniques such as mid-infrared and ultraviolet-visible spectroscopy. The way NIR spectra are collected can be divided into transmission and reflection modes.The transmission (Log (1/T)) method is used for transparent samples, and the diffuse reflection method (log (1/R)) is used for opaque or light scattering samples such as homogenates, suspensions, pastes, and solids.

1.Transmission

The NIR transmission spectrum of liquid samples is similar to other spectral analysis methods and can be performed in quartz cuvettes of different optical paths, and will not be described in detail here.

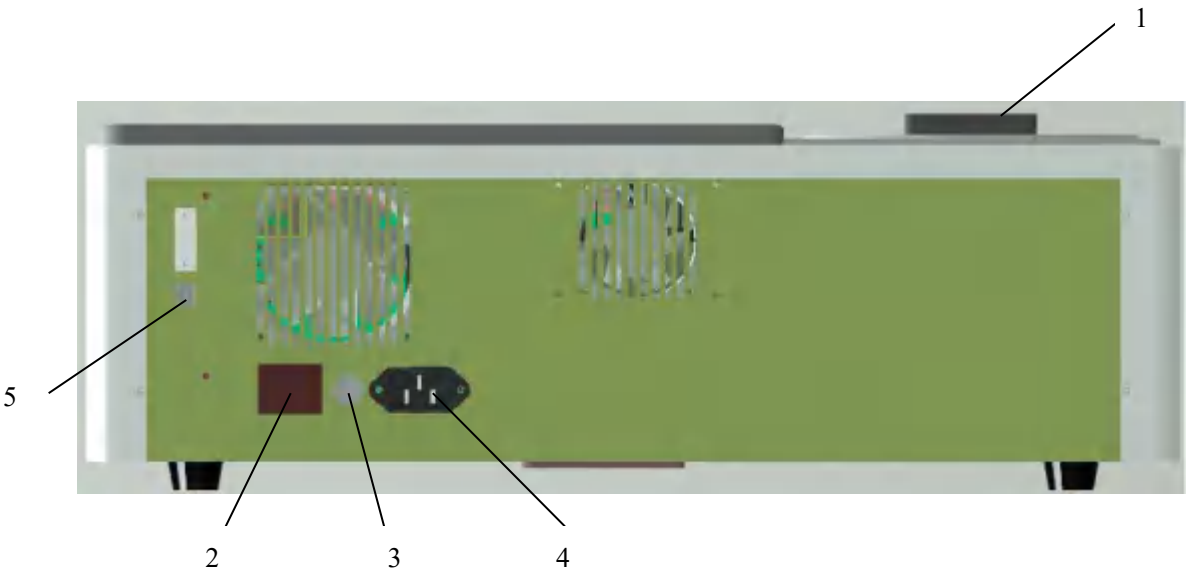
2. Reflection

The main difference between the diffuse reflectance spectrum and the conventional reflectance spectrum is that the latter light does not interact with the inside of the sample, so it does not carry the composition information of the sample. Diffuse light is the light that comes out of the light source and enters the inside of the sample. After repeated reflection, refraction, diffraction and absorption, it returns to the surface of the sample. Therefore, the diffuse light is the light that analyzes the light and the internal molecules of the sample, and loads the sample. Structure and composition information.

NIR spectra acquired by either transmission or diffuse reflection are difficult to identify characteristic spectra associated with a chemical composition. In order to improve spectral characteristics and compensate for baseline shifts, in the NIR spectrum, mathematical methods are often used to pre-process the spectra. Derivative processing is the most common and effective method. By first-order derivative or second-order derivative processing on the spectrum, the background absorption can be effectively deducted, the baseline offset and drift can be eliminated, and the overlapping spectrum can be separated.In the post-processing aspect, near-infrared spectroscopy must rely on modern chemometric algorithms and computer technology, using the full spectrum information of the near-infrared spectrum of the standard sample, that is, using the spectral data point group composed of all the data points of each sample spectrum to establish the sample. The mathematical relationship between the spectrum and the component to be tested, the so-called mathematical model, is used to calculate the near-infrared spectrum of the unknown sample to obtain the content of the component to be tested.

1.2 Appearance

Fig 1.2.1Appearance



1. Sample compartment2.Power switch3. Fuse4.Power socket 5.USB Port

Fig 1.2.2Left view

1.3

The near-infrared spectrometer adopts the integrating sphere diffuse reflectance spectrum acquisition method, which is suitable for measuring the near-infrared diffuse reflectance spectrum of powder or granular samples. The diffuse reflectance spectrum is collected from the bottom window position of the sample cup, and the sampling principle is shown in Figure 1.3.1

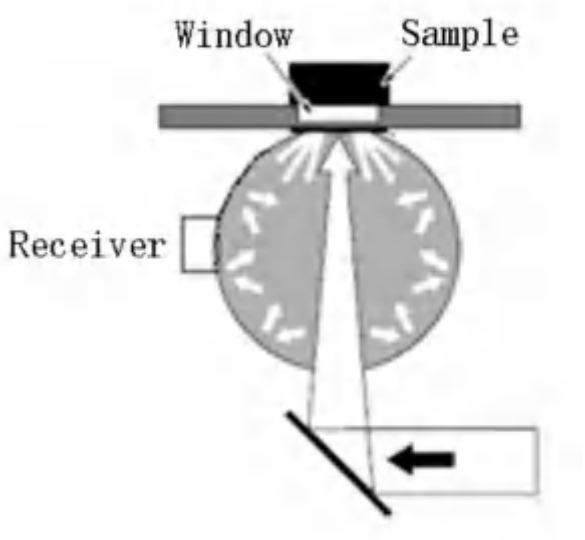


Figure 1.3.1

Load the sample into the sample cup, and the load piece is used for flattening.

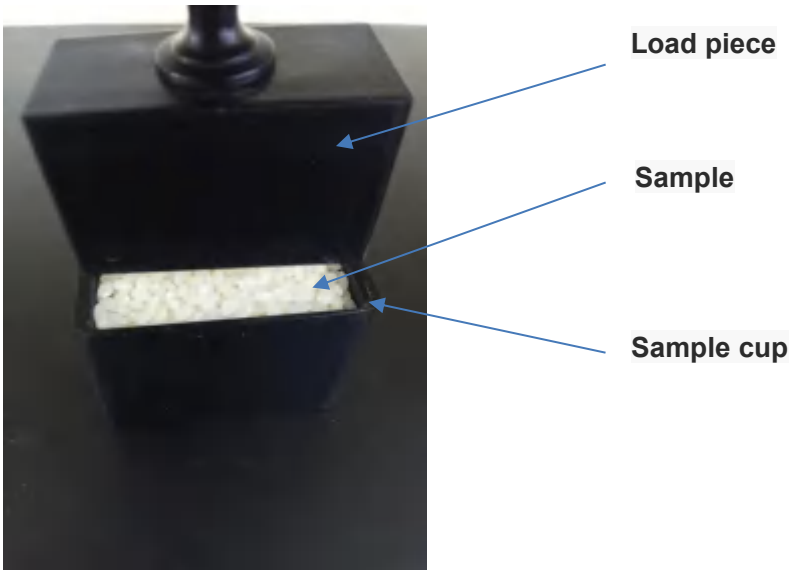


Figure 1.3.2

1.3 Performance

Measurement Method	Integrate-sphere
Bandwidth	12nm
Wavelength Range	900~2500nm
Wavelength Accuracy	≤0.2nm
Wavelength Repeatability	≤0.05nm
Stray Light	≤0.1%
Noise	≤0.0005Abs
Analysis Time	About 1 minute
Interface	USB2.0
Dimension	540x380x220mm
Weight	18kg

1.4 Packing List

1	Main instrument	set	1
2	Operation manual	copy	1
3	Certificate	piece	1
4	Software copy (In flash disk)	piece	1
5	Quartz Sample Cup	piece	2
6	Load part	piece	1
7	Brush	piece	1
8	Ear wash ball	piece	1
9	Fuse (2V)	piece	2
10	Power cable	piece	1
11	USB cable	piece	1
12	Packing list	piece	1

2 Environmental Requirements of Software

Please read the manual of Windows XP or higher version before reading this section. Windows XP is recommended.

When the operating system is Windows Vista or higher version, please run the software under administrator account. Otherwise the software may not run properly.

Please change the setting in Power Options"Put the computer to sleep" to "Never". Otherwise it may cause an error while running Prolab.

2.1 PC Requirements

2.1.1 Hardware Requirements

Hardware	Requirements
CPU	Intel 2.5GHz or same level CPU
Memory	No less than 2G
Hard drive	No less than 1G space
USB port	USB2.0
Monitor	Resolution 1024*768 or above Color 16bit or above

2.2 Install Prolab

- Boot your computer.
- Insert the Prolab disk, then open "My computer".
- Select your CD Rom in the browser.
- Double click "Setup" to install.
- Follow the steps and finish setup, then restart the computer.

3 Before Use

3.1 Connect to PC

Please use the USB cable to connect the instrument and PC. Driver installation will automatically start when first time connecting. Please run the software after driver installation is done.

3.2 How To Connect

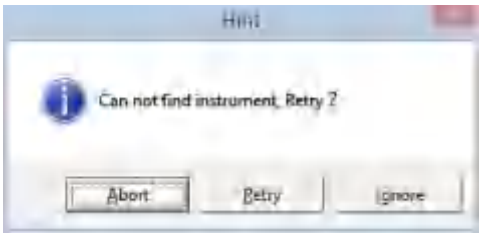
1. Plug in USB cable

Connect the instrument and PC with USB cable while the PC is on.

2. Turn on the instrument.

Turn on the instrument then run Prolab. The instrument will check if connected.

There will be a dialog pop out as below if not connected or connection error.



"Abort"：Exit the software.

"Retry"：Check again.

"Ignore"：Continue running Prolab. Other functions are available.

3. Initialization

The software will automatically start initializing and adjusting.

4. Interface.

Click  above to create a new measurement. Then select "Photometric", "Wavelength Scan", "Time Scan" or "Quantitaion" mode.

5. Shutting down

Close the software first, then turn off the instrument.

If you turn off the instrument first, there will be an error in Prolab. You need to run task manager to end the software.

4 Functions

4.1 Modes

There are 4 modes:

1. Photometric

（1） Measure the photometric data of the sample.
（2） Data display as Trans./Abs..
（3） Photometric data supports up to 26 wavelengths.
（4） support up to 10 user-defined calculation formula.
（5） Data printout available.

2. Wavelength Scan

（1） Get the spectrum of the sample.
（2） Display as Trans./Abs..
（3） Repeat scan available.
（4） Spectrum processing.
（5） Data printout available.

3. Time Scan

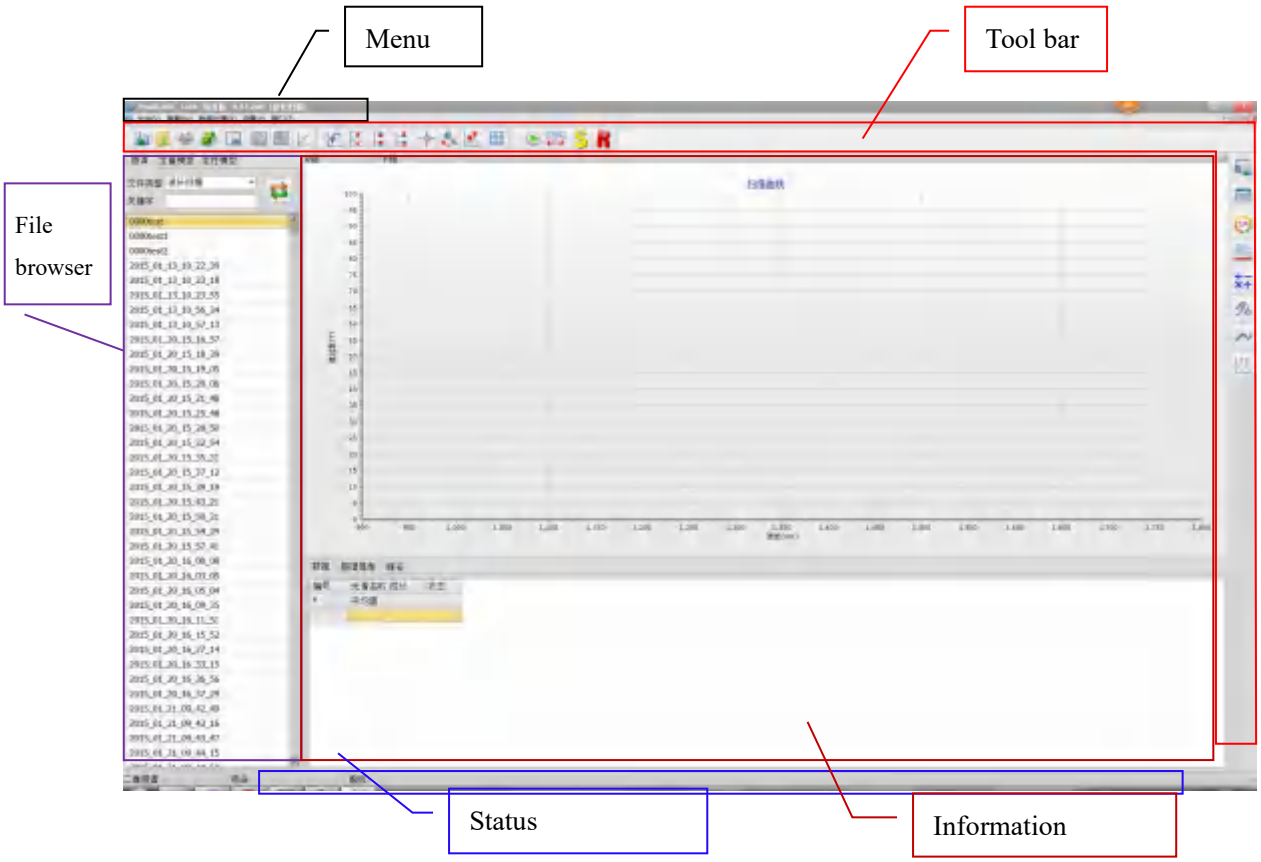
（1） Get the spectrum of sample varying by time.
（2） Display as Trans./Abs..
（3） Repeat scan available.
（4） Spectrum processing.
（5） Data printout available.

4. Quantitation

（1） Supports single-wavelength, dual wavelength and three-wavelength quantitative analysis.
（2） Supports 1 to 3 times curve fitting.
（3） Data decimal can be changed.
（4） Programmable optical gate control.
（5） Supports data printout.

4.2 Interface

4.2.1Modules



4.2.2Modules Intro

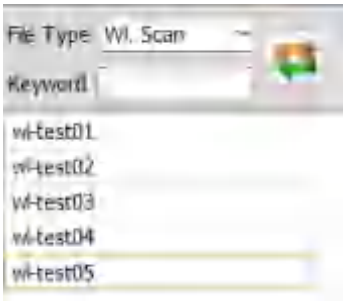
1. Menu & Toolbar

Menu & Toolbar

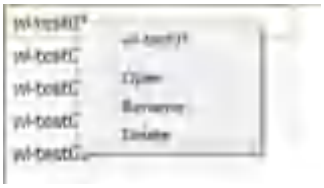
1) Provides instrument controls and settings.
2) Tool bar are shortcuts for common features.

2. Document Browser

Document Brower shows files saved in Wavelength Scan, Time Scan and Quantitative Analysis mode. Double click to open a file.



1) Double click a file to open/reset spectrum.
2) Right click a file to open, rename or delete.
3) Input keywords to search.



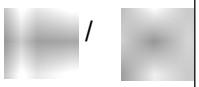
3. Spectrum Window & Information Window

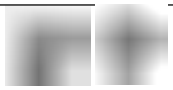
1) Information window shows current data and settings of the instrument.
2) In spectrum window, you can use mouse to zoom in and out. Press the left mouse button, drag the mouse from top left to bottom right to draw a square, then release the button. Spectrum in that square will be zoomed in. Drag the mouse the opposite way to zoom out.
3) Click “Peaks” to show the peaks in the spectrum.

4. Status Window

Status window shows the current status of the instrument.

4.2.3Icons

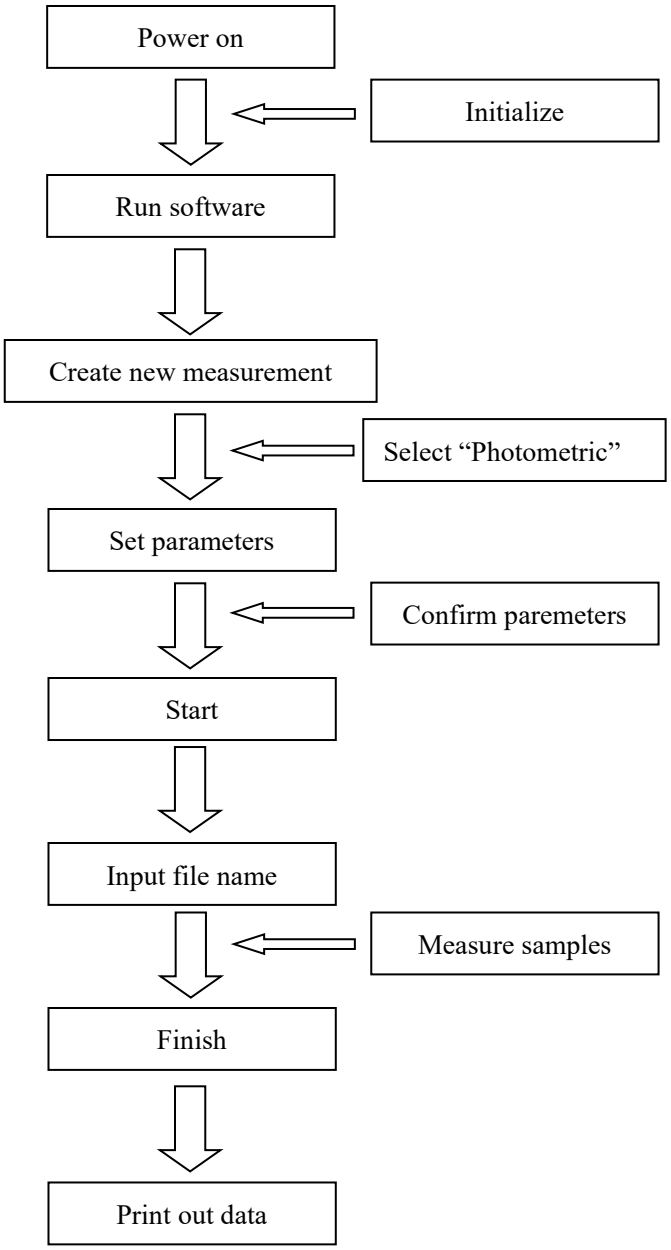
Icon	Function
	New Measurement
	Open Spectrum
	Show/Hide Status
	Show/Hide Spectrum Information
	Wavelength scan / Time scan
	Photometric window
	Quantitation window
	Back to original coordinate
	Auto coordinate
	Y-axis enlarge 2 times
	Y-axis reduce 2 times
	Get/Cancel Axis Data
	Zoom In/Out
	Show/Hide Peaks
	Show/Hide Grid
	Start/Stop

	Set wavelength
	Set 100%
	0%
	Set baseline
	Spectrum Properties
	Print Data
	Trans. / Abs.
	Move sample rack to “Sample” position
	Move sample rack to “Reference” position
	Current status online/offline

5 Software Operation

5.1 Photometric

Photometric work flow

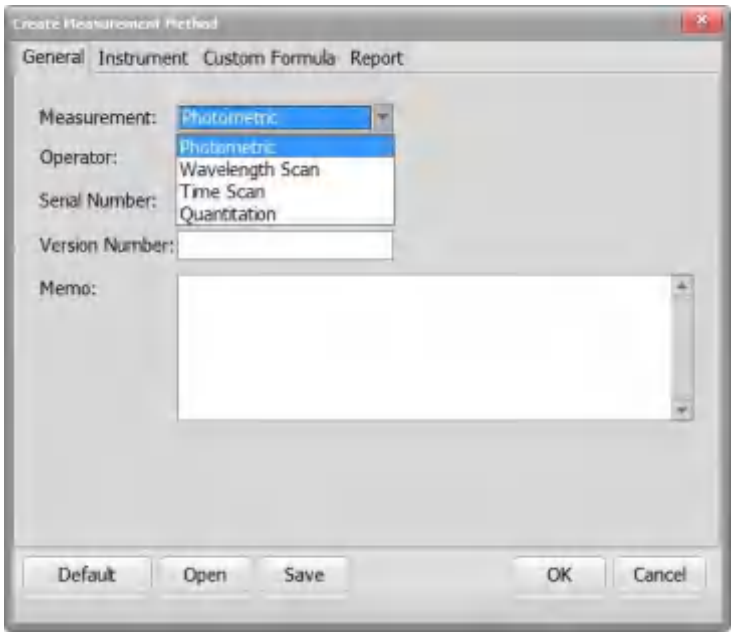


5.1.1 Create Measurement

Create a new measurement.

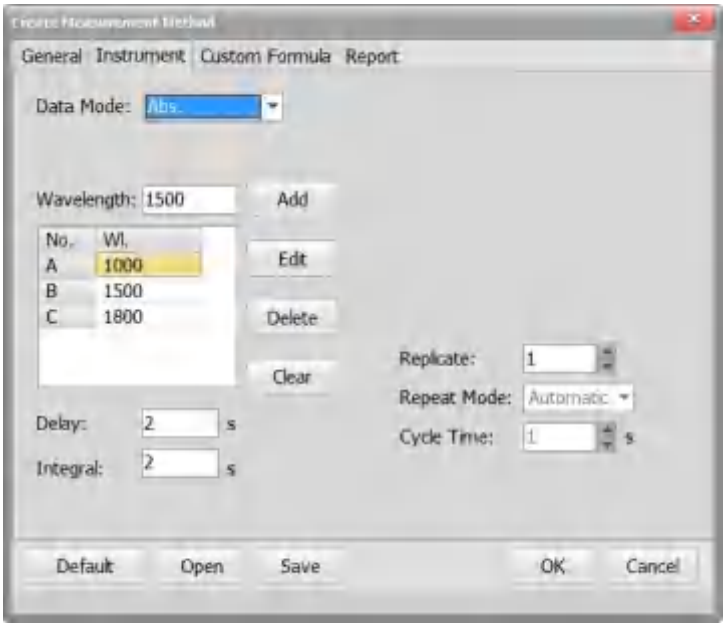
Select “Files”->“Create Method” or click  to enter Create Method Window.

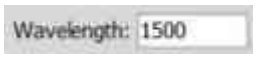
1. Measurement summary：



1) Measure Mode: Choose “Photometric”.
2) Operator: Input operator’s name.
3) Serial Number: Shows the serial number of the instrument.
4) Version Number: Shows the version of the instrument.
5) Memo: Enter a description or notes on measuring conditions.
6) Click Default to reset.
7) Click Open to open saved parameters.
8) Click Save to save the parameters.

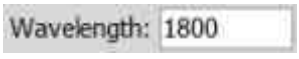
2. Instrument Tab：



1) Data Mode: Data display as Trans. or Abs.
2) Wavelength: Input wavelength in 

, then click 

to add it in the table.
3) Change wavelength:Select the wavelength in the table 

, then change the value here 

. Click 

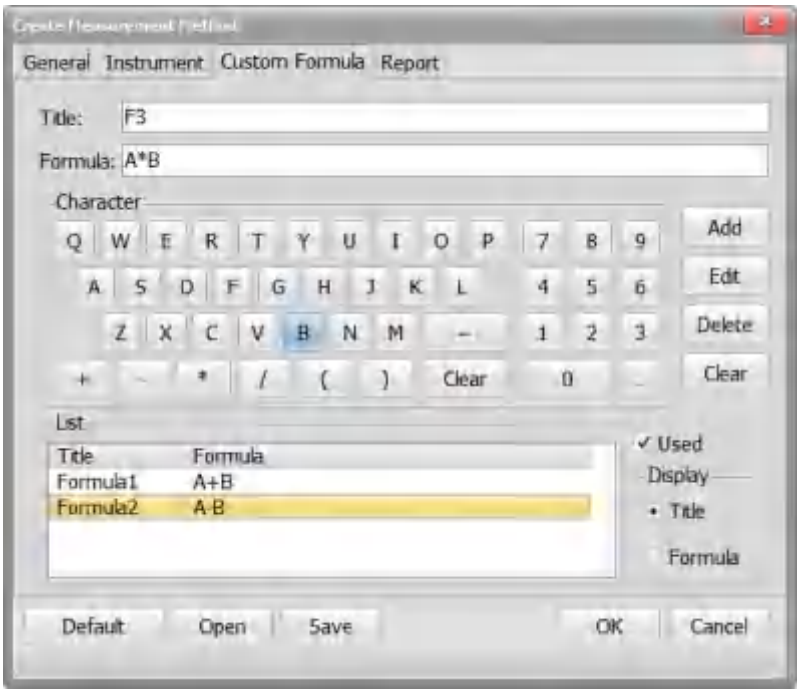
to finish.
4) Delete wavelength: Select the wavelength in the table 

. Click 

to delete it.
5) Clear:Click 

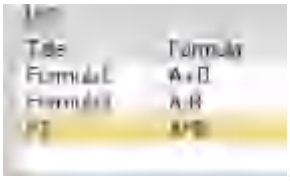
to delete all wavelengths.
6) Delay:Delay time before measuring. Usually for stabilization.
7) Integral: Data integral time.
8) Slit: Slit of the instrument.
9) Light source: Shows the switch wavelength of deuterium lamp / tungsten lamp.
10) Lamp status: Switch deuterium lamp / tungsten lamp (Not available here).
11) Gain: Set a gain to measure sample (Not available here).
12) Replicate: Set the number of repeat measurements.The instrument will only scan once when it's 1.
13) Cycle time: Set a repetition interval.
14) Auto rotate: When this option is checked, in the process of repeated scanning, the sample cup will rotate at a certain angle after scanning a spectrum, and then perform the next repeated spectrum scan. The angle of rotation is automatically calculated according to the number of repeated scans to ensure that the sample rotates for one week after completing all repeated scans. (This function is mainly used on samples with uneven distribution of components, to increase the scanning area of the spectrum on the sample, and to improve the stability and accuracy of data analysis)

3. Custom Formula Tab：

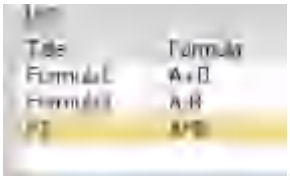


1) Title: Input formula title.
2) Formula: Use the keyboard below to input formula.
3) Add formula: Input formula here 

and click 

to add it in the list.
4) Change formula: Select the formula you want to change 
,edit it here 

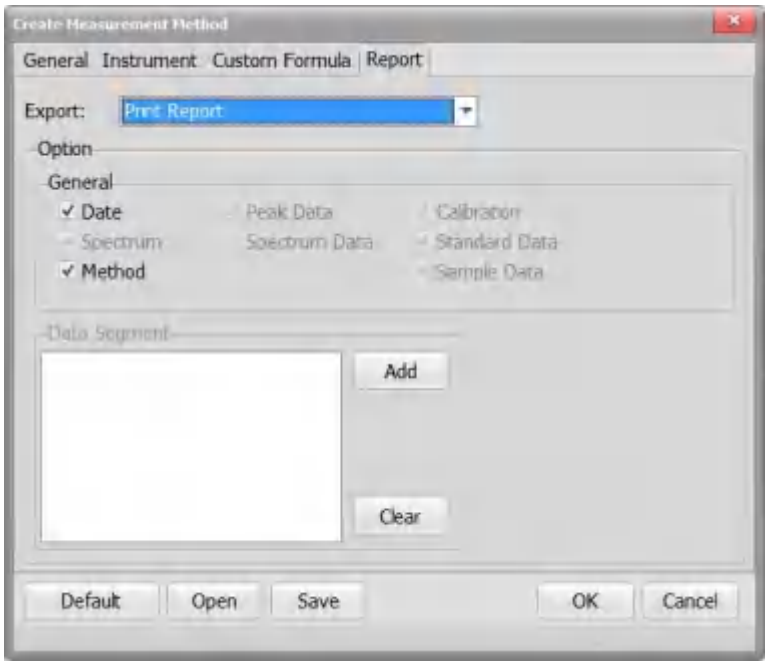
and click 

to finish.
5) Delete formula: Select the formula you want to delete 
, then click 

to delete it.
6) Clear: Click 

to delete all formula.
7) Used:Check to calculate after measurement.
8) Display: Display title or formula.

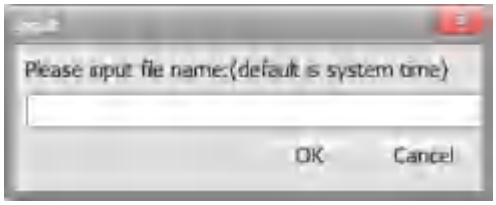
4. Report Tab：



1) Export: Choose “Print Report” or “Save as Microsoft（R）Excel file”.
2) General-Date: Add output date.
3) General-Method: Show output method.
4) Other check box not available in Photometric mode.

5.1.2Start a Measurement

1. Create Photometric measurement as 2.3.1.1.
2. Put the reference sample in the sample cell and click  to set 100% and 0%.
3. Put sample in the sample cell and click  to start measuring.
4. There will be a popout window after the first measurement. Input file name and click OK (or leave it) to save. Data will be saved in this file unless you create a new measurement.

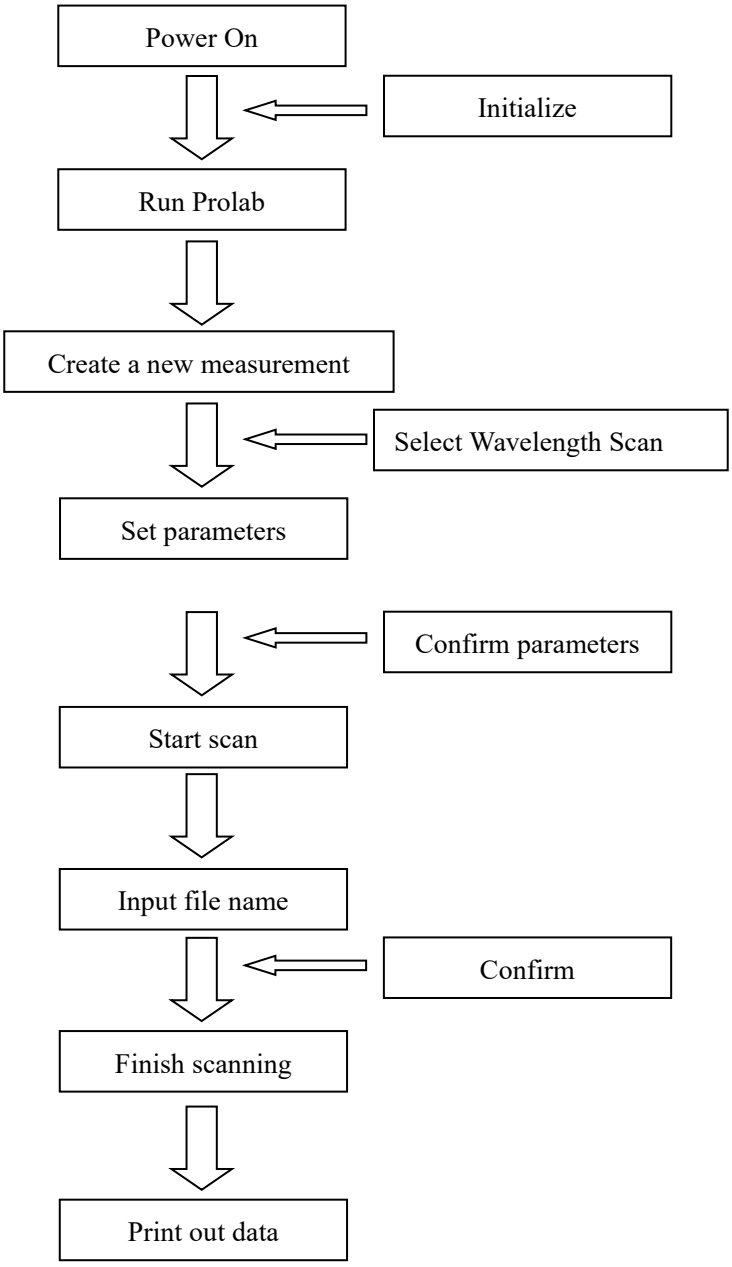


5.1.3Data Processing

1. Click  to show current method.
2. Click  to print out data.

5.2 Wavelength Scan

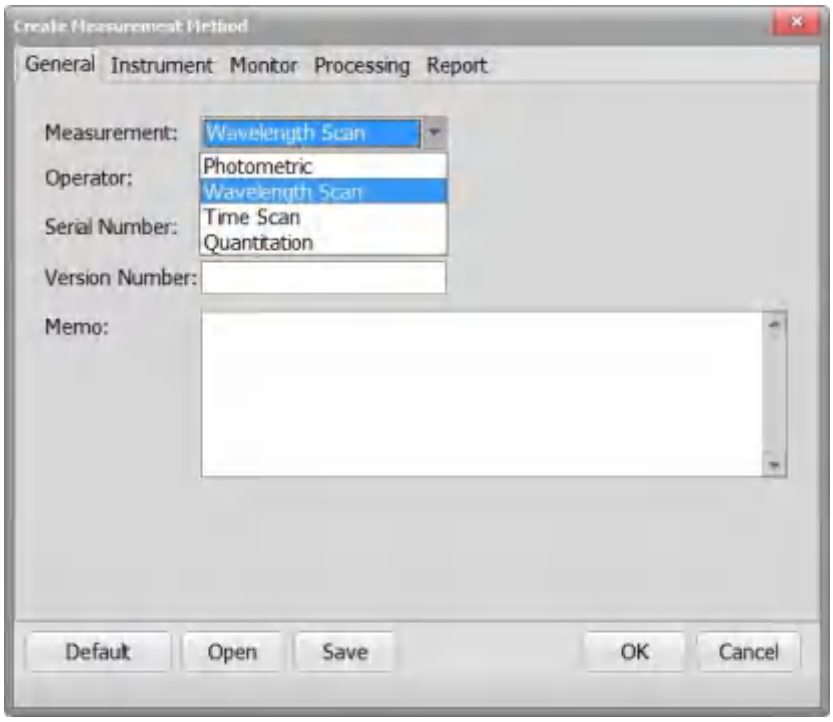
Wavelength Scan work flow



5.2.1Create a Measurement

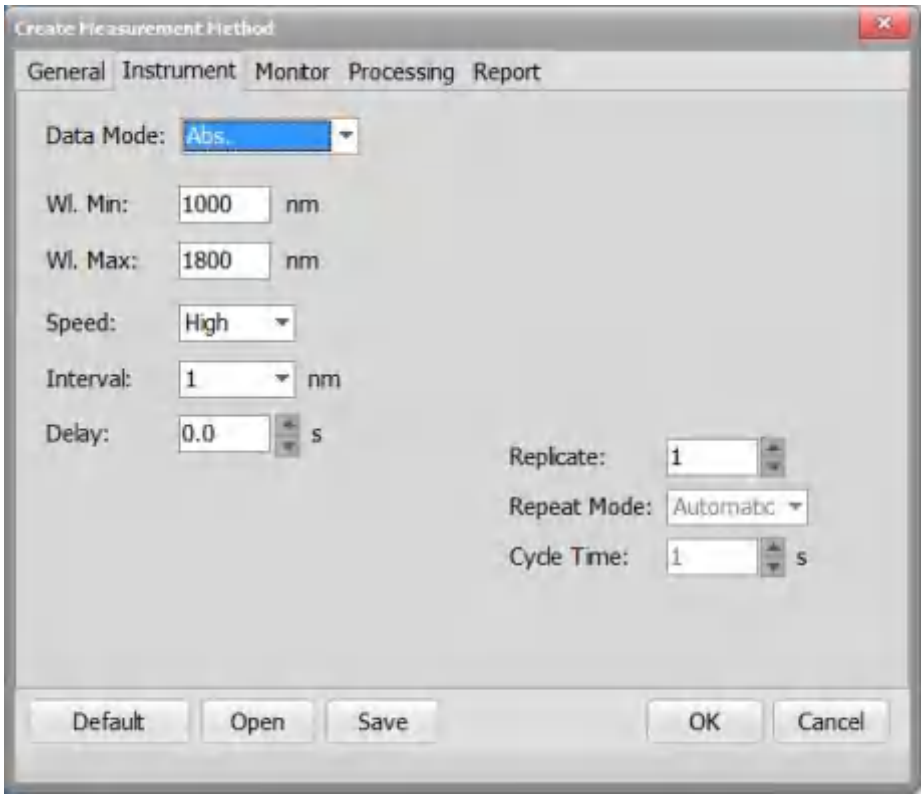
Select “Files”->“Create Method” or click  to enter Create Method Window.

1. General Tab：



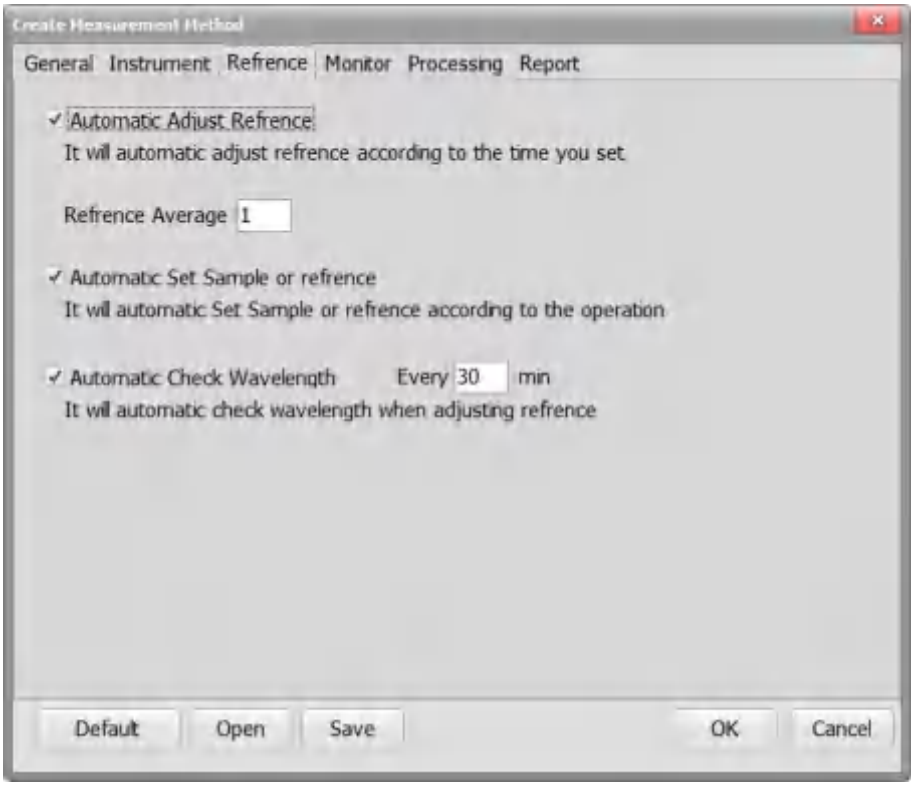
a) Measure Mode: Choose “Wavelength Scan”.
b) Operator: Input operator’s name.
c) Serial Number: Shows the serial number of the instrument.
d) Version Number: Shows the version of the instrument.
e) Memo: Enter a description or notes on measuring conditions.
f) Click  to reset.
g) Click  to open saved parameters.
h) Click  to save the parameters.

2. Instrument Tab:



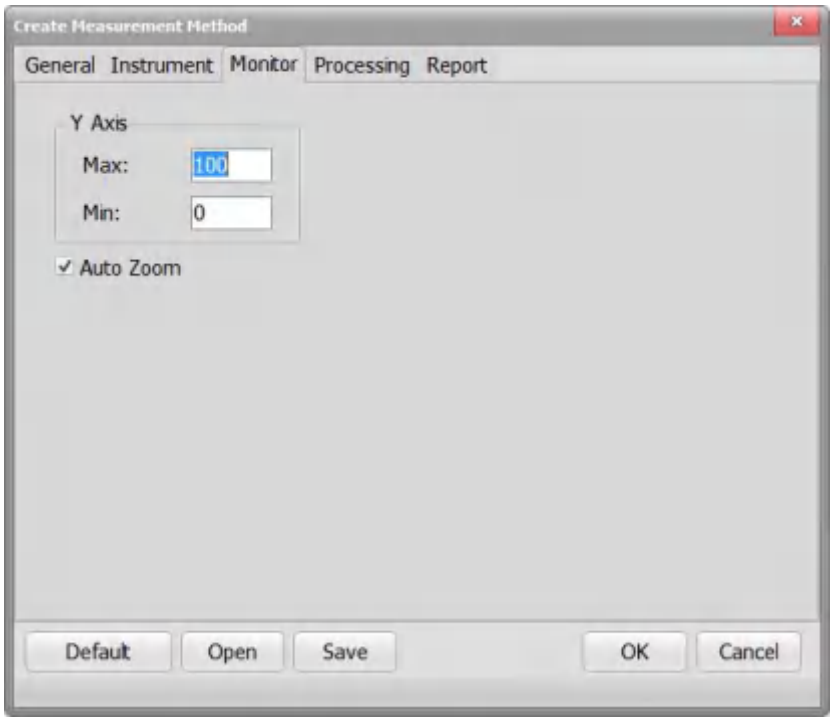
1) Data mode: Data display as Abs., Trans. or Energy.
2) WL.Min: Input the start wavelength.
3) WL.Max: Input the ending wavelength.
4) Speed: Select the scan speed. The faster the more noise appears.
5) Interval: Shows data sampling interval according to the scan speed.
6) Delay: After pressing the Measure button, measurement isstarted following the delay time set here.
7) Slit: Slit of the instrument.
8) Replicate: Set the number of repeat measurements.The instrument will only scan once when it's 1.
9) Cycle time: Set a repetition interval.
10) Auto rotate: When this option is checked, in the process of repeated scanning, the sample cup will rotate at a certain angle after scanning a spectrum, and then perform the next repeated spectrum scan. The angle of rotation is automatically calculated according to the number of repeated scans to ensure that the sample rotates for one week after completing all repeated scans. (This function is mainly used on samples with uneven distribution of components, to increase the scanning area of the spectrum on the sample, and to improve the stability and accuracy of data analysis)

3. Reference Tab:



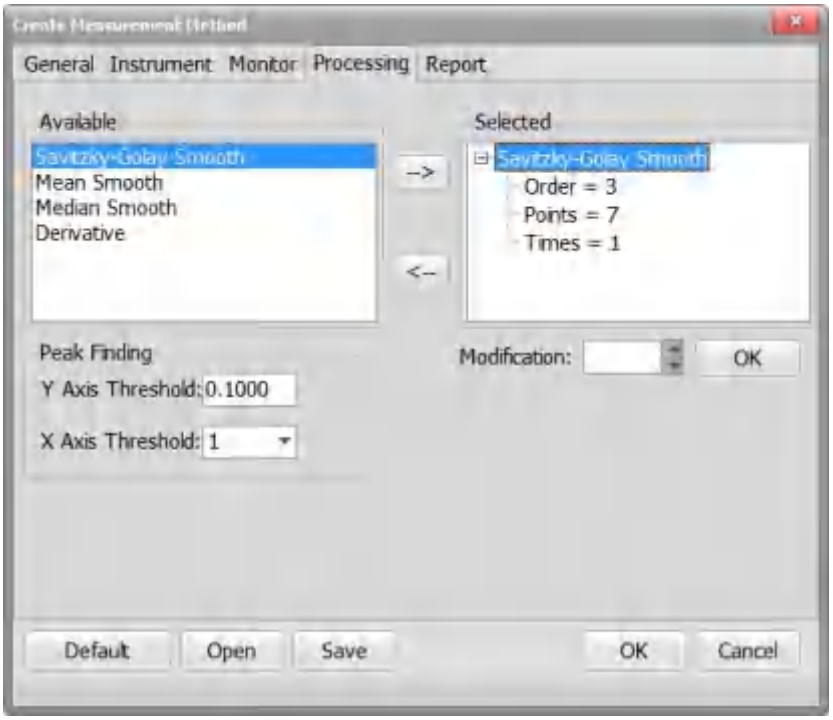
1) Automatic Adjust Reference: recommend value: 4.
2) Automatic Set Sample or reference: Automaticly move the sample or reference.
3) Automatic Check Wavelength: Every XX minutes to check the wavelength.

4. Monitor Tab



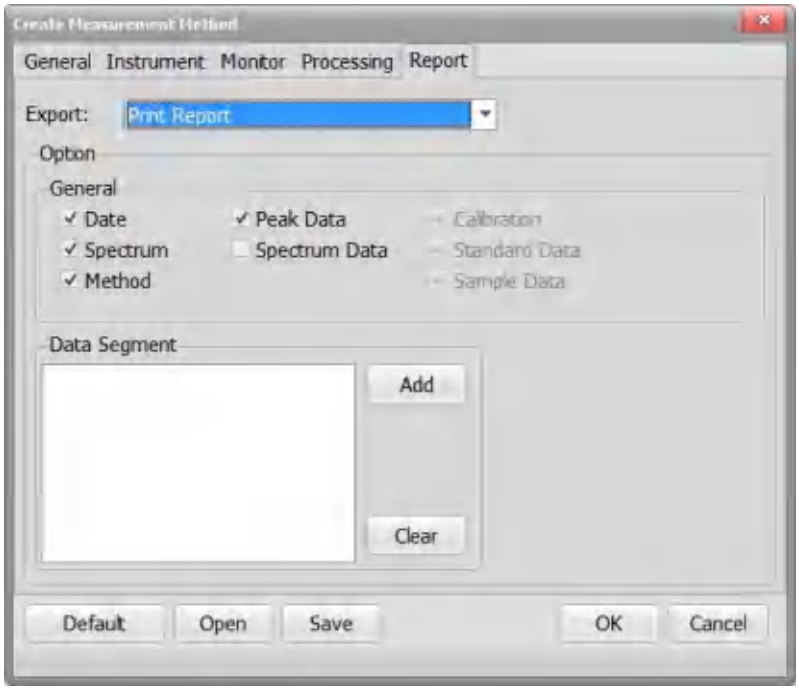
1) Y Axis: Enter the max and min point of Y axis.The max point should be larger.
2) Auto Zoom: Y axis will automatically set by spectrum data.

5. Processing Tab：



1) Available:Savitsky-Golaysmooth,Mean smooth, Median smooth and Derivative are available for data processing.
   a) Click a method in the “Available” box then click -> to put it in the Selected box.
   b) Click a method in the “Selected” box then click <- to remove it.
2) Selected: Final data will be calculated with methods in the Selected box. You can set parameters for each method.
3) Modification: Click the + to unfold the parameters of each method, click to change it in “Modification”.
4) Peak Finding: Automatically find peaks by giving threshold when the scan is complete.

6. Report Tab：

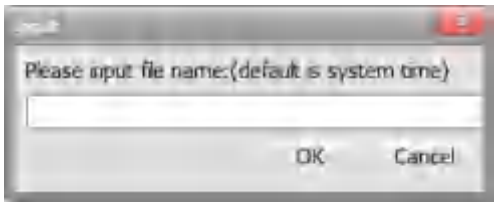


1) Output: Print Report or Save as CSV file.
2) Output options: Choose the printout data.Check the content in “Properties” button on the left after the scan.
3) Add Data: When “Spectrum Data” is checked,you can choose data section to printout.Set the start wavelength, end wavelength and interval in the pop out window,then click OK.Click the “+”to see the data section. Up to 9 sets of data.

4) Clear Data: Clear current data section.

5.2.2Start a wavelength scan

1. Create a new measurement.
2. Put reference sample in the sample cell and click  to adjust baseline.
3. Put sample in the sample cell and click  to start scanning.
4. There will be a popout window after the first measurement. Input file name and click OK (or leave it) to save.



5. Click  to stop the scan.

5.2.3Data Processing

1. Click  to show the method detail.
2. Click  to print out data.
3. Click  to reset original coordinate.
4. Click  to automatically zoom Y axis.
5. Click  to zoom in Y axis 2 times.
6. Click  to zoom out Y axis 2 times.
7. Click  /  to get/cancel axis data of the cursor.
8. Click  to zoom as set.
9. Click  /  to show/hide peaks.
10. Click  to show/hide grid.
11. Click  to move sample cell.
12. Click  to switch between Trans. and Abs.

13. Click  to run spectrum comparison.
14. Click  to run spectrum calculation.
15. Click  to run Spectrum derivation.
16. Click  to run Spectrum Smoothing.
17. Click  to find peaks.

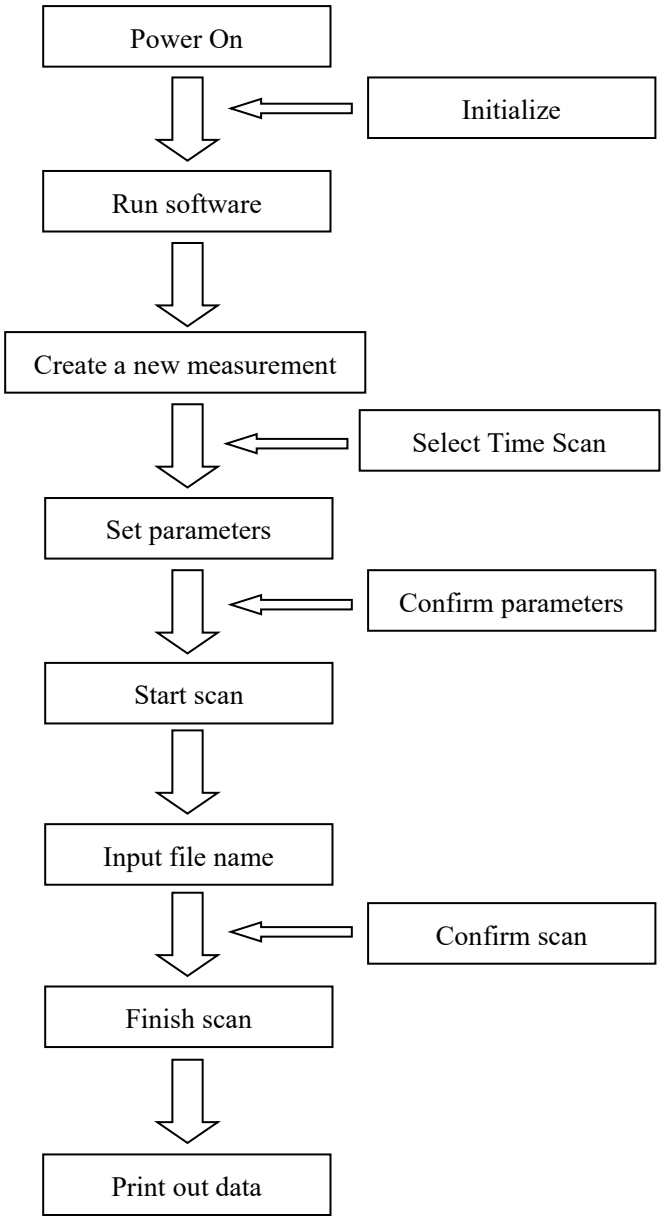
5.2.4Database

For users who need to build models for PCA, Prolab will automatically save wavelength data as .DX files in the Prolab directory/DX folder. You can also save wavelength data as .CSV files in Printout data.

We recommend using Unscramler to open the .DX files to start principal component analysis.

5.3 Time Scan

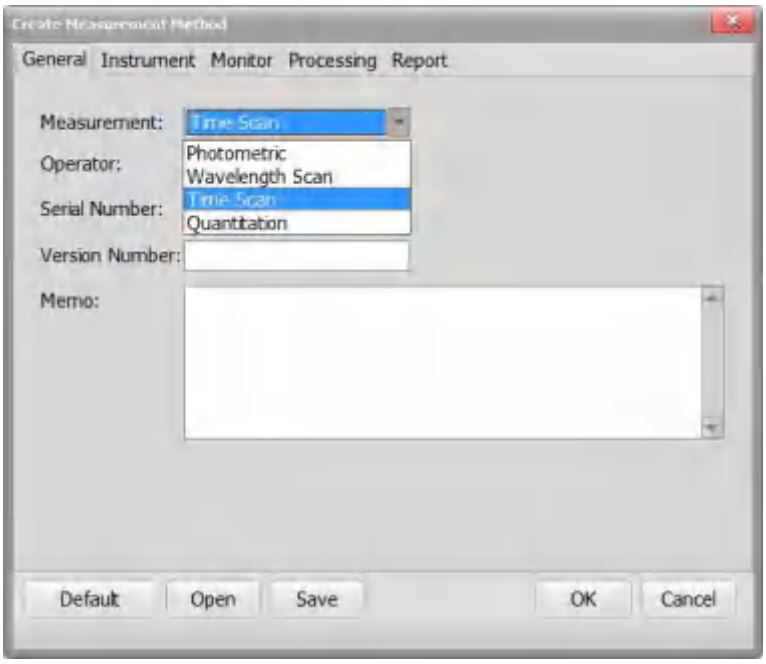
Time scan work flow



5.3.1Create a new measurement

Select “Files”->“Create Method” or click  to enter Create Method Window.

1. **General Tab：**



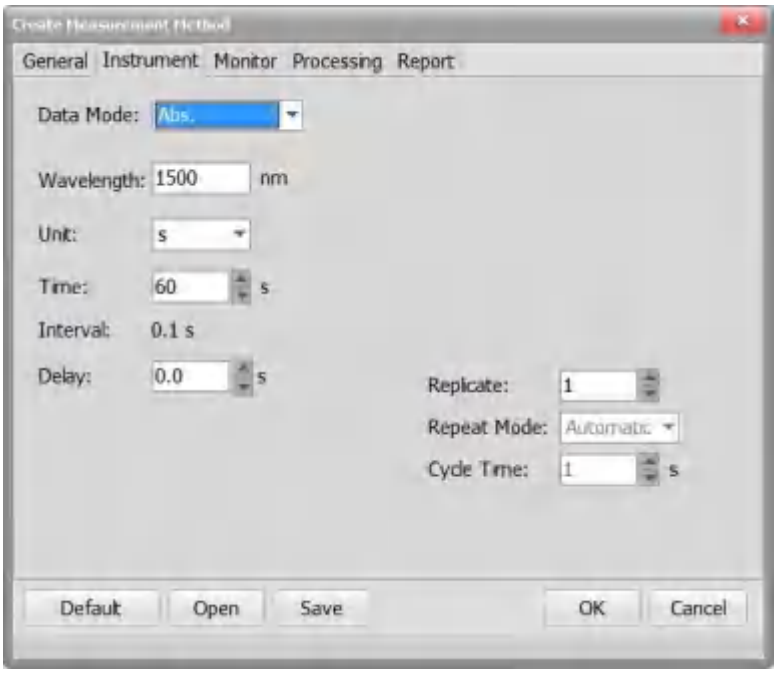
a) Measure Mode: Choose “Time Scan”.
b) Operator: Input operator’s name.
c) Serial Number: Shows the serial number of the instrument.
d) Version Number: Shows the version of the instrument.
e) Memo: Enter a description or notes on measuring conditions.
f) Click 

to reset.
g) Click 

to open saved parameters.
h) Click 

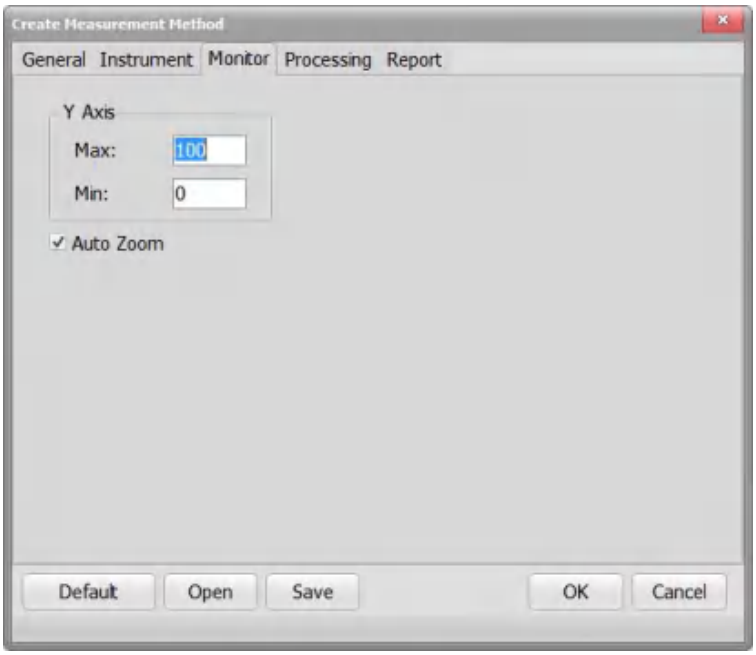
to save the parameters.

2. Instrument Tab：



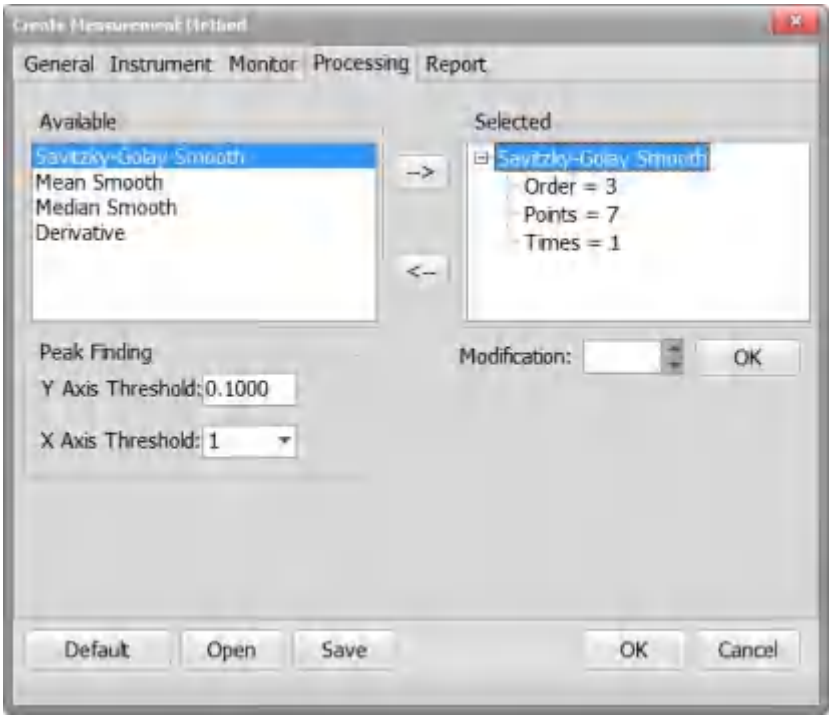
1) Data mode: Data display as Abs.,or Trans.
2) Wavelength: Input time scan wavelength.
3) Unit: Set time unit to sec or ms.
4) Time: Set the scan time.
5) Interval: Fixed at 0.1 sec.
6) Delay: Delay time before scan.
7) Slit: Fixed at 8nm.
8) Replicate: Set the number of repeat measurements.The instrument will only scan once when it's 1.
9) Cycle time: Set a repetition interval.
10) Auto rotate: When this option is checked, in the process of repeated scanning, the sample cup will rotate at a certain angle after scanning a spectrum, and then perform the next repeated spectrum scan. The angle of rotation is automatically calculated according to the number of repeated scans to ensure that the sample rotates for one week after completing all repeated scans. (This function is mainly used on samples with uneven distribution of components, to increase the scanning area of the spectrum on the sample, and to improve the stability and accuracy of data analysis)

3. Monitor Tab



1) Y Axis: Enter the max and min point of Y axis.The max point should be larger.
2) Auto Zoom: Y axis will automatically set by spectrum data.

4. Processing Tab：



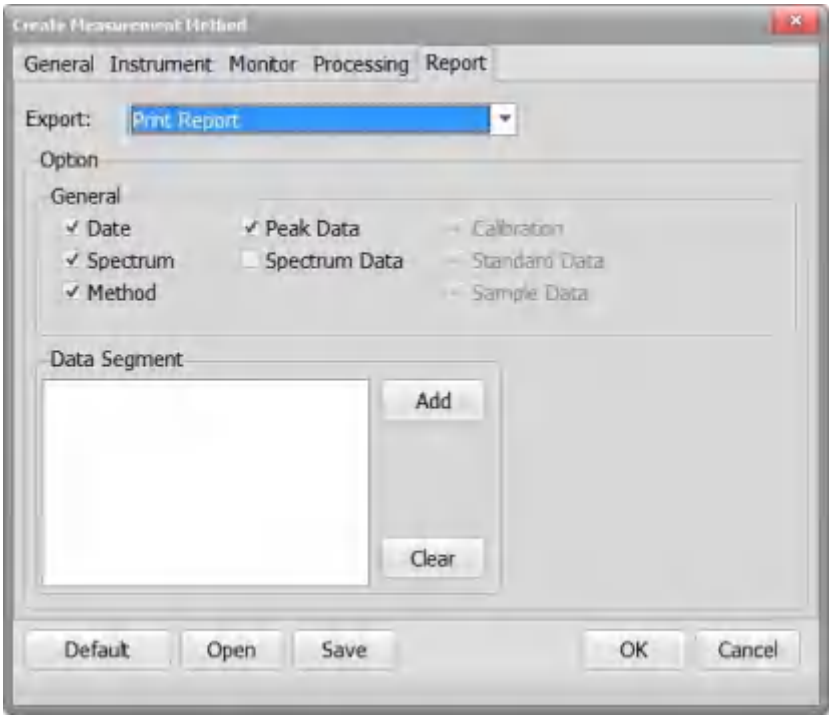
1. Available:Savitsky-Golaysmooth,Mean smooth, Median smooth and Derivative are available for data processing.

a) Click a method in the “Available” box then click  to put it in the Selected box.

b) Click a method in the “Selected” box then click  to remove it.

2. Selected: Final data will be calculated with methods in the Selected box. You can set parameters for each method.
3. Modification: Click the ⊞ to unfold the parameters of each method, click to change it in “Modification”.
4. Peak Finding: Automatically find peaks by giving threshold when the scan is complete.

7. Report Tab：

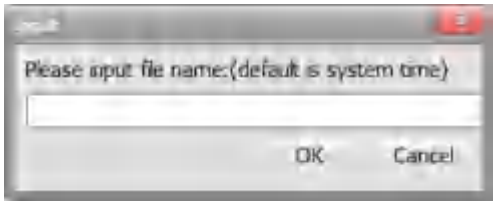


1) Output: Print Report or Export to CSV file.
1) Output options: Choose the printout data.Check the content in “Properties” button on the left after the scan.
2) Add Data: When “Spectrum Data” is checked,you can choose data section to printout.Set the start wavelength, end wavelength and interval in the pop out window,then click OK.Click the “+” to see the data section. Up to 9 sets of data.

3) Clear： Clear current segment

5.3.2 Start a Time Scan

1. Create a new time scan measurement as 2.3.3.1.
2. Put reference sample in the sample cell, then click  to set 100%.
3. Click  to set 0%.
4. Put sample in the sample cell, then click  to start scan.
5. There will be a pop-out window after the first measurement. Input file name and click OK (or leave it) to save.



6. Click  to stop the scan.

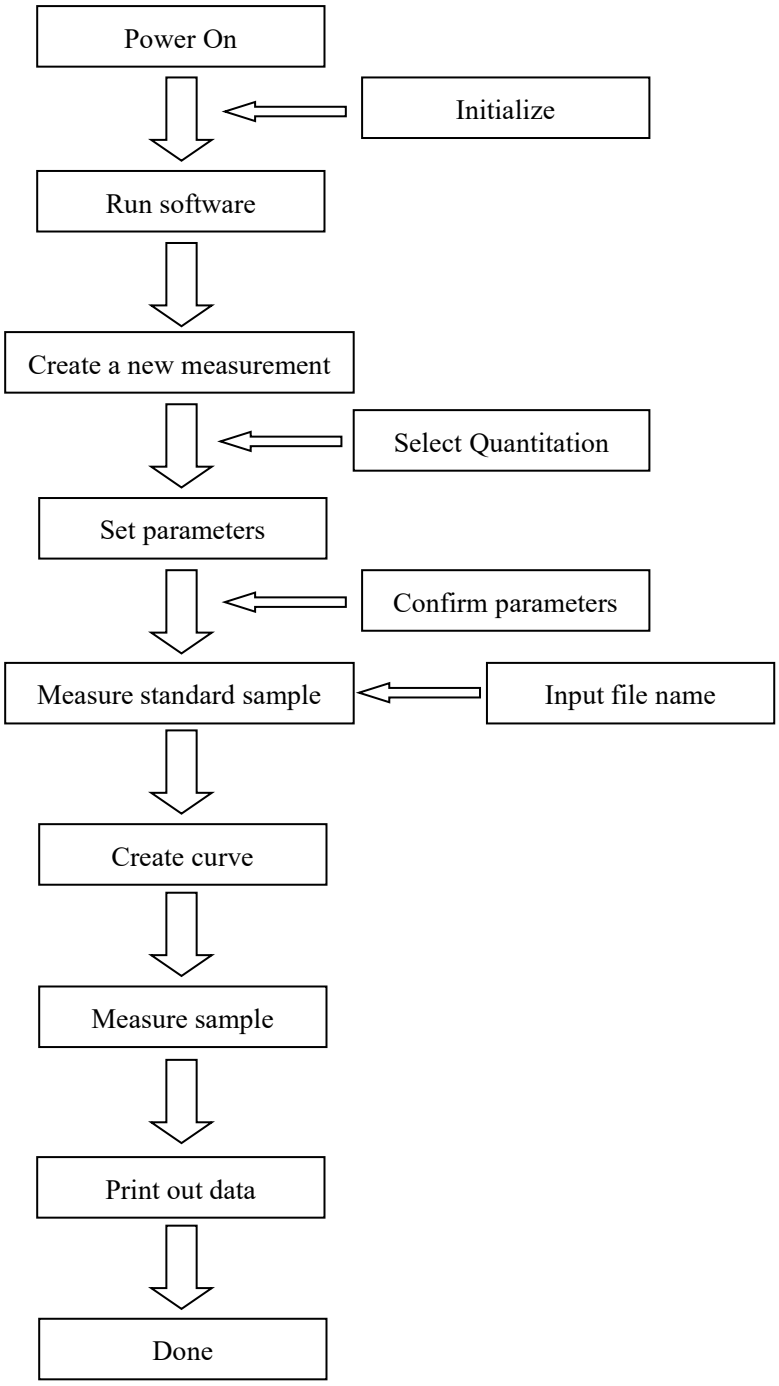
5.3.3Data Processing

1. Click  to show detail of current method.
2. Click  to print out data.
3. Click  to reset original coordinate.
4. Click  to automatically zoom Y axis.
5. Click  to zoom in Y axis 2 times.
6. Click  to zoom out Y axis 2 times.
7. Click  /  to get/cancel axis data of the cursor.
8. Click  to zoom as set.
9. Click  /  to show/hide peaks.
10. Click  to show/hide grid.

11. Click  to move sample cell.
12. Click  to switch between Trans. and Abs.
13. Click  to do spectrum comparison.
14. Click  to do spectrum calculation.
15. Click  to do spectrum derivation.
16. Click  to do spectrum smoothing.
17. Click  to run peak finding.

5.4 Quantitation

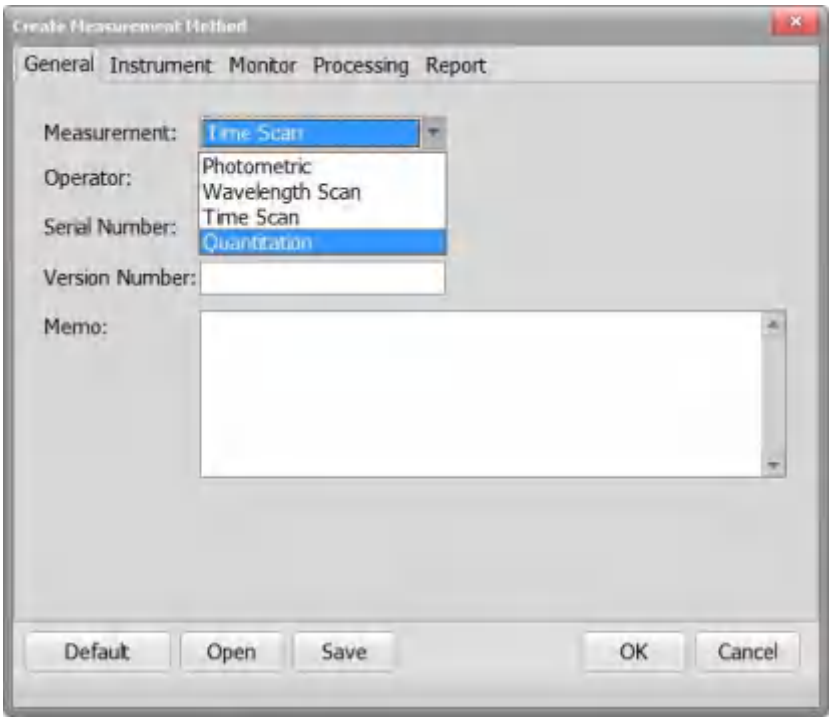
Quantitation work flow



5.4.1Create a measurement

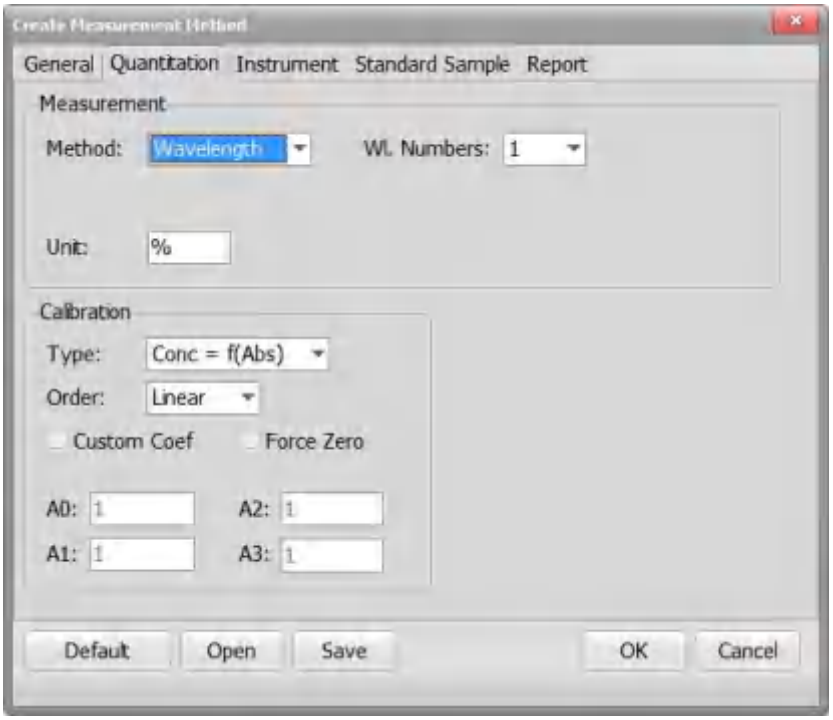
Select “Files”->“Create Method” or click  to enter Create Method Window.

1. General Tab：



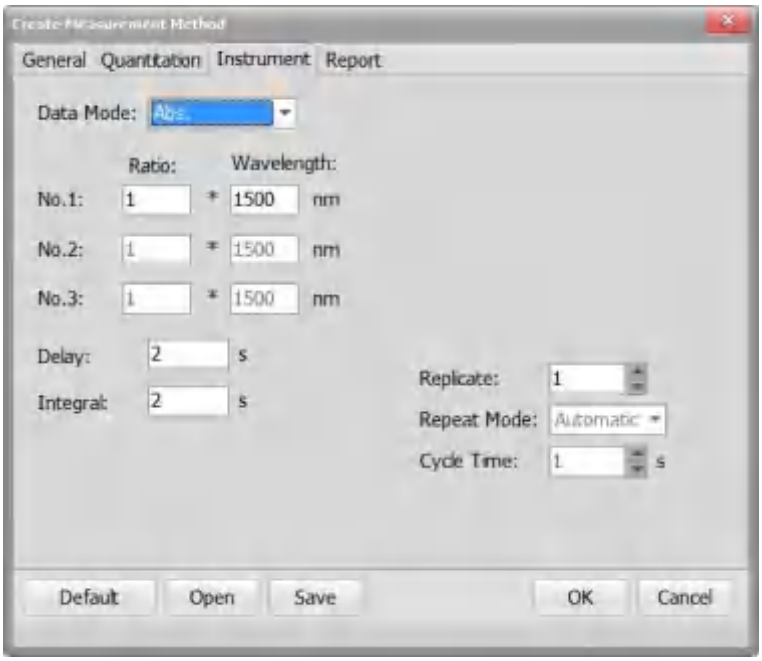
a) Measure Mode: Choose “Time Scan”.
b) Operator: Input operator’s name.
c) Serial Number: Shows the serial number of the instrument.
d) Version Number: Shows the version of the instrument.
e) Memo: Enter a description or notes on measuring conditions.
f) Click  to reset.
g) Click  to open saved parameters.
h) Click  to save the parameters.

2. Quantitation Tab：



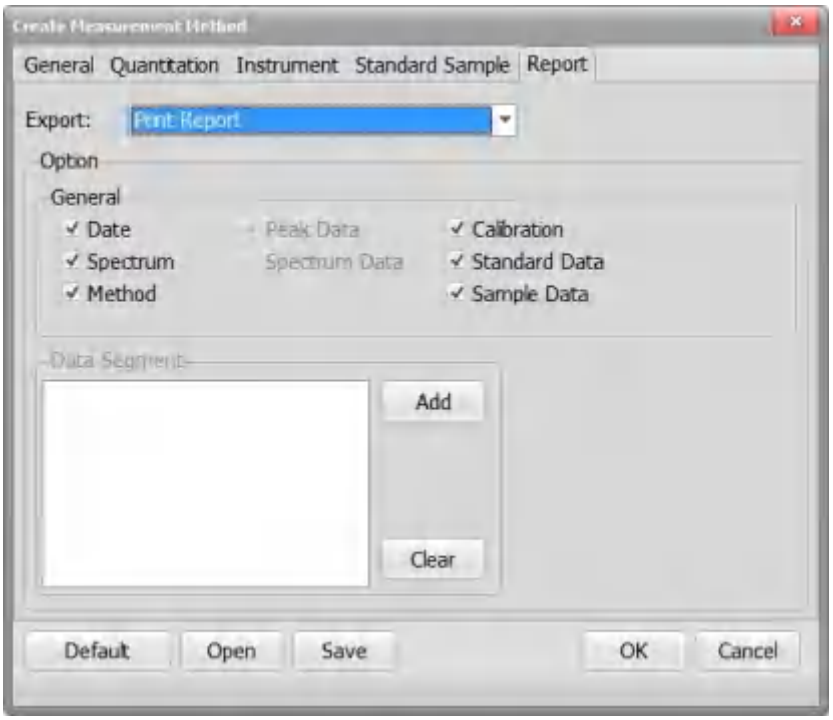
1) Method: Quantitation method. Only wavelength available now.
2) WL Number: Number of wavelengths to analyse with.
3) Unit: Concentration unit.
4) Type: The type of fomula to display.
5) Order: Linear, Quadratic and Cubic available.
6) Custom Coef: Check the box to customize equation as "$\mathrm{Conc} = \mathrm{A0} + \mathrm{A1} * \mathrm{X}^1 + \mathrm{A2} * \mathrm{X}^2 + \mathrm{A3} * \mathrm{X}^3$".
7) Force Zero: Check the box to force the (0,0) point fits the equation.

3. Instrument Tab：



1) Data mode: Choose Abs. or Trans. to display value.
2) Wavelength: Input test wavelengths based on WL numbers in Quantitation tab. When WL number is 3, the number of 3 wavelengths need to be increasing or decreasing.
3) Delay: Delay time before scan.
4) Integral: Data integral time.
5) Slit: Fixed at 8nm.
6) Replicate: Set the number of repeat measurements.The instrument will only scan once when it's 1.
7) Cycle time: Set a repetition interval.
8) Auto rotate: When this option is checked, in the process of repeated scanning, the sample cup will rotate at a certain angle after scanning a spectrum, and then perform the next repeated spectrum scan. The angle of rotation is automatically calculated according to the number of repeated scans to ensure that the sample rotates for one week after completing all repeated scans. (This function is mainly used on samples with uneven distribution of components, to increase the scanning area of the spectrum on the sample, and to improve the stability and accuracy of data analysis)

4. Report Tab：

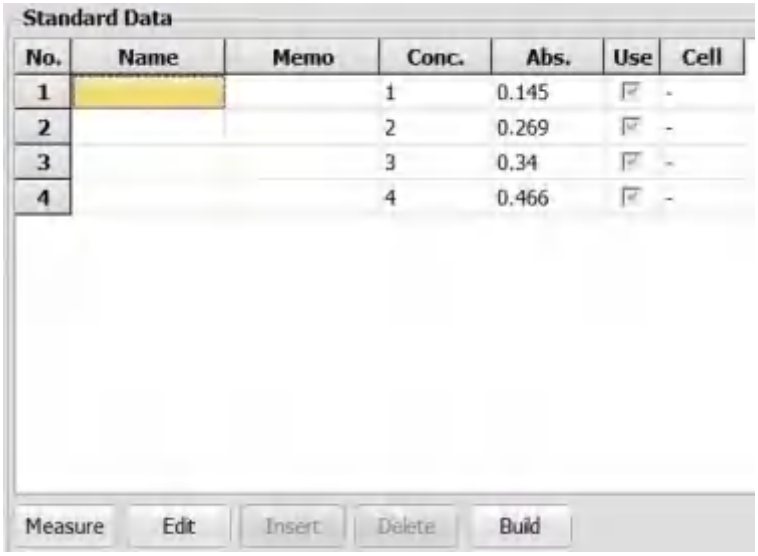


1) Export: Print Report or Export to file.
2) Date: Export with date.
3) Spectrum: Export with spectrum.
4) Method: Export with method detail.
5) Calibration: Export with equation.
6) Standard Data: Export with standard data.
7) Sample Data: Export with sample data.

8) Others are not available in Quantitation.

5.4.2Biuld Calibration Curve

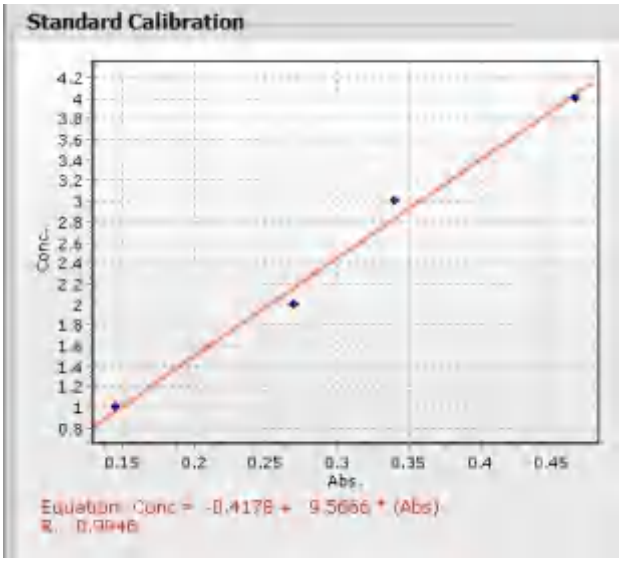
1. In the Standards window, you can modify sample name, description and concentration; add or delete sample; check the value of samples.



1) To change sample name, description and concentration: Click Edit, then double click in the table to modify the content you want. Then click OK to confirm.
2) Measure a standard sample: Click to select a sample in the table, then click Measure button. The instrument will start measurement.
3) Add Sample: Click Edit, then click Insert. There will be another line in the standards window. Click OK to finish.
4) Delete Sample: Click Edit and click a line you want to delete, then click Delete. Click OK to finish.
5) Choose the sample data needed in curve calculation: Click Edit, then click the check mark in Use row if you want to use this data for calculation.
6) Set sample cell: Click Edit and set sample cell of samples in Cell colume. "-" means do not move sample cell. Click OK to

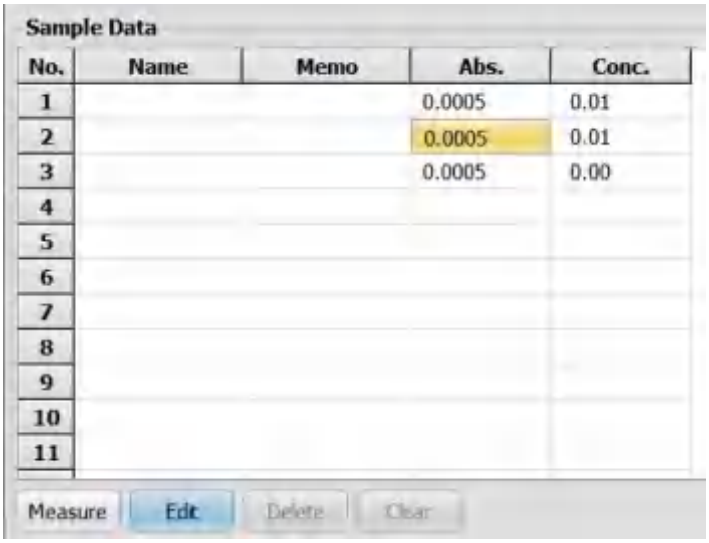
finish.

2. Click Build to build the curve of standard sample when finishing measurement.



5.4.3Measuring unknown samples

When the regression curve is created, you can start measuring the sample. Operate the test sample in samples window as below. There are functions in the sample window: Measure, Modify, Delete and Clear.



1) Change sample name & note: Click Edit button, then double click the frame you want to modify. Click OK to confirm the modification and back to test sample window.
2) Measure sample value: Click a sample value frame, then click Measure button to measure the sample. The value of the sample will be in

"Abs." and "Conc." column.

3) Delete sample: Click Edit button, then click the line you want to delete and click Delete button to delete the sample. Click OK to confirm the modification and back to test sample window.

4) Clear sample list: Click Edit button, then click Clear button. Click OK to confirm the modification and back to test sample window.

5.4.4Data Processing

1. Click to show detail of current measurement.
2. Click to print out data.

5.5 General Operation

5.5.1Wavelength

When the instrument is not measuring (shows Ready below), click  to open wavelength dialog. Input the wavelength you want then click OK to go.

Wavelength range:

- S430：1000nm~1800nm

5.5.2Set 100%

When the instrument is not measuring (shows Ready below), click  to set 100%. Status shows Adjust Full Data Set 100 below. When it shows Ready, means it is done.

5.5.3Set 0%

When the instrument is not measuring (shows Ready below), click  to set 100%. Status shows Adjust Zero Set Zero below. When it shows Ready, means it is done.

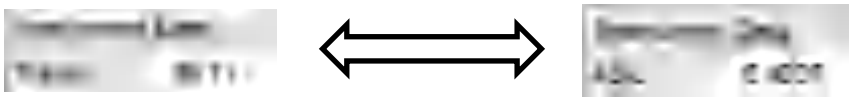
5.5.4Move sample rack

When the instrument is not measuring (shows Ready below), click  to move sample rack. Status shows Shifting Sample Cel below. When it shows Ready, means it is done.

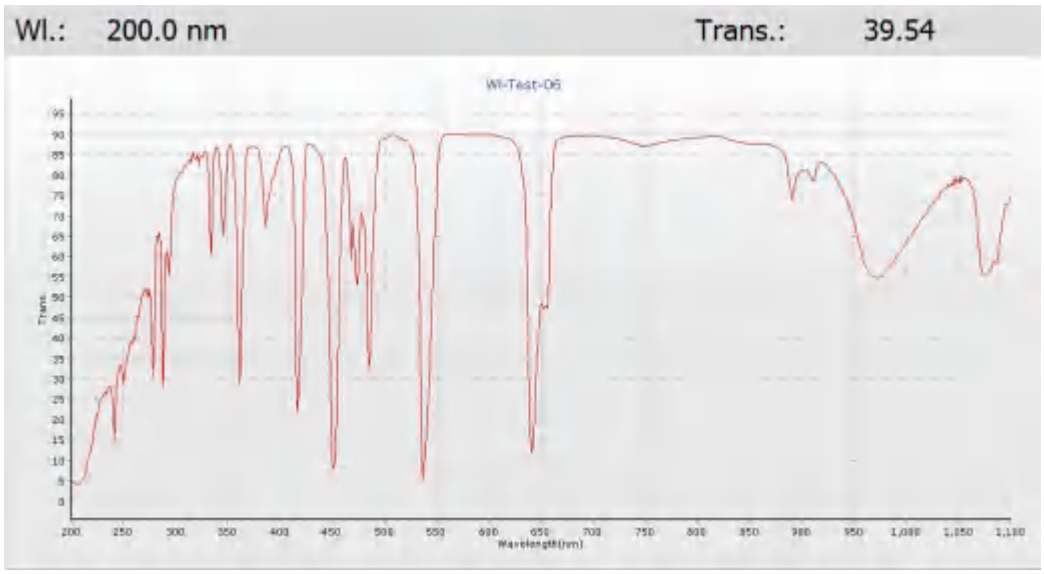
5.5.5Switch T/A

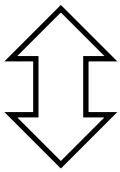
When the instrument is not measuring (shows Ready below), click to switch T/A.

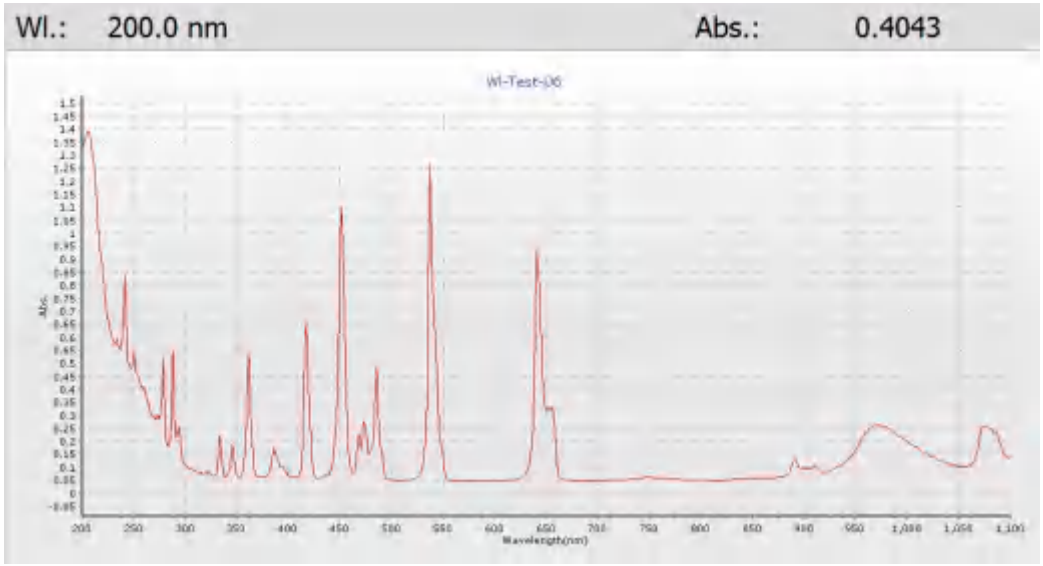
Switch current value



- Switch spectrum data

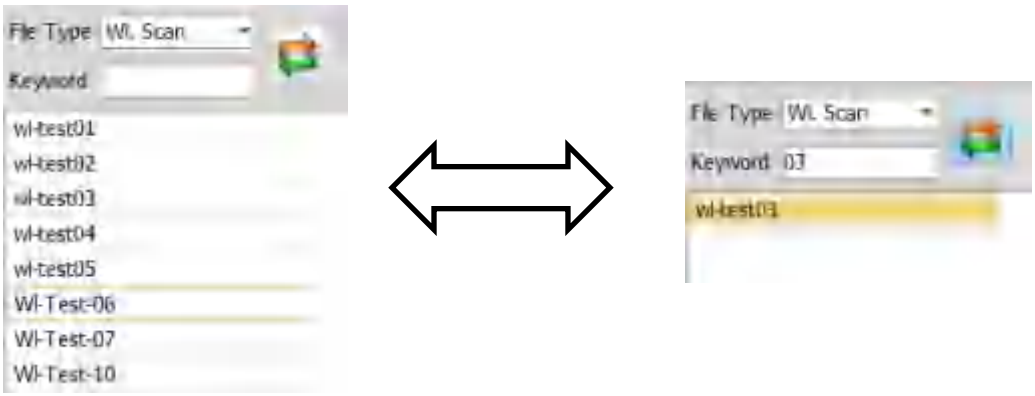






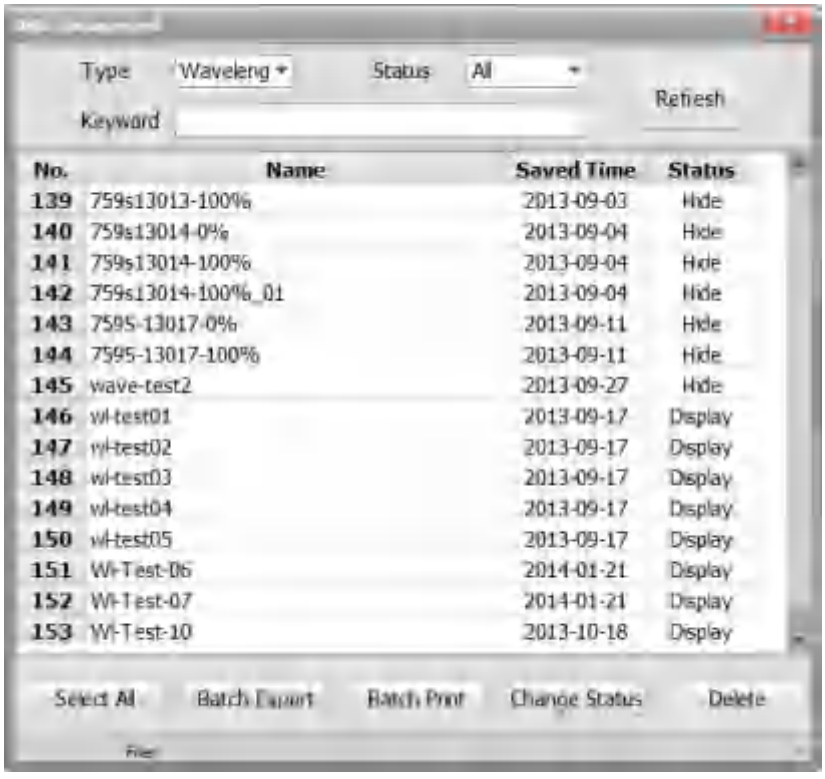
5.5.6Locate file

To locate test files, you can input keyword in keyword blank.



5.5.7Data management

Click File-Data management to enter Data management. In data management you can quickly delete, export, hide in batch.

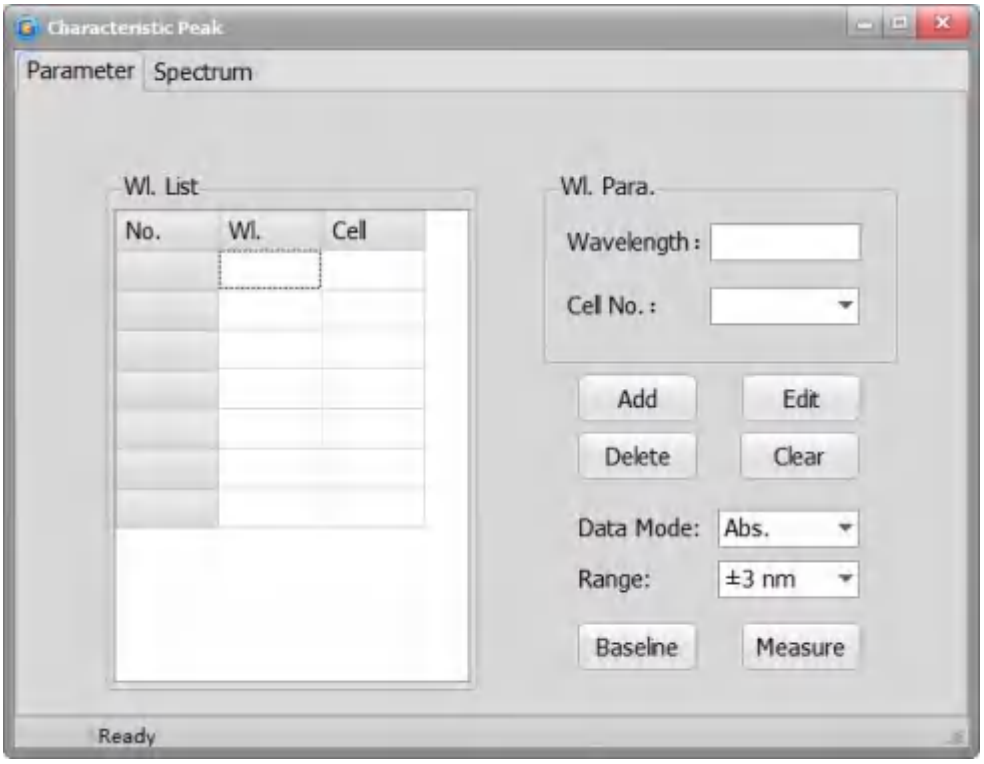


1. Refresh: Select type, status and input keyword, then click  to show the fitting files.
2. Batch Export: Select the files you need, then click  to export CSV file. This will export all data.

3. Batch Print: Select the files you need, then click Batch Print to print one by one.It will print all data in the file.
4. Change status: Switch between Display/Hide. Hidden files won't be seen in the list outside Data management.
5. Delete: Select the files you want to delete, then click Delete to delete those files.

5.5.8Characteristic Peak

Click Data Processing – Characteristic Peak to enter Characteristic Peak dialog.

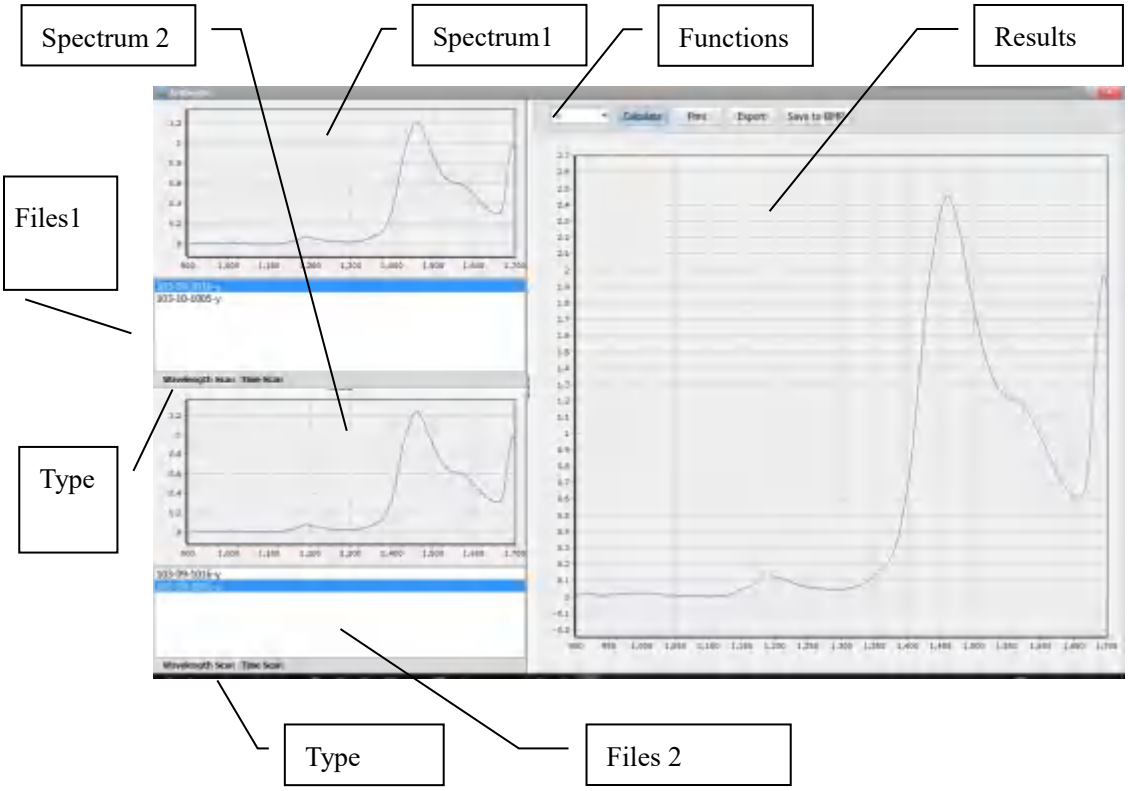


1. WL List: The wavelengths and sample cell position.
2. WL Para.: Modify wavelength and sample cell position here.
3. Data mode: Display data in Abs. or Trans.
4. Range: Choose a scan range around testing wavelength.
5. Baseline: Do baseline scan around every testing wavelength according to Range value.
6. Measure: Start scanning peaks.

5.5.9Arithmetic

Arithmetic is to do addition, subtraction, multiplication and division operations of the

same type of spectrum. Click  to enter Arithmetic.



1. Functions: Select arithmetic, calculate, save and export.

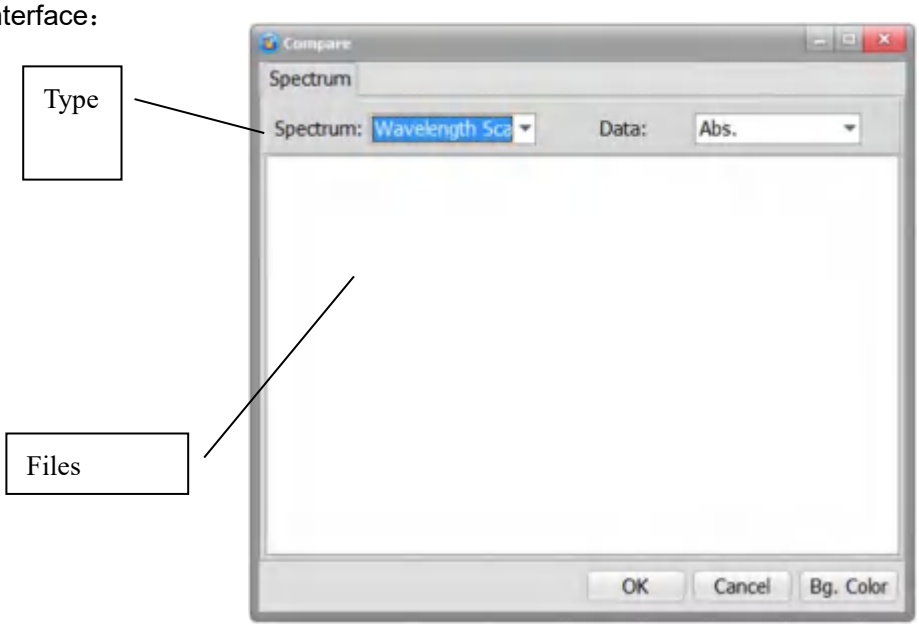
Button	Function
	Select addition, subtraction, multiplication or division
	Click to calculate the two spectrums.
	Click to save a BMP file.
	Click to print.

1. Spectrum 1 & Files 1: Shows the select spectrum in files 1.
2. Spectrum 2 & Files 2: Shows the select spectrum in files 2.
3. Spectrum type: Click to browse the same type of spectrum.
4. Results: Show the last result.
   Result spectrum =【Target spectrum 1】 +/-/×/÷【Target spectrum 2】。

5.5.10 Spectrum Compare

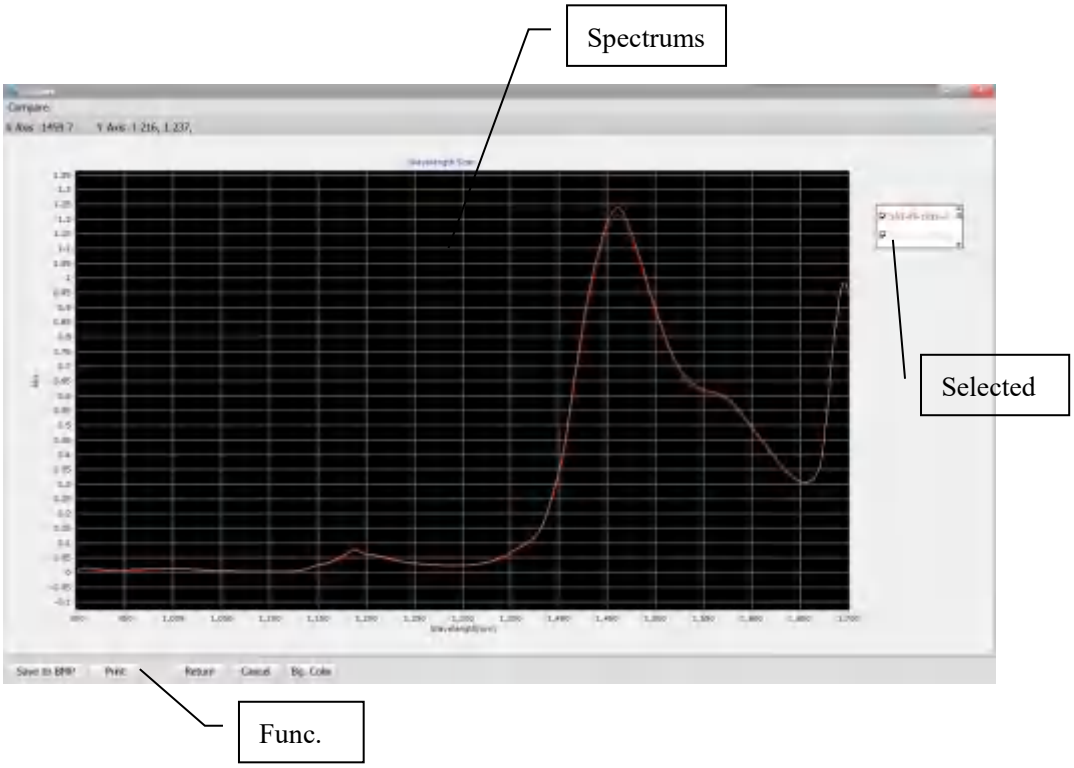
This function is to compare the same type of spectrum. Click  to enter Compare.

1. Interface：



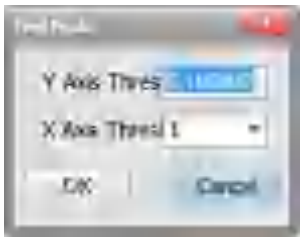
a) Type: Choose the spectrum type.
b) Files: Shows the certain type of spectrums. Hold Ctrl to select multiple spectrums.

2. Click OK to compare selected spectrums.



a) Using different colors to distinguish different spectrums in spectrum window.
b) You can check or uncheck a spectrum in the selected box.
c) Functions: Save and Print spectrum compare.

5.5.11 Find Peak



This function is to quickly find peaks of spectrum. Click  to set threshold according to current spectrum. Higher peaks need larger Y axis threshold; wider peaks need larger X axis threshold.

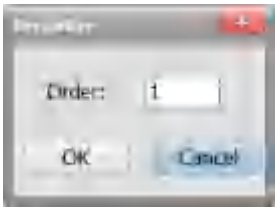
Click  to show peaks. The icon turns to  . Click it to hide peaks. Spectrum information below will show peak info.

5.5.12 Smooth

Smooth is to reduce the noise of spectrum. Click  to set smoothing parameters. Select type, Smoothing order, Number of points and Number of times then click “OK” to see the effect.

Type	Smoothing order	Number of points	Number of times
Savitsky-Golay	The highest power of the polynomial	Set the number of points to be used in calculation.(odd number)	Set the number of smoothing operations.
Mean	----------	Set the number of points to be used in calculation.	Set the number of smoothing operations.
Median	----------	Set the number of points to be used in calculation.	Set the number of smoothing operations.

5.5.13 Derivative



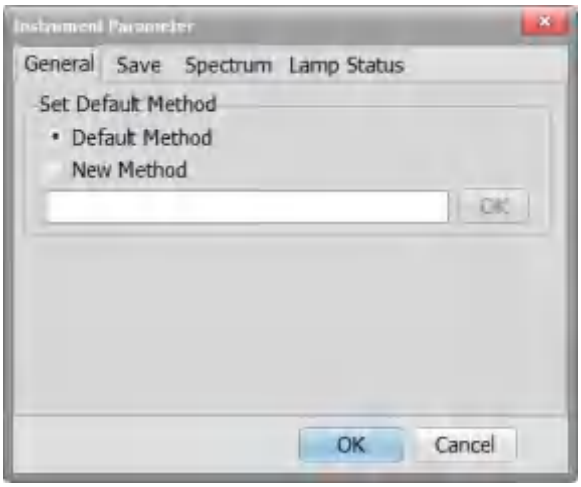
Derivative operation on spectrums is to enhance the resolution of peaks. Derivation can distinguish various disturbances affecting the shape of the spectrum peaks. Usually combining the smoothing operation.

Click  to open Derivative parameters window. Set Derivative order and click “OK” to see the result.

5.5.14 Instrument Parameter

This is to change the save path, file name and spectrum type. Click “Settings” →“Options”  to open option window.

1. **General tab**

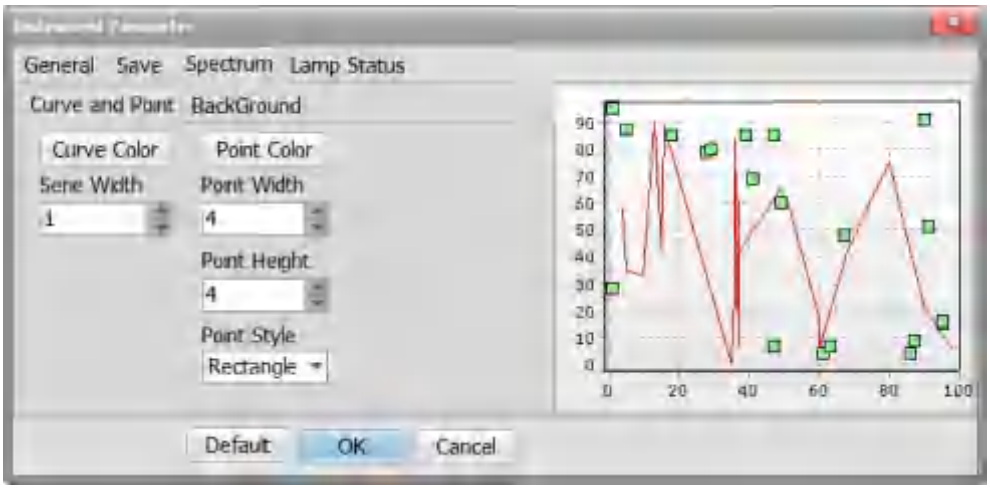


   1) Default Method: Instrument use default parameters.
   2) New method: Instrument uses specified parameters.

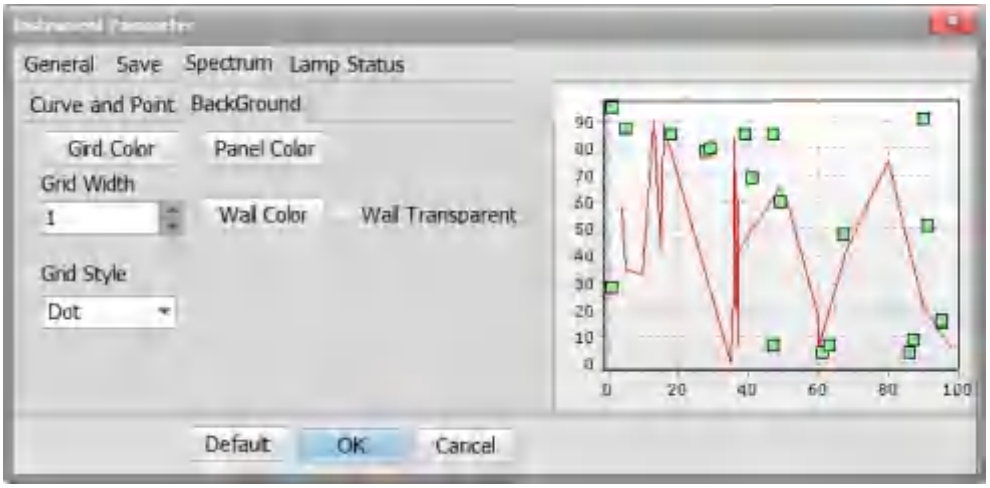
2. **Save Tab：**

   1) Automatic Increase after Scan: Automatically add a number suffix to file names.
   2) Start: Set the start number.
   3) Digit: Set number digits.
   4) Reset after rename: Auto reset number when using another name.

3. **Spectrum Tab:**

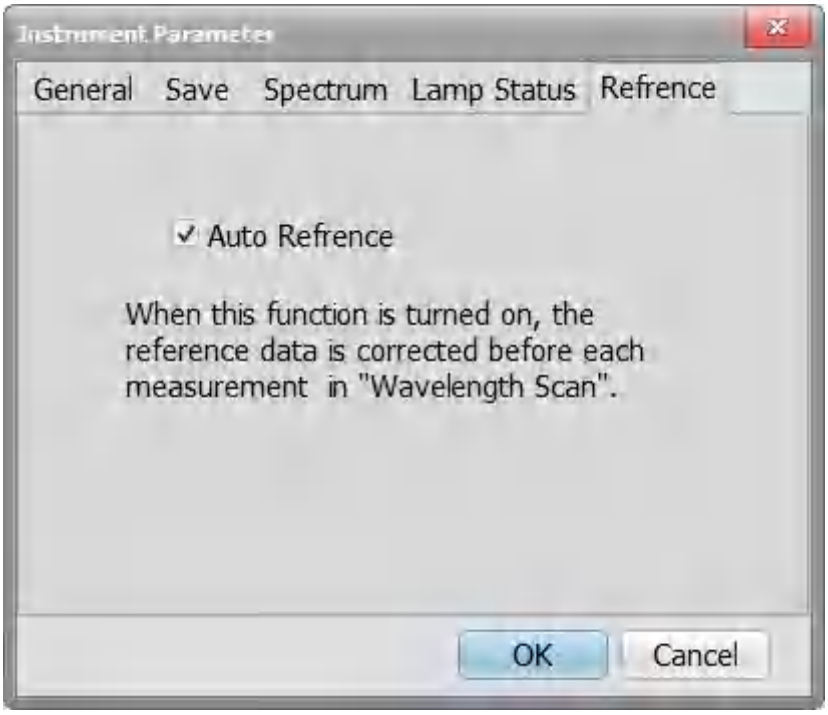


1) Curve color: Sets curve color.
2) Serie width: Sets curve width.
3) Point color: Sets dot color.
4) Point width: Sets dot width.
5) Point height: Sets dot height.
6) Point style: Sets dot shape as rectangle, circle, triangle, down triangle, cross, diagcross, star and diamond.



1) Grid color: Sets the table color in “Spectrum information” window.
2) Grid width: Sets the curve width in “Spectrum information” window.
3) Grid style: Sets table style as solid, dash, dot, dashdot, dashdotdot and clear in “Spectrum” tab.
4) Panel color: Sets the background color in “Spectrum information” window.
5) Wall color: Sets the coordinate board color.
6) Wall Transparent: Check it to make the board transparent.

4. Auto Reference Tab:



When this item is checked, the reference data is corrected before each measurement in“wavelength scan”.

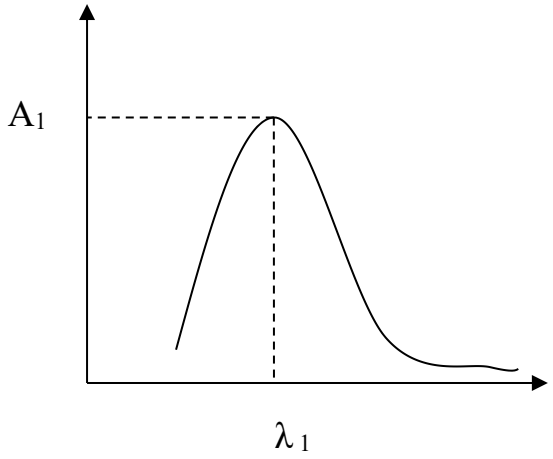
5.5.15 Rename & Delete Files

Right click on a file in file browser. You can delete or rename in the pop-out menu.

6 Appendix

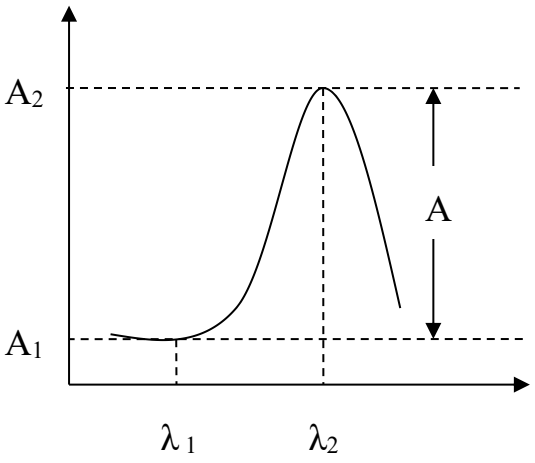
6.1 Quantitative analysis wavelength method

6.1.1 Single Wavelength



Abs. A_1 is the value on the curve at λ_1.

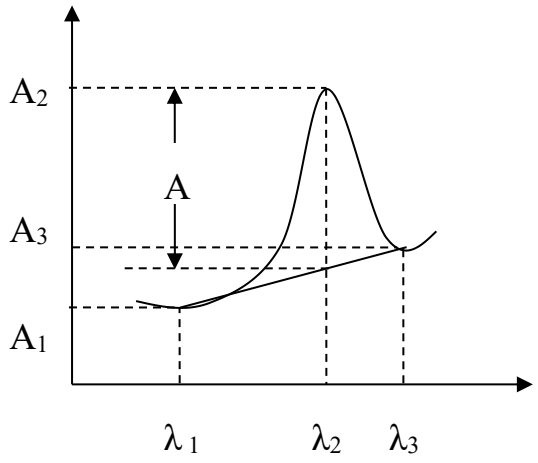
6.1.2 Double Wavelengths



A_1 and A_2 are the Fluorescence at λ_1 and λ_2.

$A=A_2 - A_1$

6.1.3 Triple Wavelengths



A_1 , A_2 and A_3 are the Fluorescence at λ_1 , λ_2 and λ_3.

$$A = A_2 - \frac{(\lambda_1 - \lambda_2) \times A_3 + (\lambda_2 - \lambda_3) \times A_1}{\lambda_1 - \lambda_3}$$

(It has to be$\lambda_1 > \lambda_2 > \lambda_3$ or $\lambda_1 < \lambda_2 < \lambda_3$)

6.2 DETAILS ON QUANTITATIVE

Prolab provides 3 calibration types: Linear working curve, Quadratic working curve and Cubic working curve. All of them are not forced through the 0 coordinates.

6.2.1 Linear Working Curve (1st order)

The calculation formula is as follow:

$$C = K_1 \times A + K_0$$

Where,

C : Concentration of each sample (input value)

A : Abs. of each sample (measured value)

K_1 and K_0 are calculated by the least squares method.

Suppose there are n data points(A_n , C_n), then

$$K_1 = \frac{\sum_{i=1}^{n} A_i C_i - \frac{1}{n}\sum_{i=1}^{n} A_i \cdot \sum_{i=1}^{n} C_i}{\sum_{i=1}^{n} A_i^2 - \frac{1}{n}(\sum_{i=1}^{n} A_i)^2}$$

$$K_0 = \frac{\sum_{i=1}^{n} C_i}{n} - K_1 \times \frac{\sum_{i=1}^{n} F_i}{n}$$

6.2.2 Quadratic Working Curve (2nd order)

The calculation formula is as follow:

$$C = K_2 \times A^2 + K_1 \times A + K_0$$

Where,

C: Concentration of standard sample

A : Abs. of each sample (measured value)

Kn are calculated by the least squares method

Suppose there are n data points(A_n ， C_n)，then：

$$K_2 = \frac{S(A^2C)S(AA) - S(AC)S(AA^2)}{S(AA)S(A^2A^2) - [S(AA^2)]^2}$$ （Formula F5-5）

$$K_1 = \frac{S(AC)S(A^2A^2) - S(A^2C)S(AA^2)}{S(AA)S(A^2A^2) - [S(AA^2)]^2}$$ （Formula F5-5）

$$K_0 = \frac{\sum_{i=1}^{n} C_i}{n} - K_1 \frac{\sum_{i=1}^{n} C_i}{n} - K_2 \frac{\sum_{i=1}^{n} F_i^2}{n}$$ （Formula F5-7）

6.2.3 The correlation coefficient

The correlation coefficient R represents how the regression curve fitting.

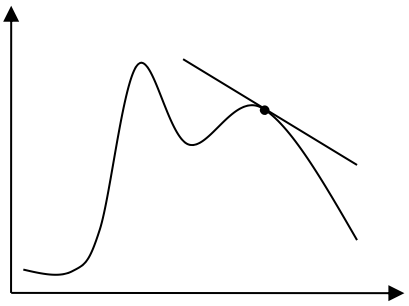
Suppose there are n data points(C_n， A_n):

$$R = \frac{\sum_{i=1}^{n} C_i A_i - \frac{\sum_{i=1}^{n} C_i \cdot \sum_{i=1}^{n} A_i}{n}}{\sqrt{\left(\sum_{i=1}^{n} C_i^2 - \frac{(\sum_{i=1}^{n} C_i)^2}{n}\right)\left(\sum_{i=1}^{n} A_i^2 - \frac{(\sum_{i=1}^{n} A_i)^2}{n}\right)}}$$ （Formula F5-13）

6.3 Derivative Operation on Spectrum

The derivative of a function of a real variable measures the sensitivity to change of a quantity (a function or dependent variable) which is determined by another quantity (the

independent variable).



Derivative of the function

There are many ways of derivative operation on spectrum. Since the x-axis(time axis or the wavelength axis, etc.) of the original spectral data are equally spaced, then

First order derivative：

$$\frac{dy}{dx} = \frac{y_{i+1} - y_i}{\Delta x}$$

Second order derivative：

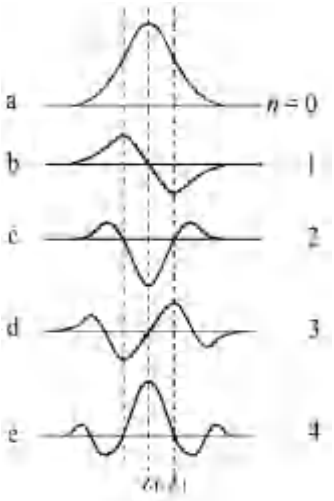
$$\frac{d^2y}{dx^2} = \frac{y_{i+1} - 2y_i + y_{i-1}}{\Delta x^2}$$ （Formula F7-2）

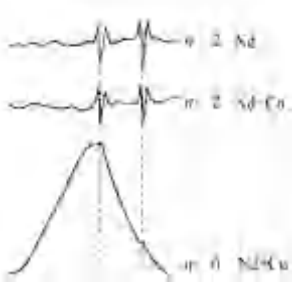
Where：

y: photometric value

x: wavelength, time, etc.

Derivative spectra not only can eliminate baseline drift or flat background interference, but also can provide a higher resolution than the original spectrum.





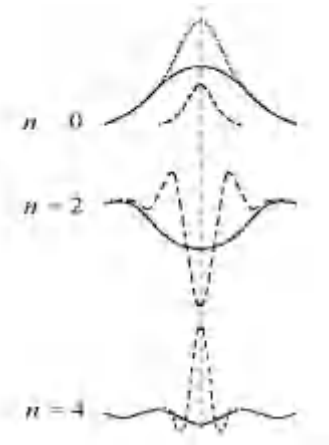


Fig. 1 **Fig. 2** **Fig. 3**

In Fig.1,there is a clear alternation of peaks. In Fig.2, the acromion is higher after derivative. Second order derivative spectrum is clearer. In Fig.3, the original spectrum two curves are seriously overlapping, but in n=2/4 the peaks are clearer.

Higher order derivative can eliminate the low order background curves. The spectrum shape is complicated after derivative, but it raises the resolution and sensitivity.

6.4 Smoothing

The basic idea of smoothing is to map a smooth point, then depicte a number of points around the smooth point to be "fit" or "average" or "sort" in order to obtain the best estimate of the value of the smooth point to eliminate random noise. With modern analytical instruments increasing speed and automation, multiple accumulate and smoothing technology has become a common method of noise reduction.

Prolab provide 3 smoothing methods: Savitsky-Golay, Mean and Median.

6.4.1 Savitzky–Golay

A **Savitzky–Golay filter** is a digital filter that can be applied to a set of digital data points for the purpose of smoothing the data, that is, to increase the signal-to-noise ratio without greatly distorting the signal. This is achieved, in a process known as convolution, by fitting successive sub-sets of adjacent data points with a low-degree polynomial by the method of linear least squares. When the data points are equally spaced an analytical solution to the least-squares equations can be found, in the form of a single set of "convolution coefficients" that can be applied to all data sub-sets, to give estimates of the smoothed signal, (or derivatives of the smoothed signal) at the central point of each sub-set.

6.4.2 Mean smoothing

Median smoothing is to sort the selected data (the number of data points is odd), then take the intermediate value as the smoothed value.

6.4.3 Median smoothing

Median smoothing is to sort the selected data (the number of data points is odd), then take the intermediate value as the smoothed value.

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