



ATR1200

Portable Raman Spectrometer



User Manual

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1. INTRODUCTION

OptoskySpectra_Raman_V3.0 is a program software for Raman spectral data acquisition and analysis.

There are some significant changes in this version that are different from the previous versions. The users used OptoskySpectra_Raman_V1.75 or earlier version in PC, so the following major differences shall be noticed by users.

- The software can load multiple curves at one time, supporting the txt/csv format and data format generated by our handheld Raman spectrometer.
- There are 3 methods for saving data: “save all spectra(automatic)”, “save selected. Every data will be saved in separate file folder. There are notes adhere to spectral data to make it easier to know.
- Add a series of algorithms for data analysis, which can implement derivative, normalization, smoothing, translation, spectrum calculation, etc.
- Function “Method”-”New” allow you to create new methods based on your own experimental requirements.
- There are huge changes and improvements in the interface.

Of course, the software changes are not only mentioned as the above. More changes your slow discovery. In short, the new version of the software will never let you down.

1.1.Purpose

This manual is used to guide users to correctly configure and use the ATR series Raman spectrometer.

2.Product operating environment

2.1.Hardware environment

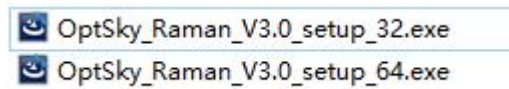
- Operating temperature range: $-10^{\circ}\text{C} \sim 40^{\circ}\text{C}$
- Storage and transportation temperature: $-20^{\circ}\text{C} \sim 70^{\circ}\text{C}$
- Working voltage: 5V, 9V (specific reference model), 50 / 60Hz

3.Driver installation

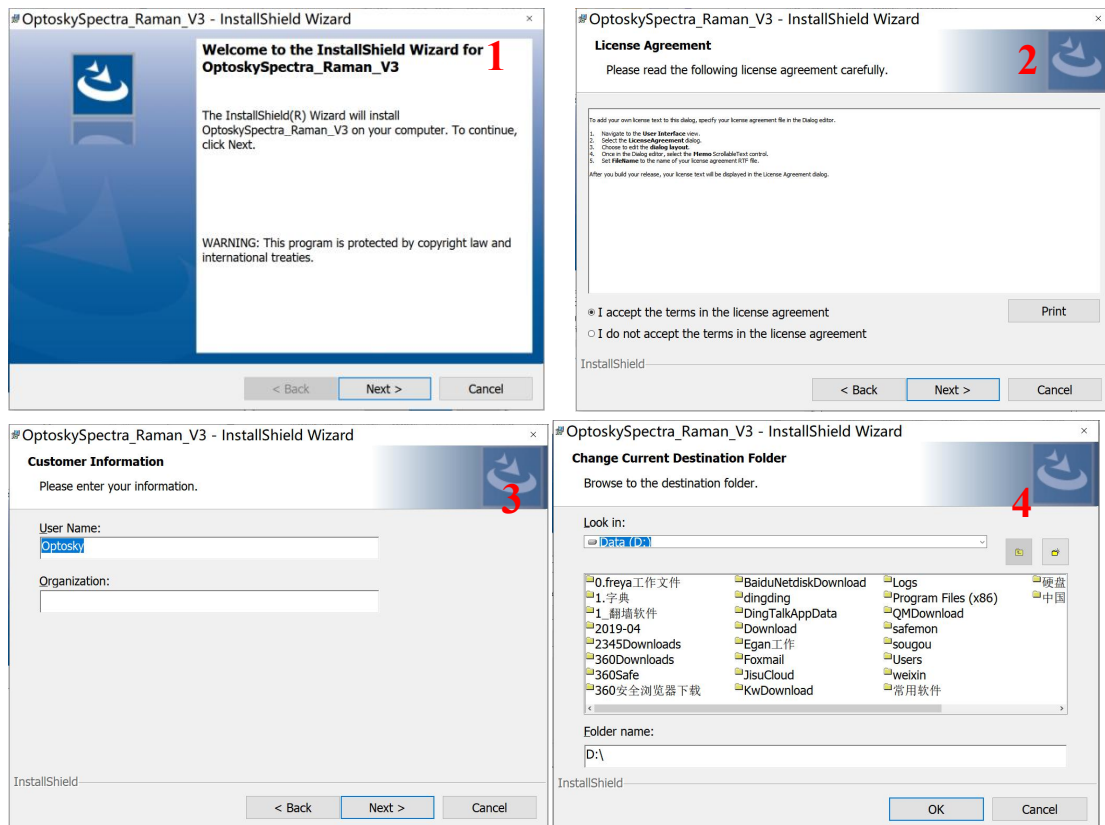
3.1.Driver Installation

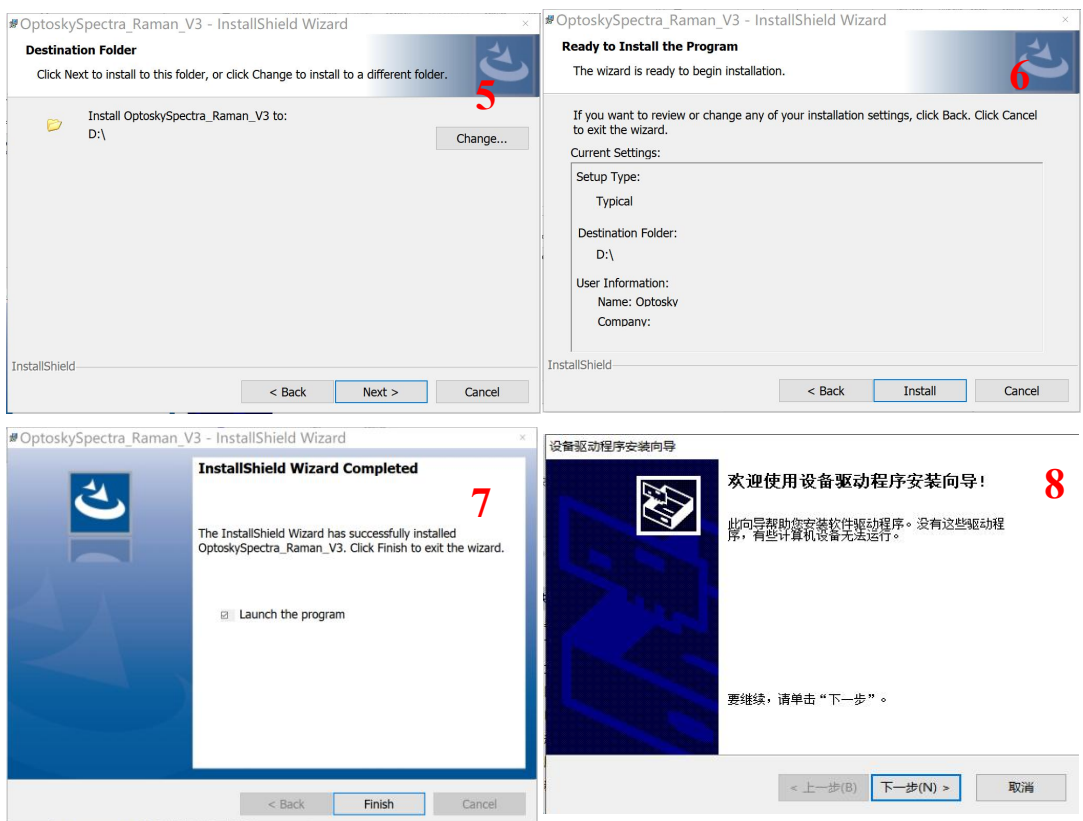
- Double-click **OptSky_Raman_V3.0_setup_32.exe** to install the driver for 32-bit Windows system.

Double-click **OptSky_Raman_V3.0_setup_64.exe** to install the driver for 64-bit Windows system.



- After about 30s, the following installation interfaces pops up step by step, and you can install the driver step by step.





3.2. Notes on operation

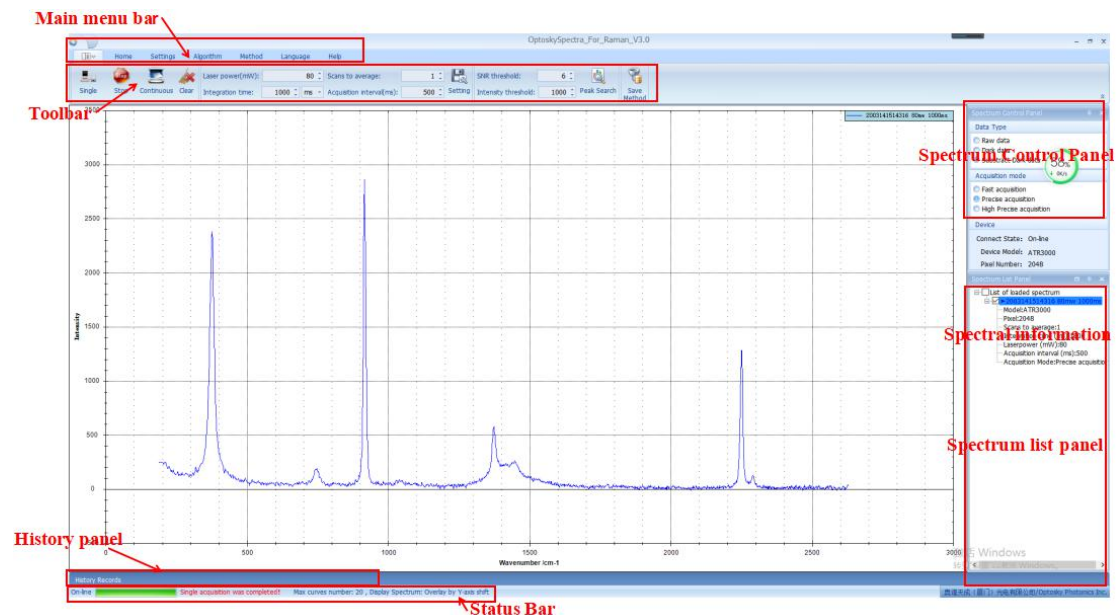
The laser probe of the ATR series Raman spectrometer should be coiled in the shape of a ring. Do not fold it or pull it strongly to prevent the fiber optic cable from breaking.

4. Support operating systems

- Windows 7 (32-bit or 64-bit)
- Windows 8 (32-bit or 64-bit)
- Windows 10 (32-bit or 64-bit)

5. Main interface

A brief visual overview of the OptoskySpectra_Raman_V3.0 main interface is shown below. The main toolbars, panels, and tabs are highlighted, see the corresponding section for more detailed information.

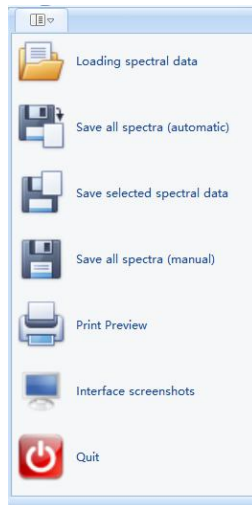


6. Main menu Bar



- Below we will introduce in detail the sub-menus after each main menu drop-down.

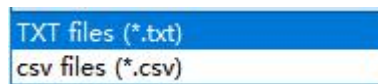
7. File



7.1. Loading spectral data

Loading spectral data means importing previously saved spectral data into the software first and presenting it on the main interface. The software can import single or multiple pieces of data at one time. The following data formats can be imported.

- TXT File (*.txt)
- CSV File (*.csv)
- The data generated by Raman instruments produced by our company.



7.2. Save all spectra (automatic)

- Save all spectra (automatic) means to save all data in the spectrum list. You can select the save path and data format.



- There are two formats for saving data: txt and csv. The specific style is as follows.

Data Generated by Optosky
 File Version;1.2
 Name;2003141514316 80mw 1000ms
 Creator;admin
 Description;11
 Created;2020/3/14 15:14:31
 Integration Time(ms);1000
 Laser Power(mW);80
 Average Number;1
 Scan Mode;Precise Scan
 Scan Interval;500
 Device Model;ATR3000
 Pixel Num;2048
 Device Sn;ATR30007
 Pixel;Raman Shift;Raw;Dark;Dark Subtracted
 1;188.5048;2807.0000;2557.0000;250.0000
 2;190.0056;2807.0000;2557.0000;250.0000
 3;191.5061;2807.0000;2557.0000;250.0000
 4;193.0063;2807.0000;2557.0000;250.0000
 5;194.5061;2807.0000;2557.0000;250.0000
 6;196.0056;2807.0000;2557.0000;250.0000
 7;197.5048;2807.0000;2557.0000;250.0000

txt format

Data Gene	Optosky				
File Vers	1.2				
Name	2003141514316 80mw 1000ms				
Creator	admin				
Descripti	22				
Created	#####				
Integrati	1000				
Laser Pow	80				
Average N	1				
Scan Mode	Precise Scan				
Scan Inte	500				
Device Mo	ATR3000				
Pixel Num	2048				
Device Sr	ATR30007				
Pixel	Raman Shi	Raw	Dark	Dark	Subtracted
1	188.5048	2807	2557	250	
2	190.0056	2807	2557	250	
3	191.5061	2807	2557	250	
4	193.0063	2807	2557	250	
5	194.5061	2807	2557	250	
6	196.0056	2807	2557	250	
7	197.5048	2807	2557	250	

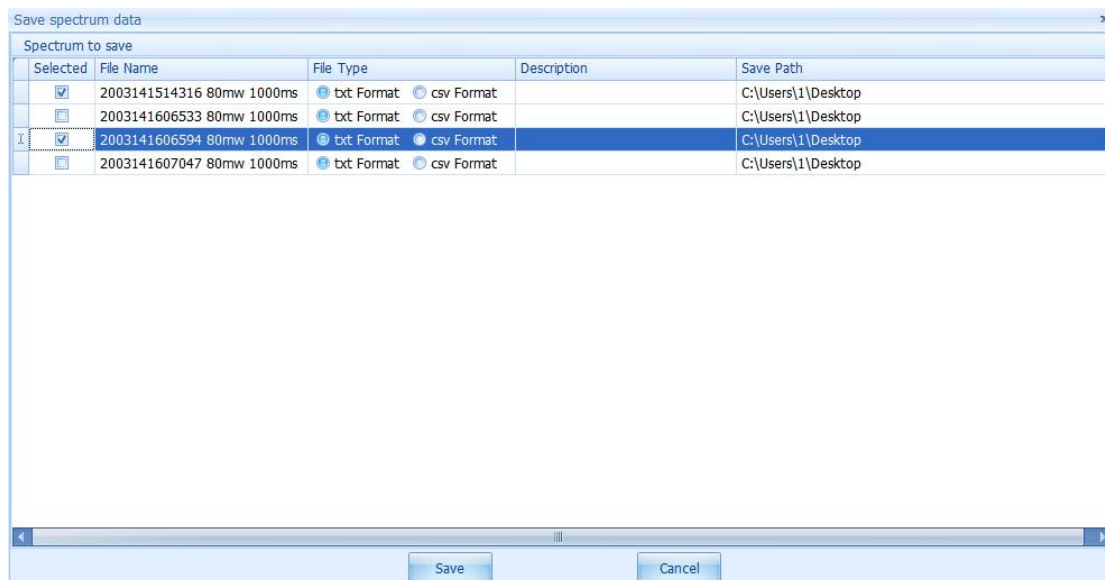
csv format

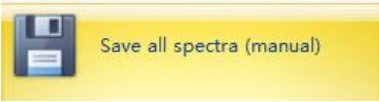


Save selected spectral data

7.3. Save selected spectral data

- Save selected spectral data means to save spectrum data that you have selected in the list. You can change the file type, save path, file name, description for every data sheet. The format of the saved data is the same as in 7.2.





7.4. Save all spectra (manual)

- Save all spectra (manual) means to save all spectrum data by user. The file name, file type, description, save path of each spectrum data can be changed manually. The format of the saved data is the same as in 7.2.

Save spectrum data			
Spectrum to save			
File Name	File Type	Description	Save Path
> 2003141514316 80mw 1000ms	☒ txt Format ☒ csv Format		C:\Users\1\Desktop
2003141606533 80mw 1000ms	☐ txt Format ☐ csv Format		C:\Users\1\Desktop
2003141606594 80mw 1000ms	☐ txt Format ☐ csv Format		C:\Users\1\Desktop
2003141607047 80mw 1000ms	☐ txt Format ☐ csv Format		C:\Users\1\Desktop

Save

Cancel



7.5. Print Preview

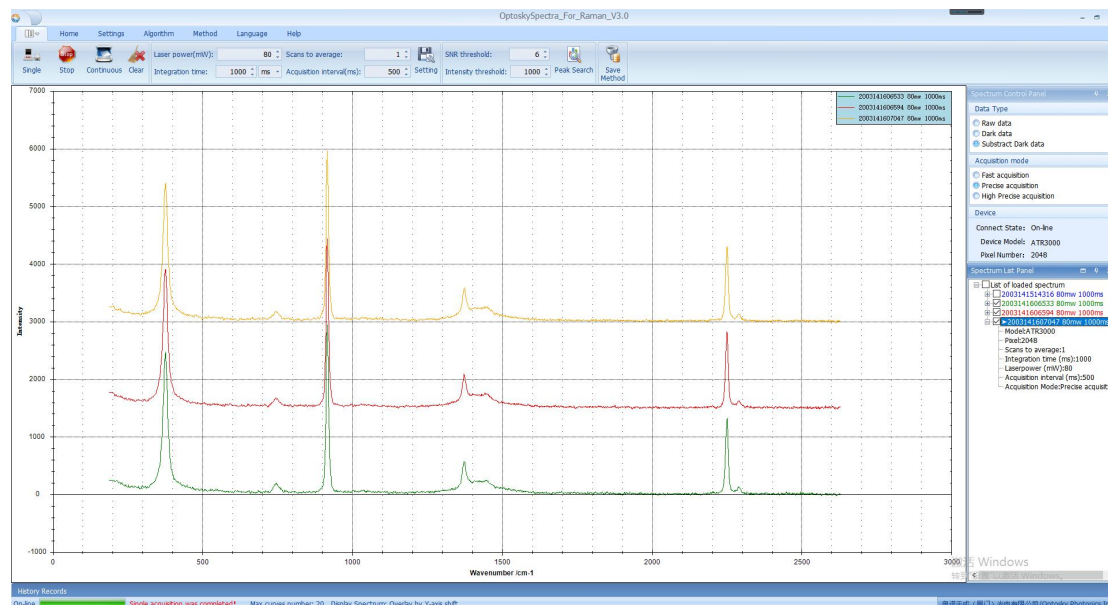
- The report can be printed and the print preview function is shown as below



7.6. Interface screenshots



- Interface screenshot refers to the screenshot of the entire interface of the software, the style is shown as below

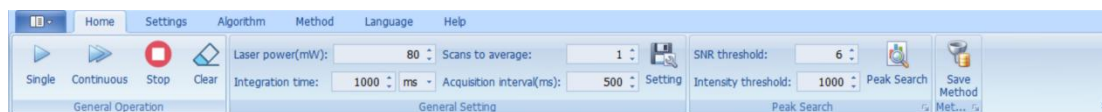


7.7. Quit

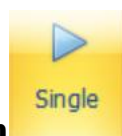


- Quit means closing the software.

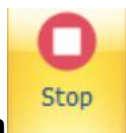
8. Toolbar under the homepage



8.1. Single Acquisition

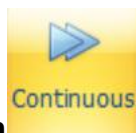


- Single acquisition means to obtain spectral data by measuring sample in single time.
- Start single acquisition of spectral data: Click the "single" button to start single spectral acquisition.
- Stop single acquisition of spectral data: Click the "Stop" button to stop.



8.2. Stop acquisition

- Click the "Stop" button to stop the ongoing spectral data acquisition process.



8.3. Continuous acquisition

- Continuous acquisition is the behavior of continuous Raman data acquisition of the measurement sample by the spectrometer. Through continuous acquisition spectral data, users can comprehensively view the performance of Raman data of measurement samples and identify the information of measurement samples.

Start continuous acquisition of spectral data: Click the "Continuous Acquisition" button to start continuous acquisition.

Stop continuous acquisition of spectral data: Click the "Stop" button to stop.



8.4. Clear graph

- Click the "Clear" button to clear the collected spectral data graph in the interface.

8.5. Laser power

Laser power(mW):

- Laser power refers to the working power of a semiconductor laser. (Mw)

Integration time: ms

8.6. Integration time

- The integration time refers to the integration time for a single scan. (S or ms)

8.7. Scans to average

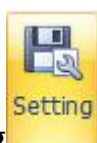
Scans to average:

- Number of averages refers to the average number of acquisitions set to perform the spectrum.

8.8. Acquisition interval

Acquisition interval(ms):

- The acquisition interval refers to the time interval(ms) when running continuous acquisition.



8.9 Setting

- Click this button and we can see the laser emitting. At this time, the laser cannot be directed to

human eyes.

8.10. SNR threshold

SNR threshold: 6

- SNR threshold, the threshold of the peak signal to noise ratio.

8.11. Intensity threshold

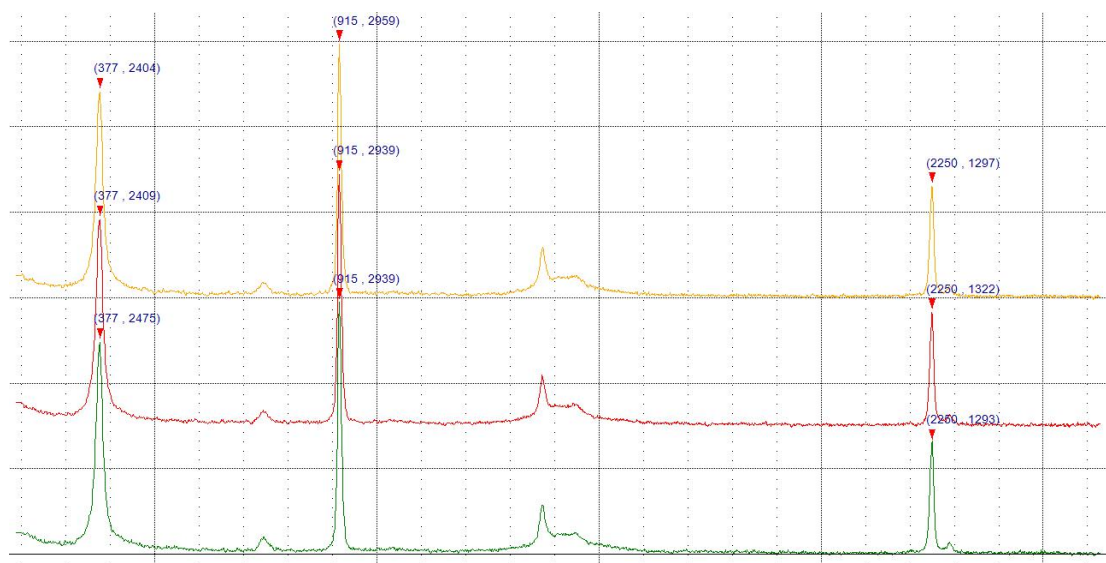
Intensity threshold: 1000

- Enter a threshold value. Only peaks with intensity value greater than this threshold will appear in the spectrum.



8.12. Peak Search

- Click this button, and the software will search the spectral peak according to the threshold and peak width setting parameters.
- The search results are shown in the figure below. Not only the peak points matching the parameters will be marked in the figure, but also the corresponding table will correspond one by one. The color of the spectrum is the same as the module color of peak finding results after the peak search. To make it appear or not on the spectrum easily.
- Meet the needs of different users.



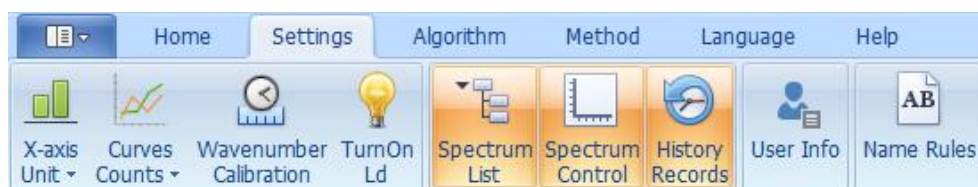
Peak finding results								
☒ Show wave crest labels								
Spectrum:2003141606533 80mw 1000ms			Spectrum:2003141606594 80mw 1000ms			Spectrum:2003141607047 80mw 1000ms		
Show	Wavenumber /...	Intensity	Show	Wavenumber /...	Intensity	Show	Wavenumber /...	Intensity
☒	377	2475	☒	377	2409	☒	377	2404
☒	915	2939	☒	915	2939	☒	915	2959
☒	2250	1293	☒	2250	1322	☒	2250	1297



8.13. Save method

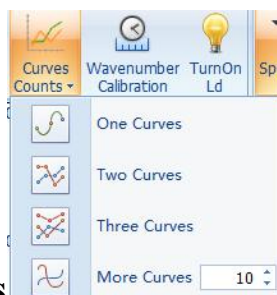
- The **save method** here can directly save the parameters of the spectrum tested in the main interface at this time as a method, and you can click **Apply** directly in the method interface next time.

9. Settings



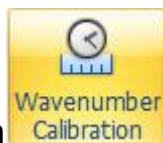
9.1.X-axis unit

- We can switch the abscissa between pixels and wave numbers.



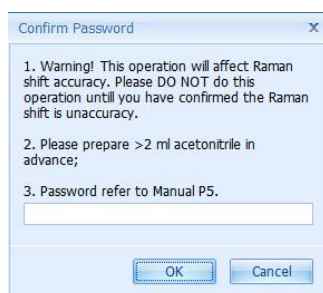
9.2.Curves Counts

- Number of curves: Set the maximum number of spectral curves that can be displayed during spectrum acquisition (up to 30 curves can be displayed at the same time). If we set 1 or 2 curves, the spectrum area can only show 1 or 2.

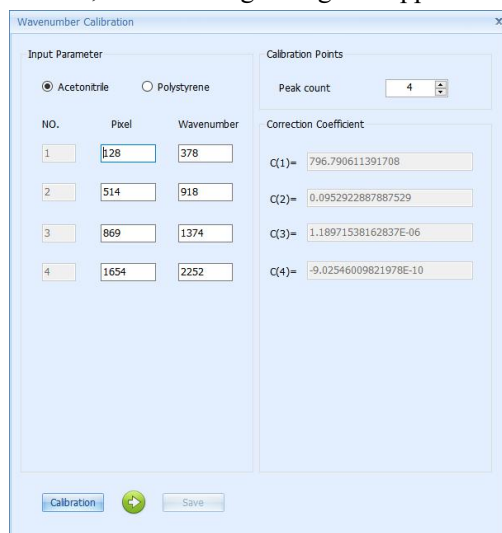


9.3.Wave number Calibration

Click the **wave number calibration** to pop up a dialog box that requires a password verification. The instruments will perform wave number correction before leaving the factory and saved to the instruments. Users generally do not need to perform wave number correction. It is recommended that users perform wave number correction once every 2-3 years to ensure the wave number No drift. Please use it carefully if you do it yourself, prepare acetonitrile before calibration, password: optosky888.



After entering the password, the following dialog box appears.



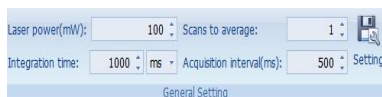
Here is an example of the calibration, sample is acetonitrile:

- Point the probe at acetonitrile sample and click on a single acquisition to scan the spectrum.
- After the spectrum has been displayed on the program interface, set the proper peak threshold and peak intensity value, click "Peak Search", and the program will display the peaks according to the peak threshold and peak intensity threshold set by the user.
- In the dialog box above, the value in the "Wave number" column is read-only, and the four characteristic peak wave values of acetonitrile are fixed. The user only needs to enter the pixel values corresponding to the four characteristic peaks of acetonitrile in the "pixel" column. (note: the abscissa unit is pixel)
- After calibration, click **save** to finish this process.

9.4. Turn on the laser



- Click  to turn on the laser, then the laser emit, and click  to turn off the laser.

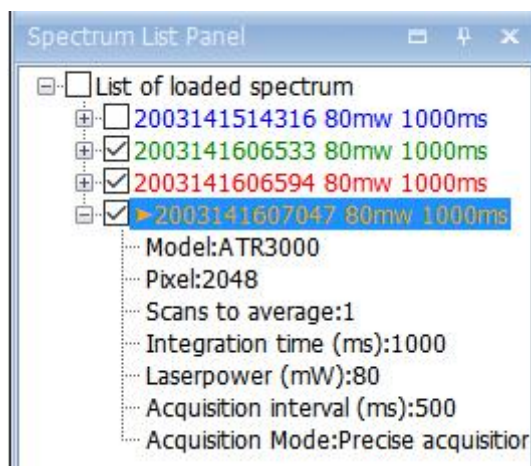


- Clicking **"setting"**, the laser will also light up.
- The laser will also light up automatically during acquisition.



9.5. Spectrum list Panel

- Load the selected spectrums together to check at one time instead of loading one by one.
- Click "+" or "-" to expand or merge the spectrum detailed information.
- Double-click the spectrum name to rename.
- Right-click the spectrum name to remove the spectrum.



9.6. Spectrum Control Panel

- The data type can be switched at will among 3 types: raw data, dark background data, and

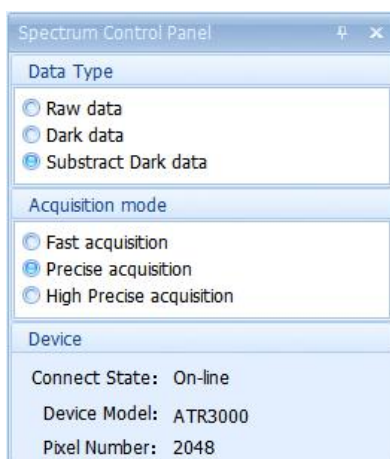
subtract dark background.

- The sampling mode can be switched at will among fast acquisition, precise acquisition and high-precision acquisition.

(1) Fast sampling mode: When collecting spectral data, you need to save the dark background spectrum collection before collecting the spectral data, and then directly turn on the laser for collection. After collection, and the collected results will deduct the saved dark background.

(2) Accurate sampling mode: When collecting spectral data, the dark background data is collected firstly, then the laser on and the sample/background spectral data collected, then the dark background collected is subtracted from the collection result to get the real spectral data of sample.

(3) High-precision sampling mode: When collecting spectral data, dark background collection is performed firstly before every collection, and then the laser is turned on, waiting for 5s to ensure that the laser is stable, and finally, the collection result will deduct the dark background collected in real time.



9.7. History Records

- In the historical record, we save the collected data, and do not save the data processed afterwards.
- The main page history shows the last 30 entries. If you want to see more history, you can click more to search.
- In the history control panel, you can modify the file name, user notes, and save methods.

History Records									
You can pull the column header to the area to group the list									
Spectrum Name	User remarks	Integration T...	Laser power(...)	Baseline ...	Acquisition ...	Scans to ...	Smooth...	Acquisition Time	Acquisit...
2003141607947 80mw 100...		1000	60		Precise acq...	1		2020-03-14 16:0...	2020-03-14
2003141605594 80mw 100...		1000	60		Precise acq...	1		2020-03-14 16:0...	2020-03-14
2003141606533 80mw 100...		1000	60		Precise acq...	1		2020-03-14 16:0...	2020-03-14
2003141514316 80mw 100...		1000	60		Precise acq...	1		2020-03-14 15:1...	2020-03-14
2003141513497 80mw 100...		1000	60		Precise acq...	1		2020-03-14 15:1...	2020-03-14

All Historical Records

Select All Unselect All Select Unselect Delete Selected

You can pull the column header to this area to group the list

Se...	Spectrum Name	用户备注	Integration...	Laser power...	Baseln...	Acquisition...	Scans ...	Smoot...	Acquisition Time	Acquisitio...
>	2003141607047 80mw 1000...		1000	80	☒	Precise acq...	1	☒	2020-03-14 16:07...	2020-03-14
☐	2003141606594 80mw 1000...		1000	80	☐	Precise acq...	1	☐	2020-03-14 16:07...	2020-03-14
☐	2003141606533 80mw 1000...		1000	80	☐	Precise acq...	1	☐	2020-03-14 16:06...	2020-03-14
☐	2003141514316 80mw 1000...		1000	80	☐	Precise acq...	1	☐	2020-03-14 15:14...	2020-03-14
☐	2003141513497 80mw 1000...		1000	80	☐	Precise acq...	1	☐	2020-03-14 15:13...	2020-03-14
☐	2003141512519 80mw 1000...		1000	80	☐	Precise acq...	1	☐	2020-03-14 15:12...	2020-03-14
☐	2003141506319 80mw 1000...		1000	80	☐	Precise acq...	1	☐	2020-03-14 15:06...	2020-03-14
☐	2003141506097 80mw 1000...		1000	80	☐	Precise acq...	1	☐	2020-03-14 15:06...	2020-03-14
☐	2003141505589 80mw 1000...		1000	80	☐	Precise acq...	1	☐	2020-03-14 15:05...	2020-03-14
☐	2003101007435 80mw 1000...		1000	80	☐	Precise acq...	1	☐	2020-03-10 10:07...	2020-03-10



9.8. User Information

- User information can be set here, and the saved data(txt/csv format) will also include the operator name.

Operator Information

Operator:

Organization:

Work Tel:

Word Addr:

Save Cancel



9.9. Name Rules

- Before collecting spectra, you can set the name rules firstly, so that all spectra collected will be named according to the rules, which can reduce the time for renaming subsequent spectrum one by one.

Spectrum name rule setting

Prefix content: 1111

☒ Spacer 1: -

☒ Date format: yyyyMMdd

☒ Spacer 2: -

Serial number length: 4

Example of effect

1111-20200314-0001

Application(A) Save(S)



9.10. Matching results

- The matching result is added to the view panel. When we select the matching result, the result will be displayed on the right side of the main interface. The premise of displaying the result is that we need to add the spectrum library in advance, set whether to recognize this substance, and what the threshold is. We will talk about the addition and setting of the spectrum library later.
- Click details, we can know the substance name, customs code, CAS, Raman shift range, chemical formula, hazard category, physical and chemical properties, main uses, hazard characteristics, etc.

Match Result

Match Result Spectrum ... Spectrum ...

N/A
n/a

Rate
0%

Detail

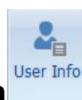
Match Result

Match Result Spectrum ... Spectrum ...

CaCO3
n/a

Rate
79%

Detail



9.11. User information

User information can be set here, and the saved data will also extract the operator name.

Operator Information

Operator: admin

Organization:

Work Tel:

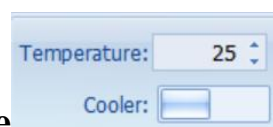
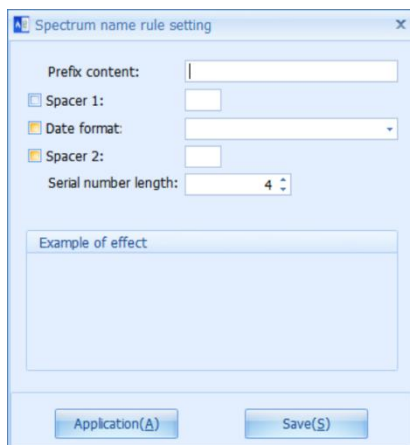
Work Addr:

Save Cancel



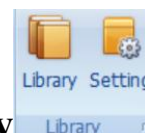
9.12. Name rule

Before collecting the spectra, you can set the naming rules first, so that all the collected spectra will be named according to the rules, which can reduce the time of renaming one spectrum after another.



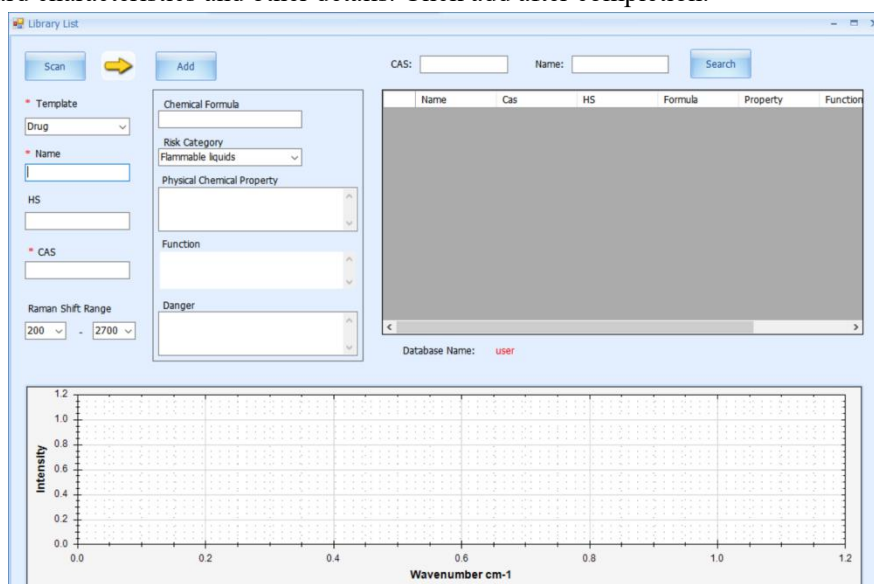
9.13. Setting of refrigeration temperature

To set the cooling temperature of CCD, we can set - 5-25 °C to reduce the noise. Generally, only 1064nm excitation wavelength needs refrigeration.



9.14. Setting & management of spectrum library

Place the sample, click Scan, and then edit the template, substance name, customs code, CAS, Raman shift range, chemical formula, hazard category, physical and chemical properties, main uses, hazard characteristics and other details. Click add after completion.



To query the entered spectrogram, first select the template, then input CAS and substance name, and click query.

Template: 毒品 CAS: Name: Search

Name	Cas	HS	Formula	Property	Function
------	-----	----	---------	----------	----------

Database Name: 111

Click database to create a new database.

Library List

111
user

New
Select
Delete

When setting the material identification, check whether to identify the material and match the threshold setting.

Material Match Setting

☒ Match Material

Match Threshold1(%): 60

Match Threshold2(%): 40

Key Point Threshold: 0

OK Cancel

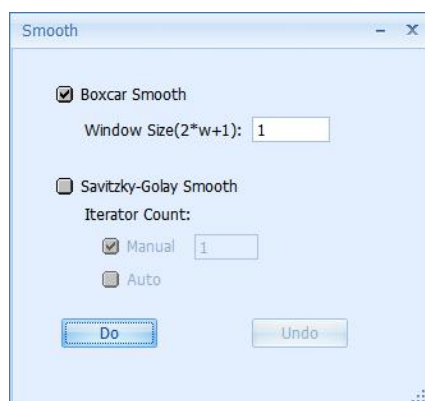
Only when the spectrogram database is established, can we present the matching information of substances on the right side of the main interface.

10. Algorithm



10.1. Smoothing

- Smoothing is an algorithmic operation. By choosing a smoothing algorithm, our curves can be made smoother and more beautiful. Our software has two smoothing algorithms to choose and applies.
- Smoothing can be applied regardless of the Y-axis data type is set to be raw data, or dark background data, or subtracted dark background.

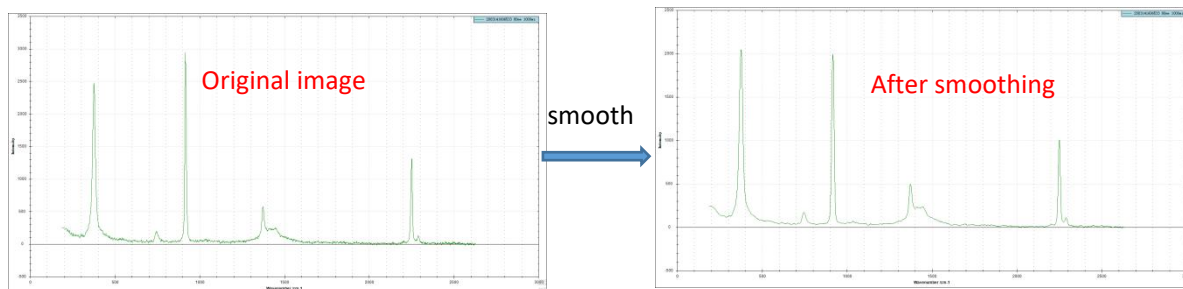


- Boxcar smooth

Boxcar smoothing can make the data collected by the modular equipment more extensive. Boxcar smoothing function eliminates high frequency noise and makes the collected data clearer. When collecting weak signals, it can be used to increase vertical resolution, reduce noise, improve dynamic characteristics such as signal-to-noise ratio (signal-to-noise ratio), and stray-free dynamic range. It uses digital signal processing to average the data collected at adjacent sampling points to improve vertical accuracy. The disadvantage of the Boxcar smoothing function is that it smooths the waveform and effectively filters out high-frequency signals, and some content may be lost.

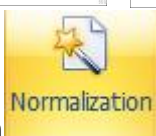
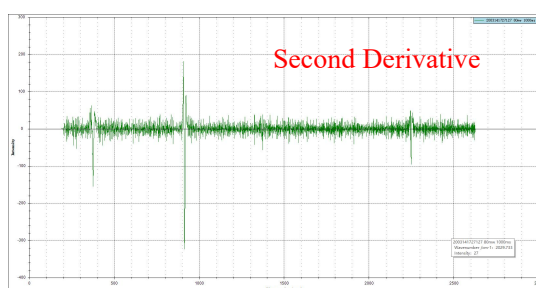
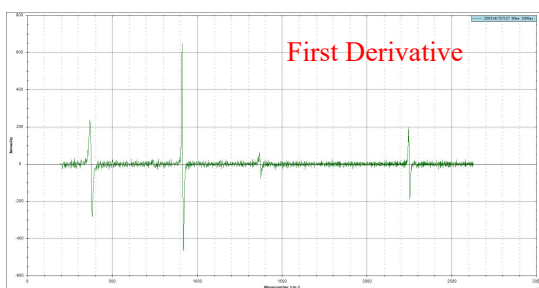
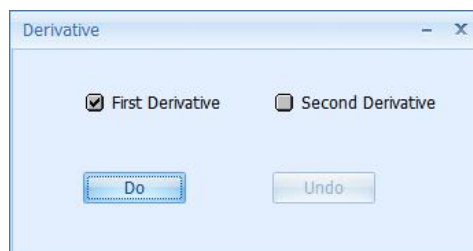
- Savitzky-Golay smooth

Savitzky-Golay smooth filtering is one of the pre-processing methods commonly used in spectral analysis. Smoothing filtering by the Savitzky-Golay method can improve the smoothness of the spectrum and reduce the interference of noise, which will cause less distortion and reduce the spectral resolution. The effect of S-G smooth filtering varies with the selected window width, which can meet the needs of many different occasions.



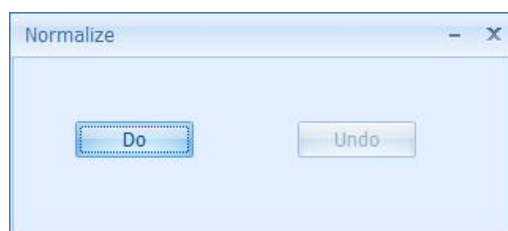
10.2. Derivative

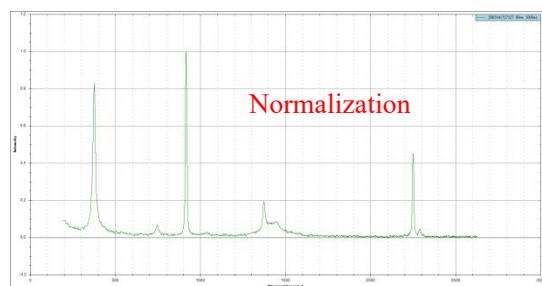
- Our instrument has two differentiating algorithms to choose and applies to all spectra in the interface.
- This function can be applied regardless of the Y-axis data type is set to be raw data, or dark background data, or subtracted dark background.



10.3. Normalization

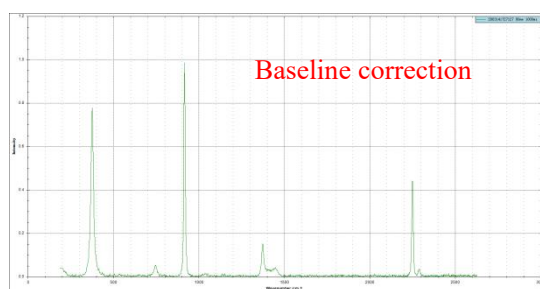
- The normalization algorithm is applied to all spectra in the interface.
- This function can be applied regardless of the Y-axis data type is set to be raw data, or dark background data, or subtracted dark background.





10.4. Baseline correction

- The normalization algorithm is applied to all spectra in the interface.
- This function can be applied regardless of the Y-axis data type is set to be raw data, or dark background data, or subtracted dark background.

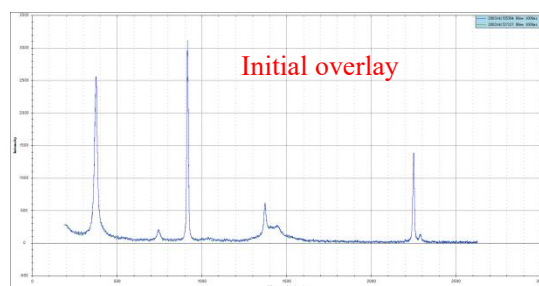


10.5. Undo

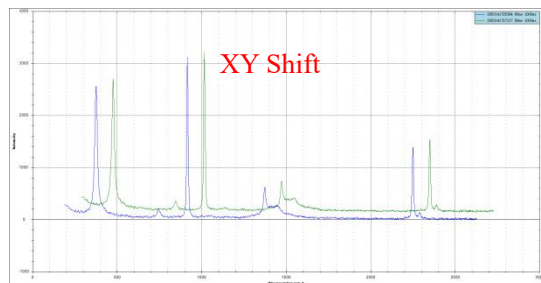
- The above algorithm process can undo by click this panel.



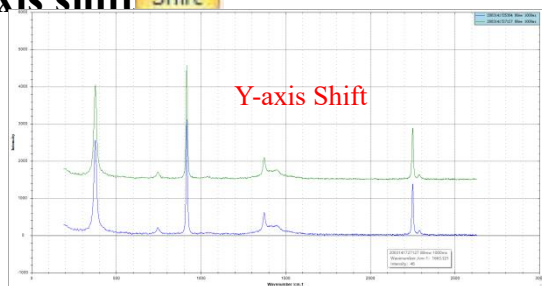
10.6. Initial overlay



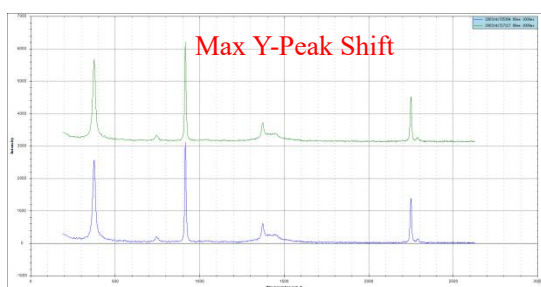
10.7.XY Shift



10.8. Y-axis shift



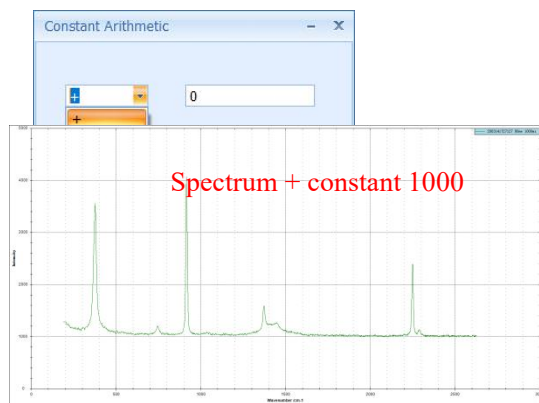
10.9. Max Y-Peak shift



10.10. Constant Arithmetic

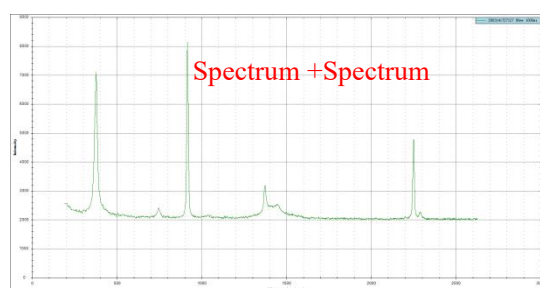
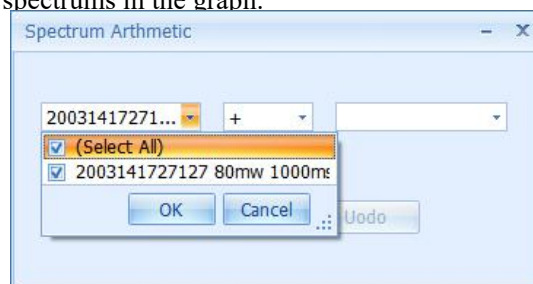


- Adding(+), subtracting(-), multiplying(x) and dividing(/) can be done to the spectrum.



10.11. Spectrum Arithmetic

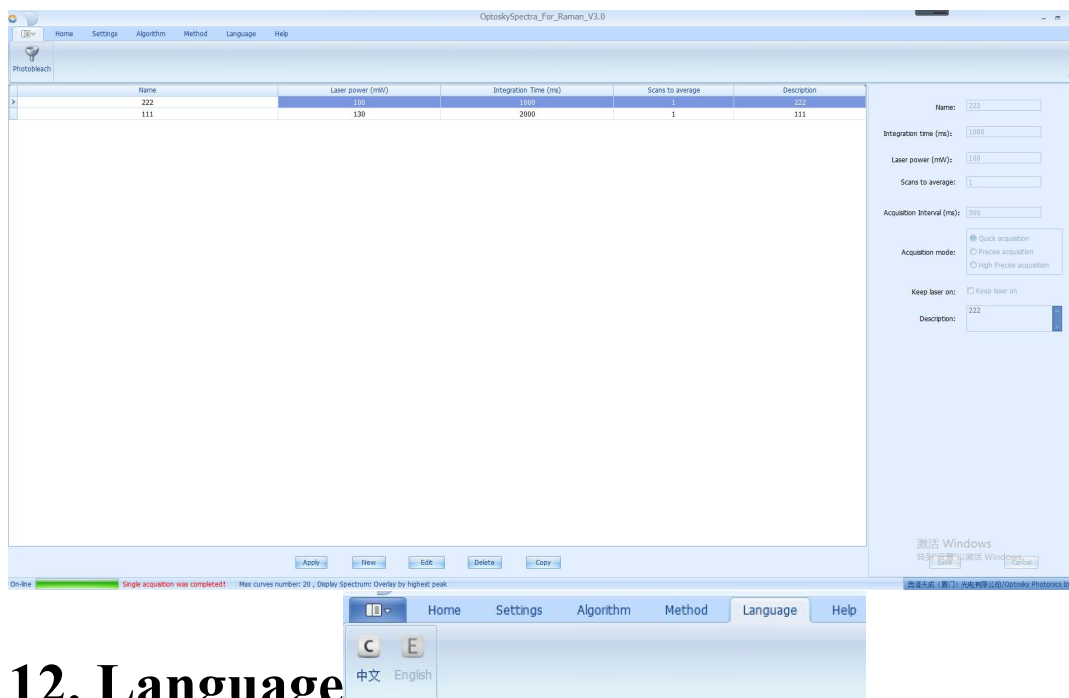
- Add, subtract, multiply, and divide a single spectrum in the graph to single or multiple spectra in the graph.



11. Method



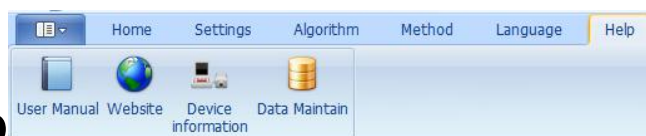
- Implement functions such as method creation, modification, copy, delete, and apply, making it more convenient for users.



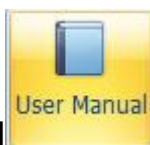
12. Language

- Switch between Chinese and English

13. Help



13.1. User Manual



- The user manual is actually a user instruction manual to help everyone use the software more easily.

13.2. Company Website



- It is convenient for everyone to connect to our website with clicking **Website**, to know our products, company culture, etc.



13.3. Device Information

- It is convenient for everyone to query the device information.



13.4. Data Maintenance

- The purpose of data maintenance is to make our software running smoothly.
- Clear history is to delete history records, data shrink is to reduce the disk space occupied by history.

