



Benchtop Raman Spectrometer

PeakSeeker User Manual

Version 2.0

1/3/2021



Document Number: UM20210103.002

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1. Laser Safety and Precautions

The PeakSeeker™ and PeakSeeker Pro™ series of instruments complies with DHHS Radiation Performance Standards 21 CFR (J) for Class IIIB Laser products. It contains a laser light source that emits visible and/or invisible laser radiation at a power level which can be user adjusted from 5 mW – 300 mW. The upper end of this range is approximately 100 times the power output of a typical laser pointer. The user must be aware of the dangers associated with equipment of this type and must be experienced in practices and processes associated with handling such products.

We recommend the following safety precautions while operating the laser. This is only a recommended list and by no means comprehensive:

1. Post warnings in the area where the instrument is to be used.
2. Allow access only to authorized personnel.
3. Do not look directly in the path of the beam.
4. Always wear safety goggles (provided with the instrument) while using the system.

Safety Notice

All Raman Systems are equipped with an electronic shutter which prevents laser emission when measurements are not being made. During a sample scan, the red LED on the panel will illuminate, indicating laser excitation of the sample under measurement.



WARNING!

An illuminated RED LED on the instrument panel indicates active laser emission!

Sample burning

It must be noted that dark materials will absorb the laser energy much more efficiently than transparent materials. Such materials will therefore heat up more quickly and may become more sensitive to thermal damage and possibly incite ignition or detonation.

Moreover, very high laser power focused on a very small spot (100 μm diameter is typical) implies very high power density which can cause the sample damage.

Disclaimer:

Photonwares Inc. assumes that the user of the instrument has read and is familiar with all precautions that need to be exercised, while operating an instrument with a class IIIB laser. Photonwares is not responsible for any damage caused to personnel, equipment, or samples arising from incorrect use of the laser or the instrument.

2. Software and Drivers installation

This section is to introduce the first-time installation or a reinstallation of RSIQ software on the new computer. The PeakSeeker and PeakSeeker Pro instruments are normally supplied with dedicated notebook computers preloaded with RSIQ software. You could skip this section if you already purchased the Raman Spectrometer with laptop. The installation procedure applies to installation on user supplied computers. Software is provided on a USB flash drive with each instrument when delivered.

- ❖ The manual is based on using Windows 10 (64 bit) as the operating system.
- ❖ The RSIQ software needs .NET framework version 4 or newer.

2.1 Software Installation

1. Power on the computer only, DO NOT connect the Raman instrument to computer.
2. Insert the USB flash drive into the computer and open the drive folder. The installation file is in the folder Setup. There is a copy of the installation files on the laptop's folder D:\Setup, too.

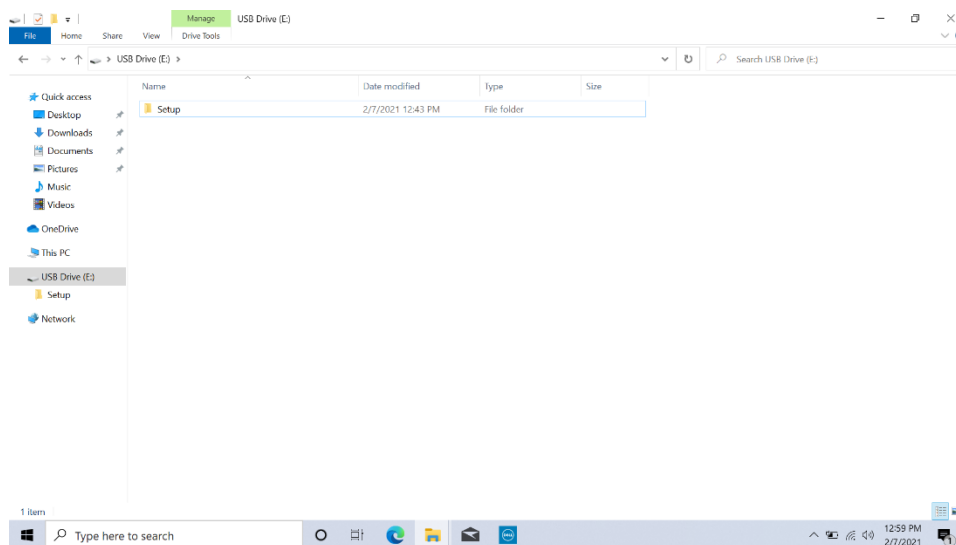


Figure 2.1 Installation Folder

3. Double click the “RSIQ_Setup” file, the installation will start as a setup wizard. Click “Next>”:

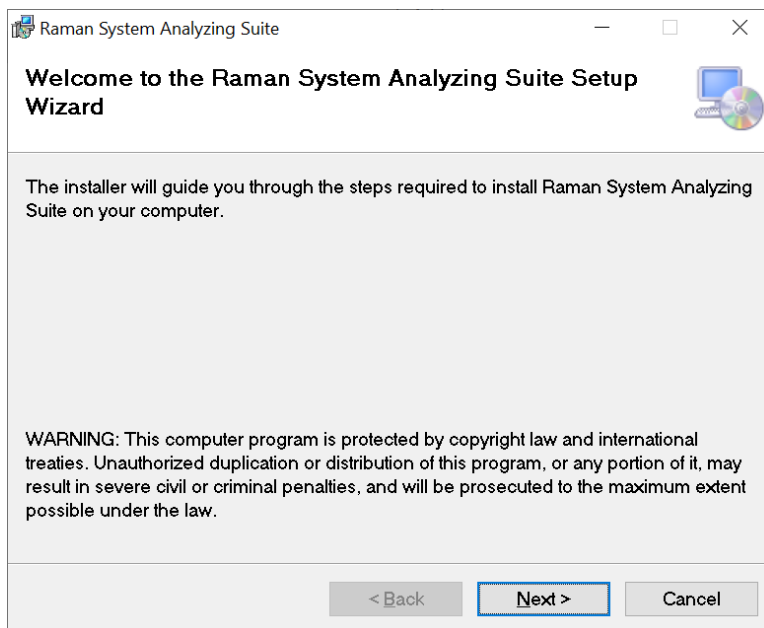


Figure 2.2 RSIQ Setup Wizard

4. The wizard asks to select the file folder location to install the software, click 'Browse' to change the default folder or click "Next>":

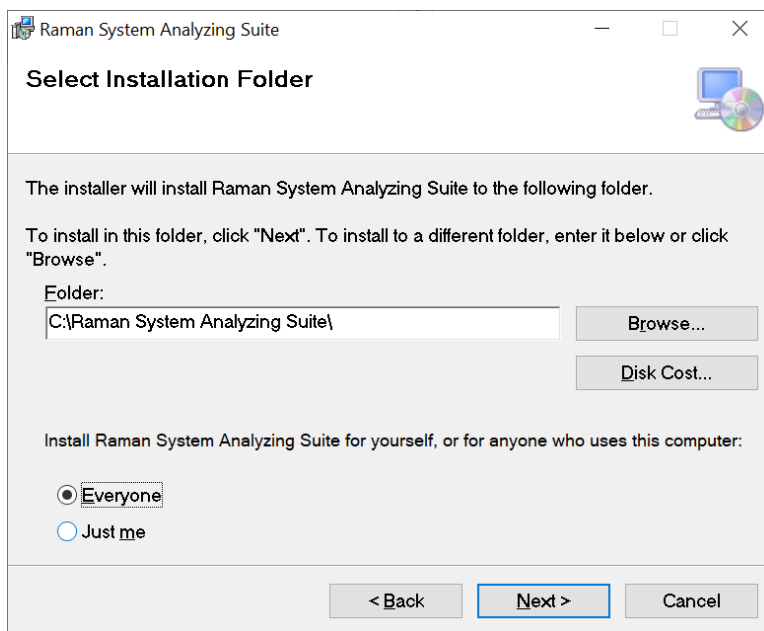


Figure 2.3 Installation folder

5. Confirm the installation and click "Next>". If you want to change the selection, click "<Back":

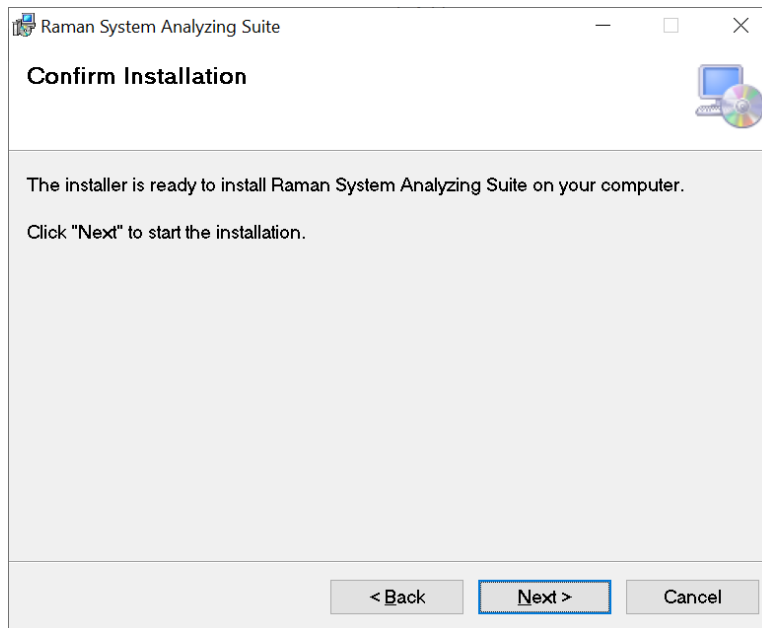


Figure 2.4 Confirm

6. After the installation is finished. Click "Close" to exit.

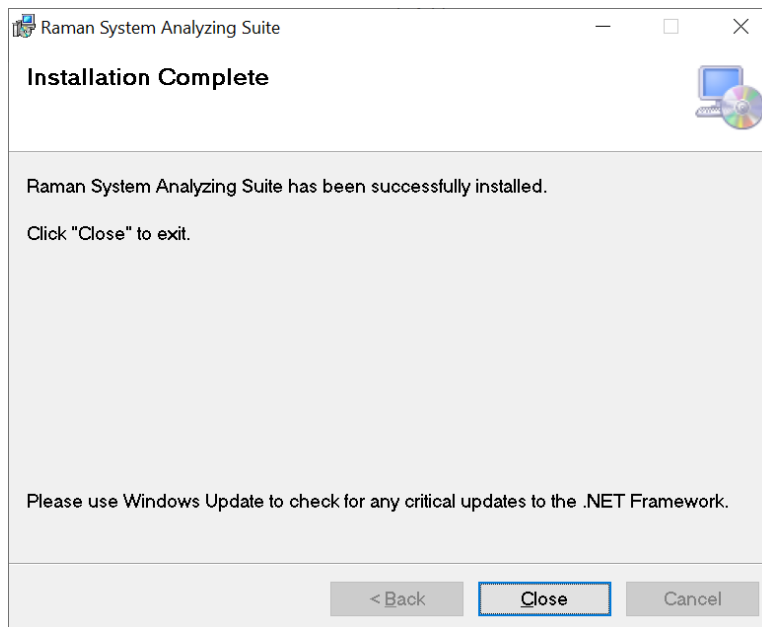


Figure 2.5 Installation complete

7. After the installation is finished the software will create a shortcut on the desktop.

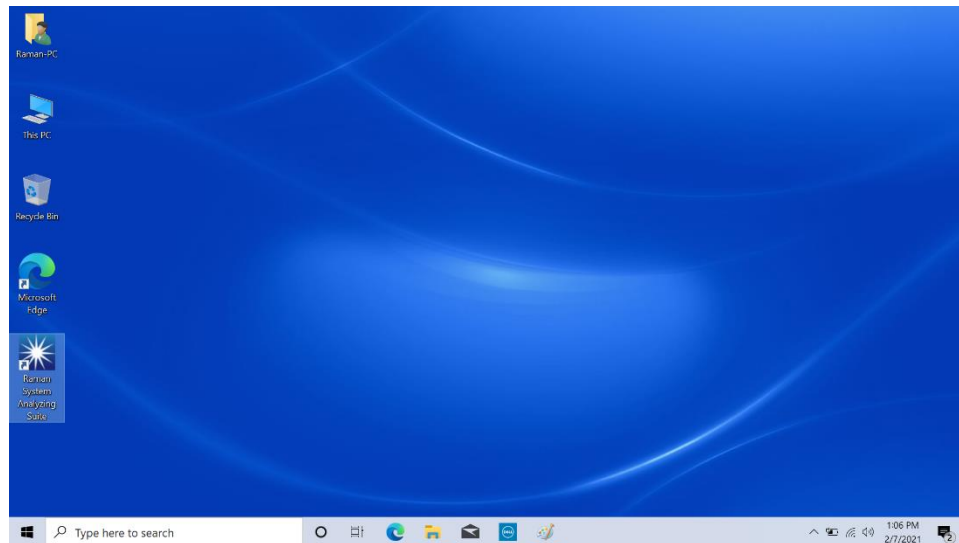


Figure 2.6 Desktop Shortcut

2.2 Spectrometer Driver Installation

Please operate the computer only, DO NOT connect the spectrometer to the computer.

1. Double click the 'Drivers' folder under the 'Setup' path

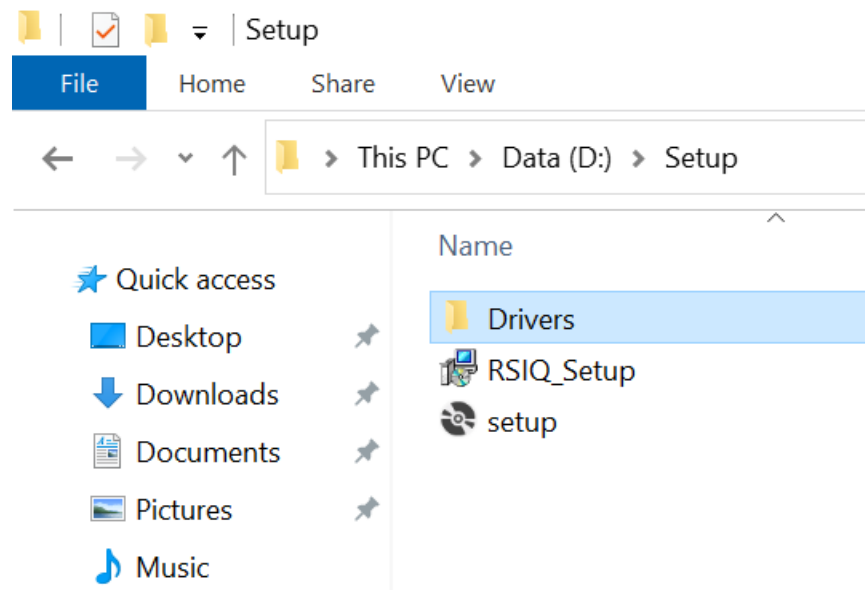


Figure 2.7 Driver Folder

2. Go to 'Spectrometer Driver' folder, the spectrometer needs both 32bit and 64bit drivers installed on the computer.

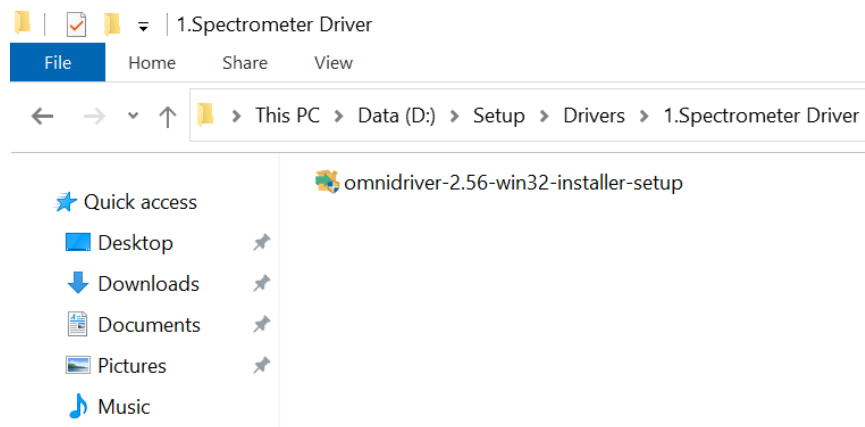


Figure 2.8 Spectrometer Driver Folder

3. Double click to start the installation. It supports a lot of languages, English is recommended.

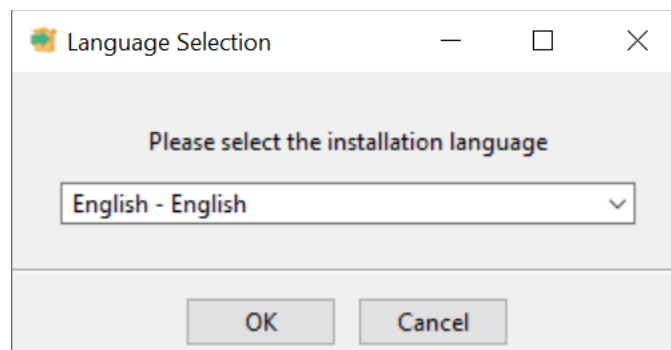


Figure 2.9 Language Selection

4. Follow the hint on the screen to finish the installation

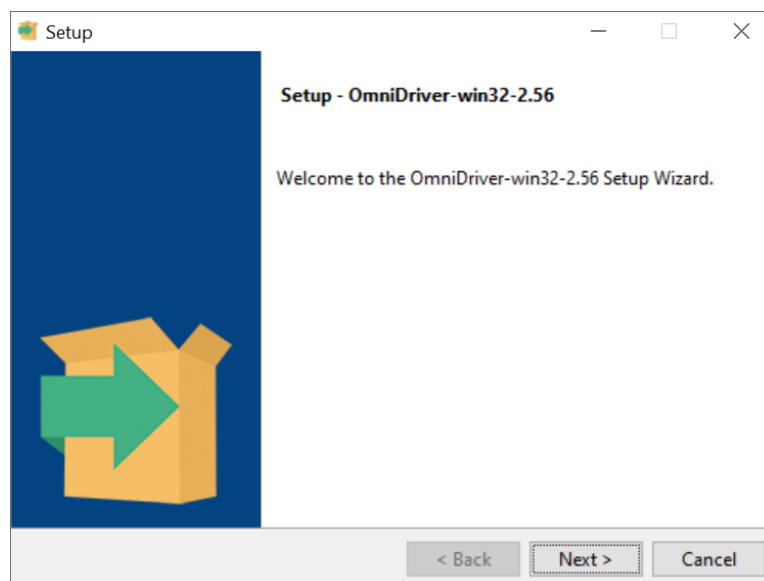
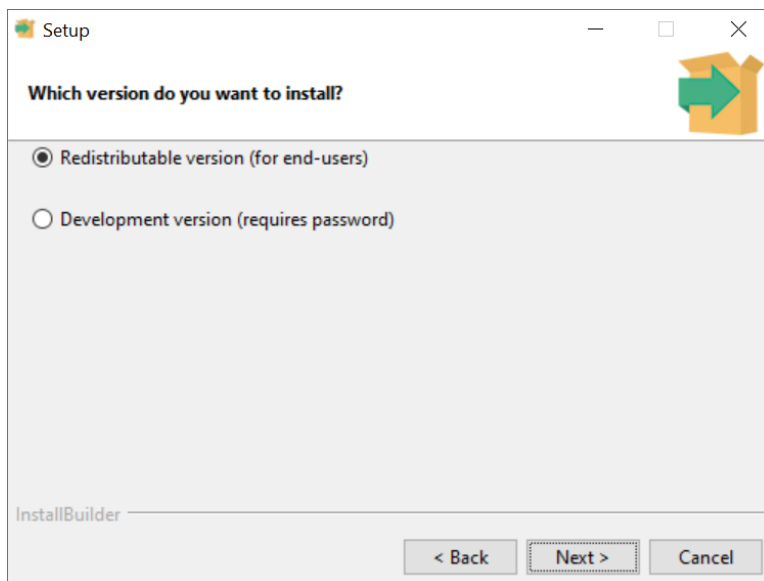
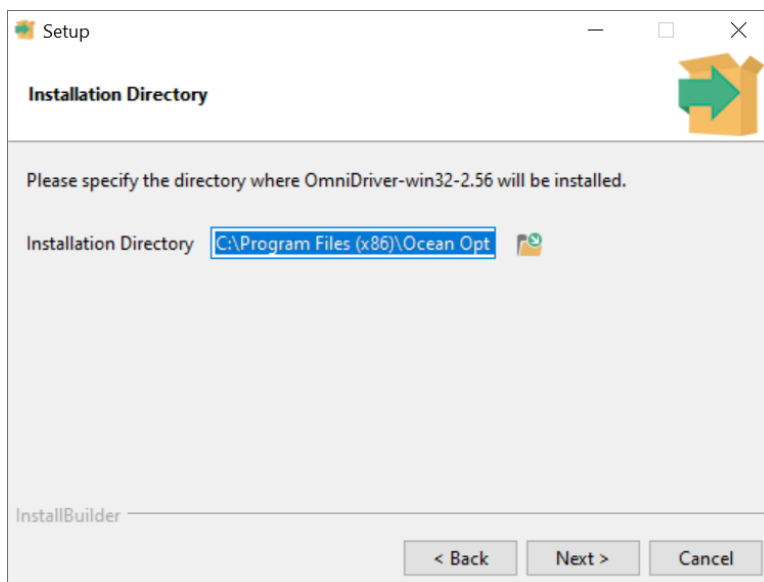


Figure 2.10 Setup Wizard

5. Choose 'Redistributable version' and click 'Next>'

**Figure 2.11 Version Selection**

6. Use the default installation directory and click 'Next>'

**Figure 2.12 Installation Path**

7. Use the default setting and click 'Next>'

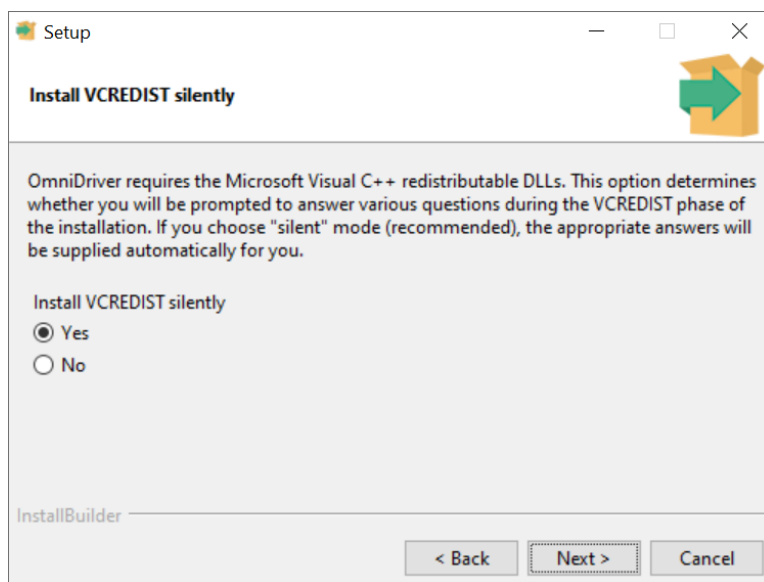


Figure 2.13 VCREDIST

8. For Windows 10 and future OS, please choose the default WinUSB drivers. EzUSB works for old OS like windows XP or vista. Click 'Next>' to finish installation

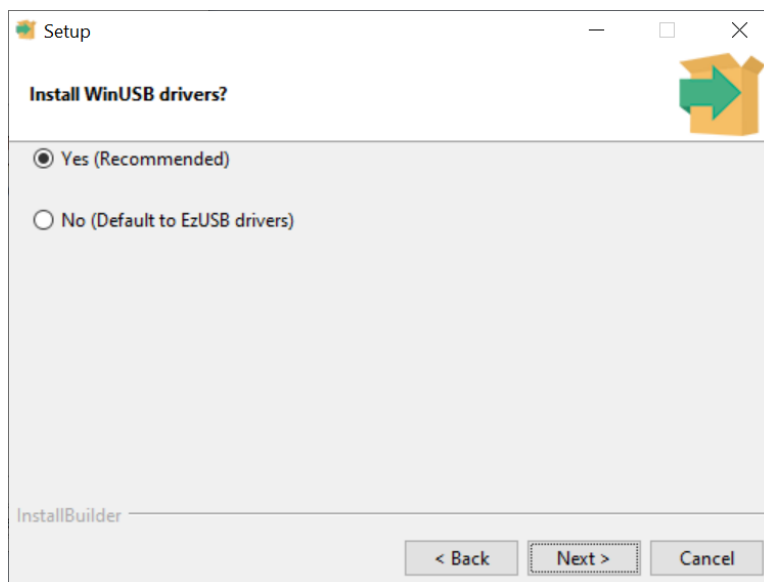


Figure 2.14 Driver selection

9. The installation is in processing

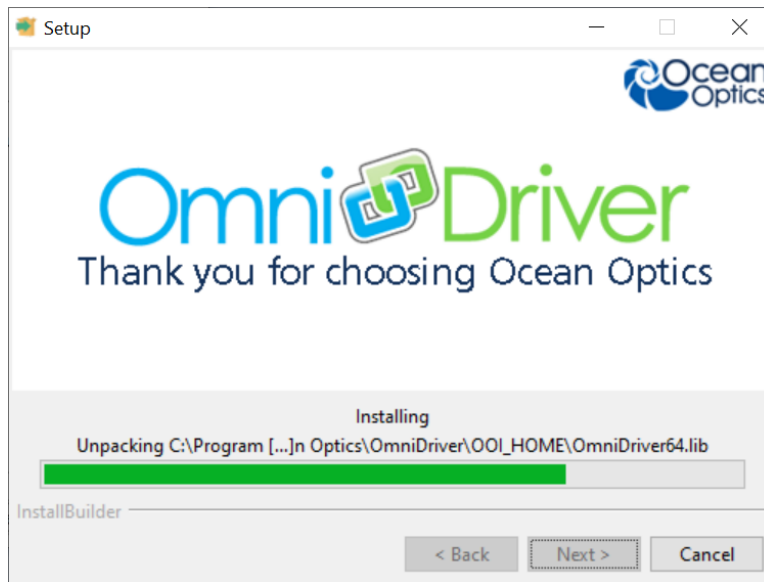


Figure 2.15 Installing

10. For Window 10 system, because the .Net Framework is 4.0 by default but the driver needs the 3.5 version, click 'Download and install this feature'. Otherwise, the system may not work properly.

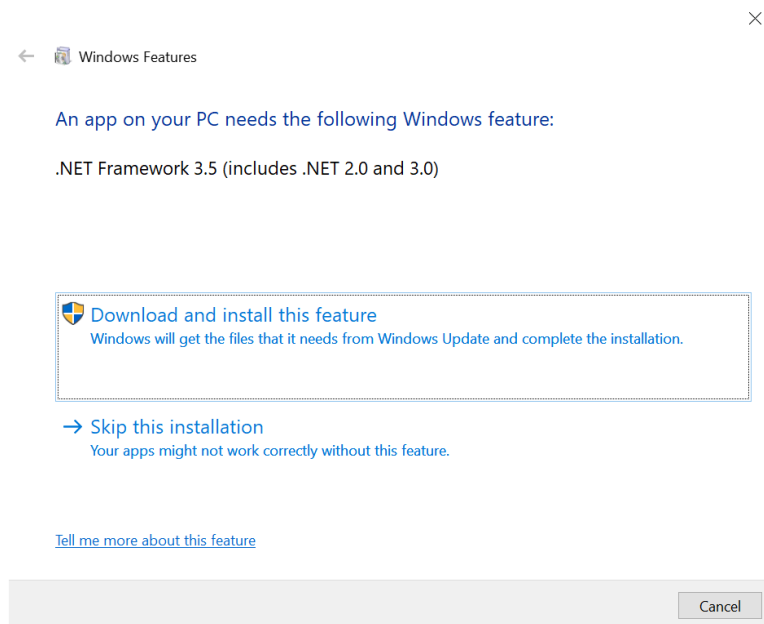


Figure 2.16 .Net Framework installation

11. Wait for the installation

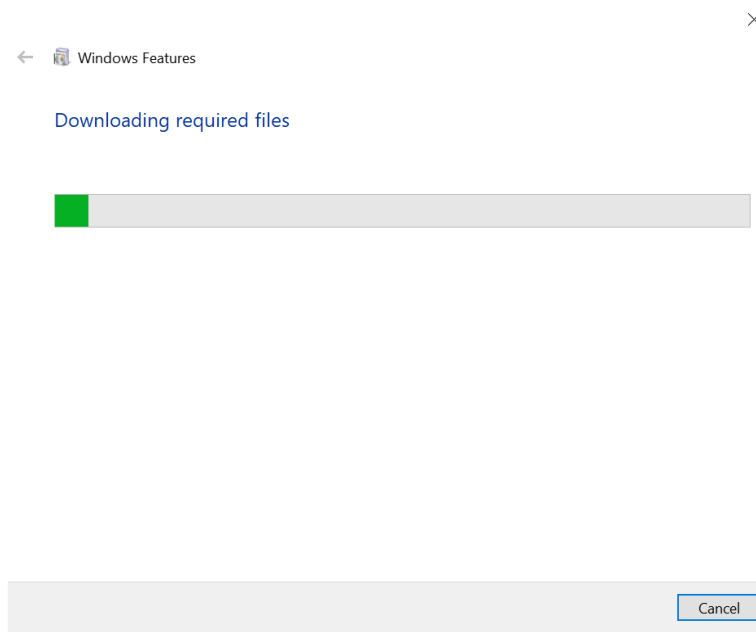


Figure 2.17 .Net Framework installation

12. Successfully installed the .Net Framework

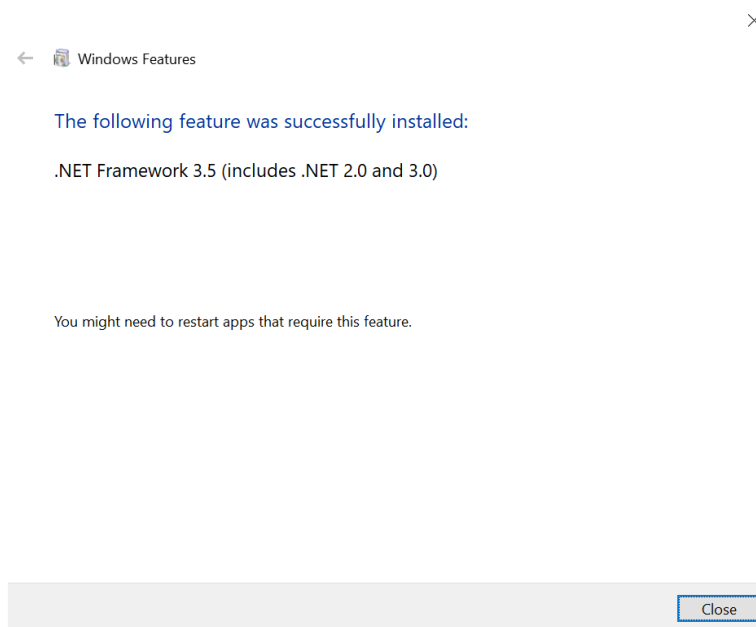


Figure 2.18 .Net Framework installed

13. Click finish to complete the installation

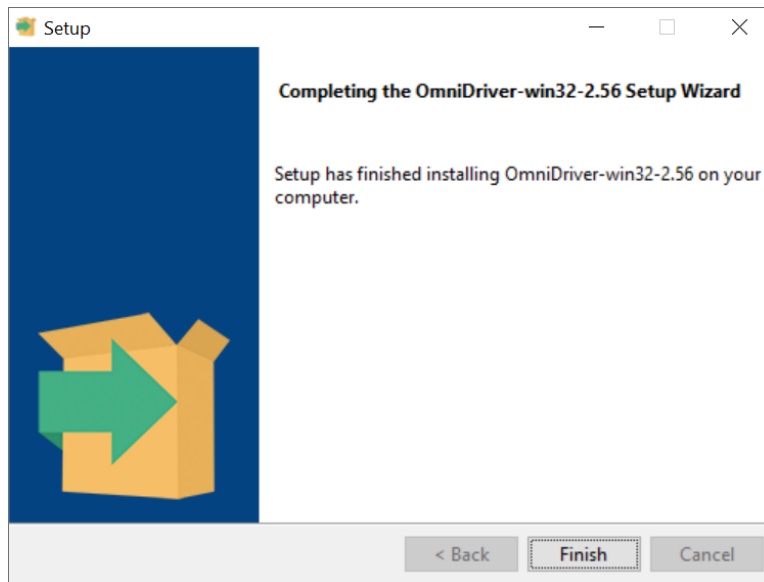


Figure 2.19 Driver installed

2.3 System Main board Driver Installation

Now connect the spectrometer with the provided USB cable to finish the installation of main board driver.

The spectrometer is equipped with a class 3b laser, please always wear a safety goggle when turning on the system power.

1. Plug in the 12V DC power supply.
2. Turn on the power switch.
3. Check the green LED on the front panel, if it turns on then the spectrometer is powered on. The green LED will only be turn on when the system is powered on and the USB cable is plugged into the computer. The system will never work if there is no USB cable plugged into a computer.
4. The Window system may automatically install the drivers from windows update server and show messages like this:

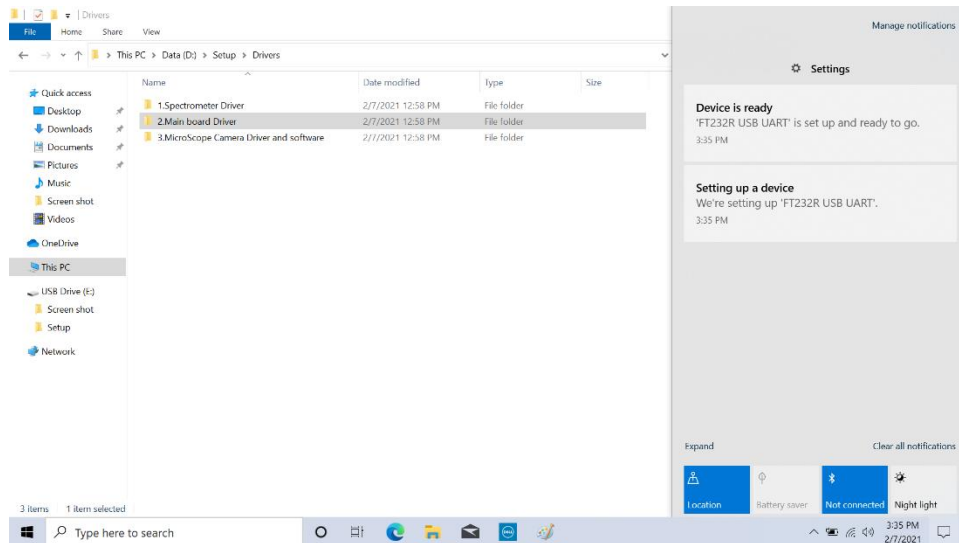


Figure 2.20 Main Board Driver

5. To verify the driver is installed correctly, please go to desktop and right click on 'This PC' and click 'Properties'

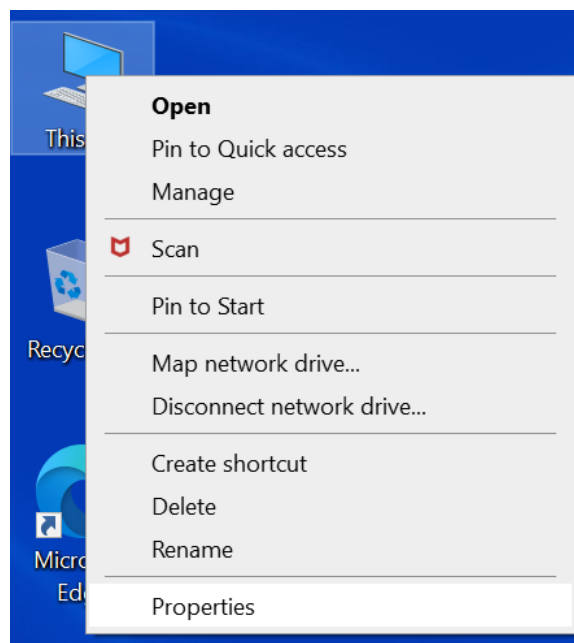


Figure 2.21 Find Device Manager

6. Click 'Device Manager' to check the installed drivers:

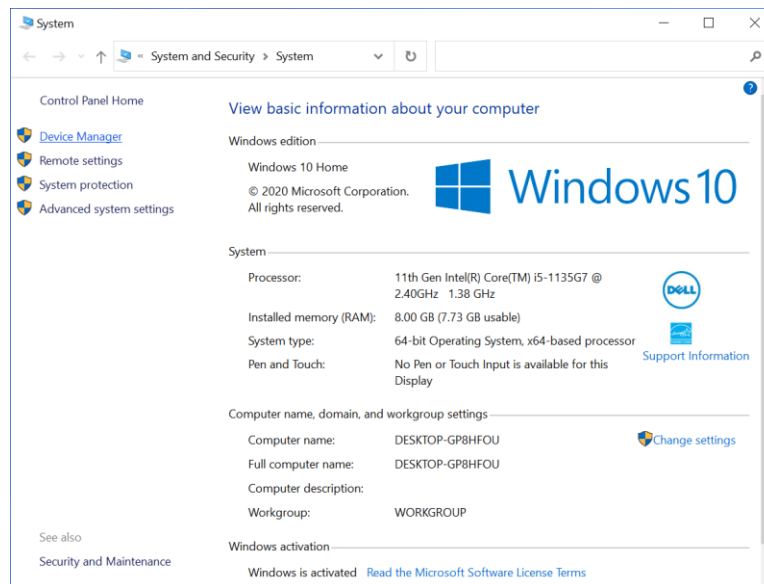


Figure 2.22 Find Device Manager

7. In this case, the spectrometer's driver installed correctly. But there is a yellow '!' in front of 'FT232R USB UART', that is the driver needed to control the laser

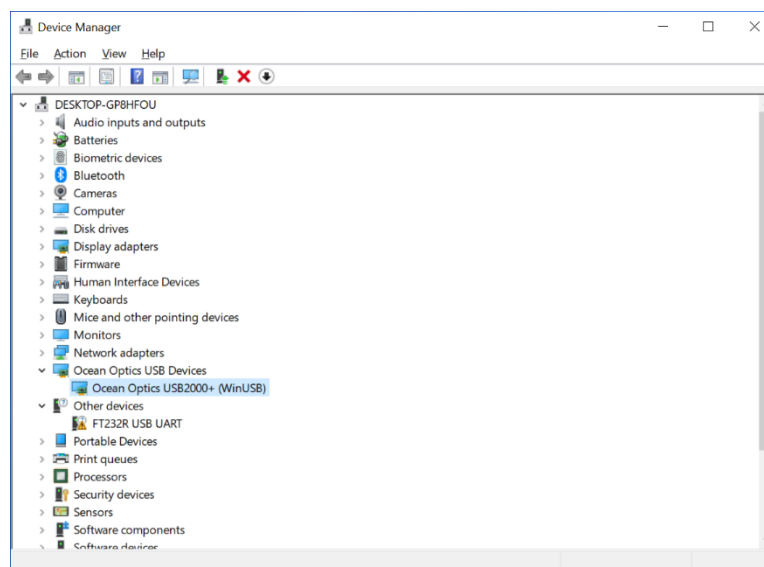


Figure 2.23 Check Installed Drivers

8. Right click on 'FT232R USB UART', select 'Update driver'

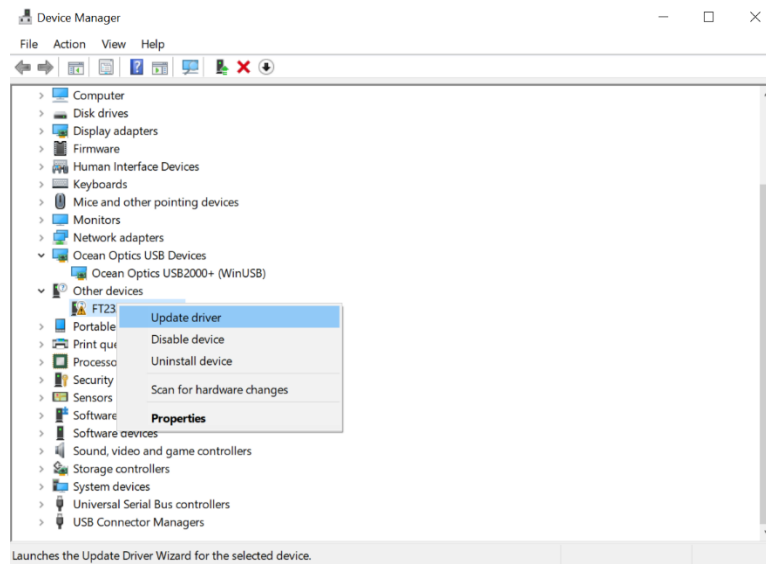


Figure 2.24 Update driver

9. Click 'Browse my computer for drivers'

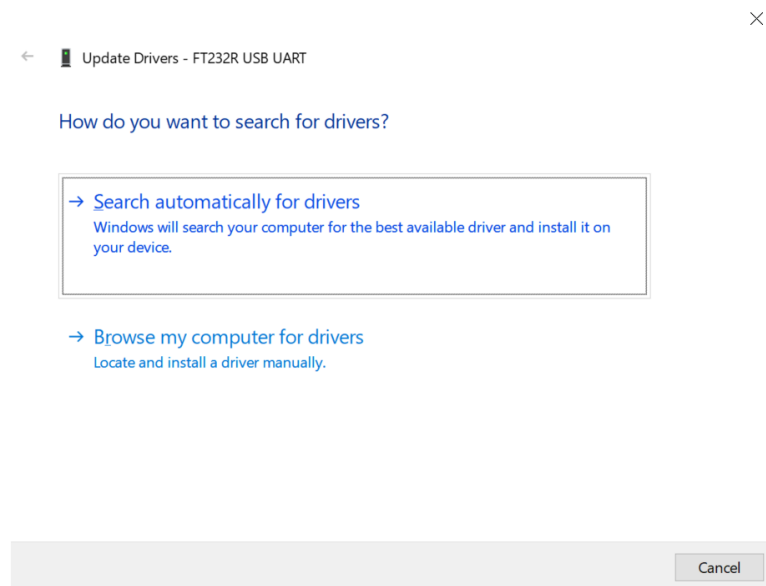


Figure 2.25 Choose the installation method

10. Click 'Browse' to select the driver location:

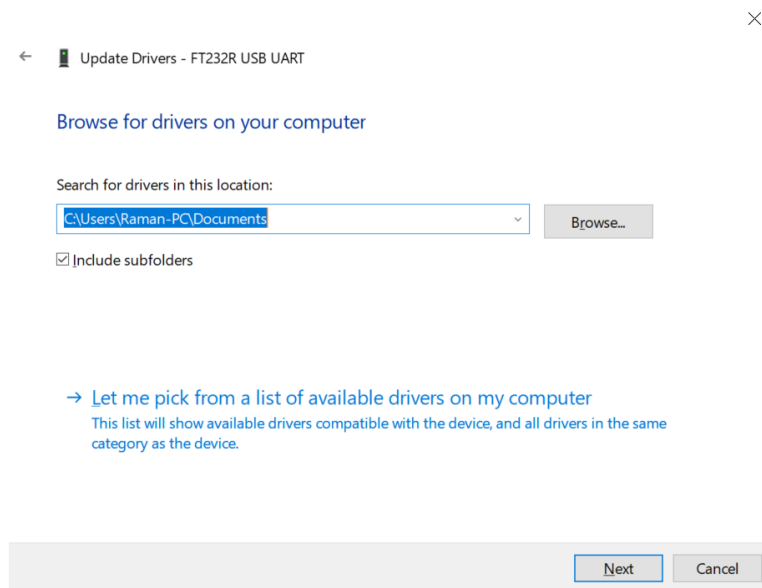


Figure 2.26 Choose the driver location

11. The default driver path is 'D:\Setup\2.Main board Driver'

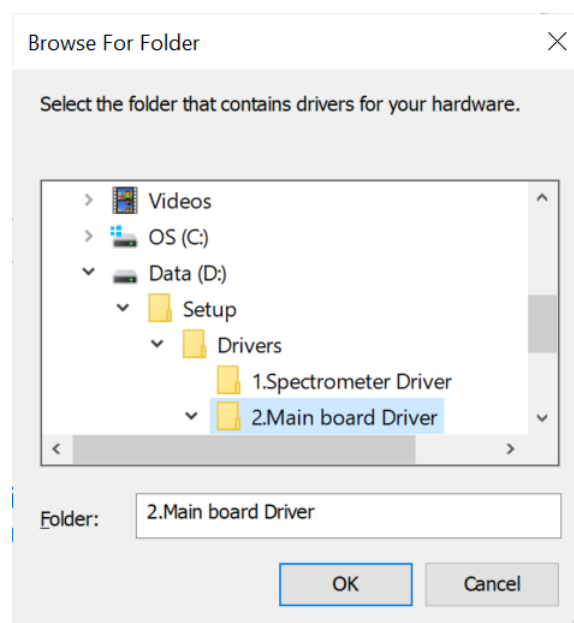


Figure 2.27 Driver location

12. Click 'Next' to finish the installation

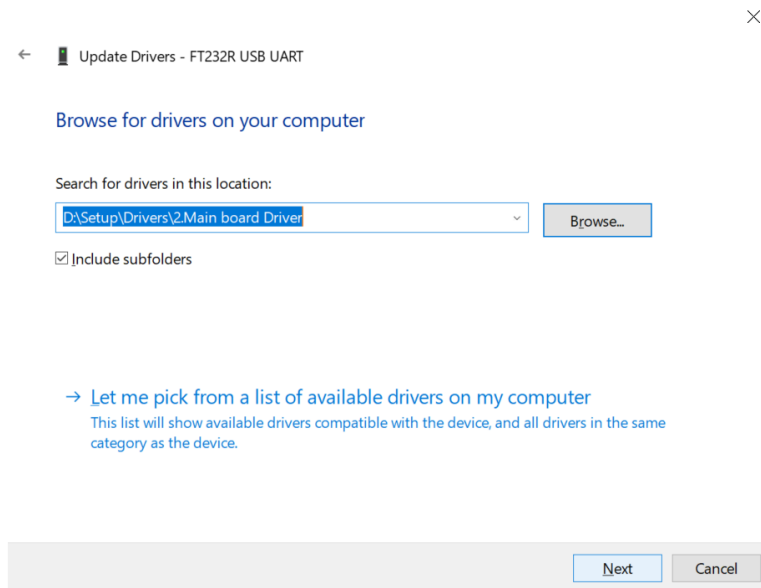


Figure 2.28 Set the driver location

13. Click 'Close' to complete the installation

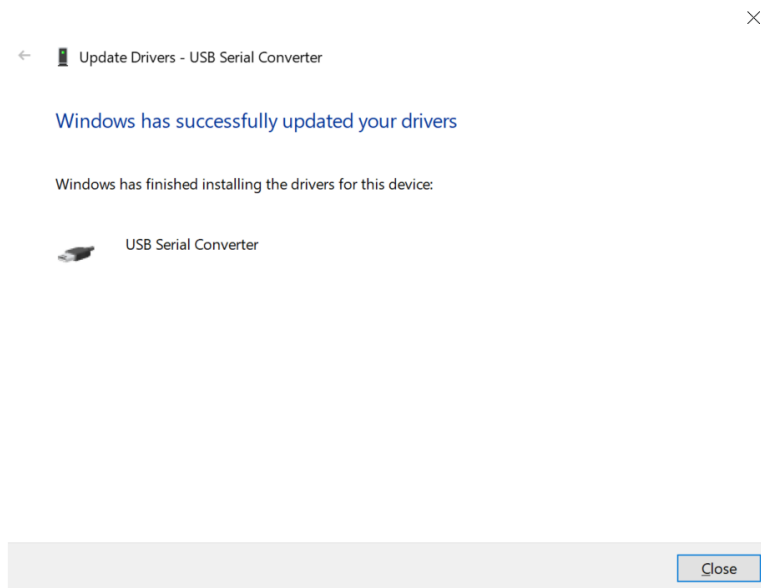


Figure 2.29 Finish the installation

14. Go to 'Device Manager' to check the hardware list, it shows another yellow '!' in front of 'USB Serial Port' this time.

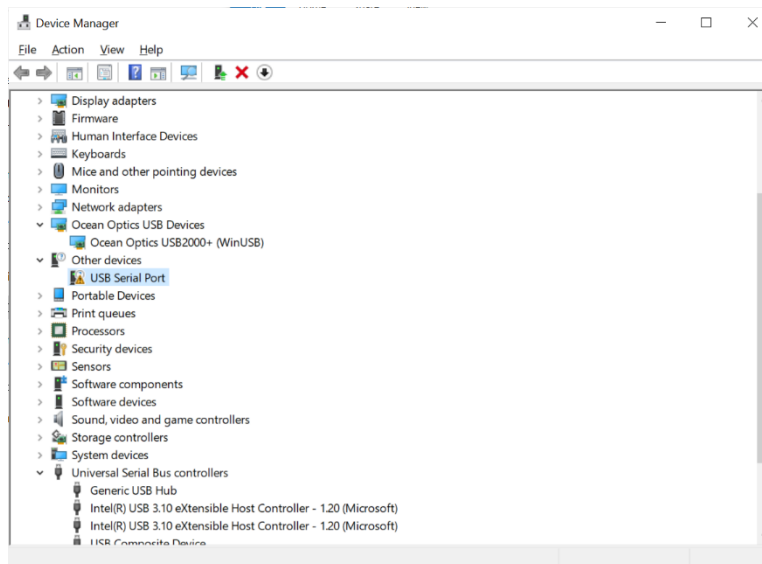


Figure 2.30 Check the hardware list

15. Repeat steps 8~14 to install the driver. Finally, it will show the USB serial port is successfully updated.

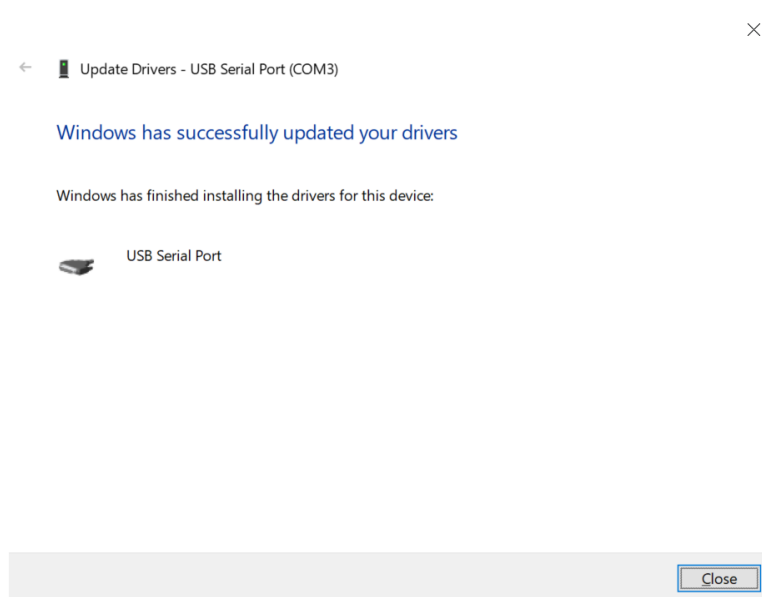


Figure 2.31 Finish the installation

16. Go to 'Device Manager' to double check all the drivers are installed correctly

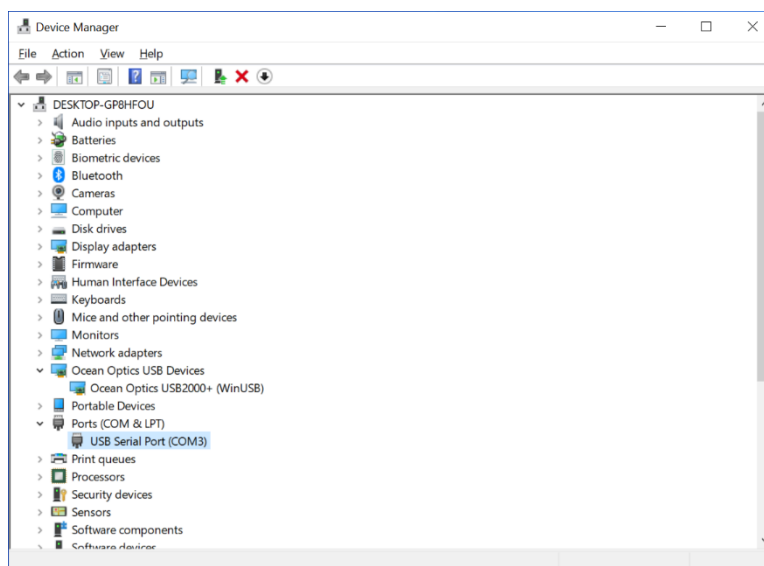


Figure 2.32 Double check the hardware list in the Device Manager

The 'USB Serial Port (COM3)' indicates that the installation is completed. Now the system is installed and ready to use.

3. User interface and operation

3.1 Quick Guide

A complete Raman spectrometer kit contains the Raman spectrometer, cabled probe, notebook computer, AC power supply, sample compartment, 2 probe measurement caps---L for liquid samples and S for solid samples, 2 keys for laser activation, 2 interlock connectors---a blank one for customizing and a soldered one for default using, USB cable.

If you want to use your own computer, please read through section 1 “How to install the RSIQ software”.

- 1) Plug the USB cable into Raman spectrometer and the computer. Plug the soldered male interlock into the female part on the back panel and a key into the laser lock switch. Plug in the power supplies for both the Raman spectrometer and computer.
- 2) Wear the safety goggles before the next step.
- 3) Turn on the power switch at the back of Raman spectrometer. The fan will work and the green LED on the front panel will illuminate.
- 4) Turn on the laser key switch. For safety reasons and lower power consumption, the laser will not be turned on at this time.
- 5) Turn on the computer and run the RSIQ software. While the software starts, there will be a screen to show the spectrometer which is detected. If it does not show the serial number or displays 'No systems detected!', please unplug the USB cable and plug again.

The first step in measuring a sample is to collect the dark scan from the sensor. After setting the integration time and clicking 'Collect spectrum', a dark scan initiates. After recording the dark scan, the laser will turn on and the red LED on the front panel will illuminate to indicate the status of laser. After the scan is complete, the laser will turn off and the Raman spectrum of the sample will be displayed.

3.2 Power up the instrument

1. The 12V DC Adapter supplied with the unit plugs into the Power Input Port located in the back of the instrument as shown in the picture.

*****The PRO-532 uses a universal 110~240V power supply which is built into the system. Please plug the wall outlet power cord into the power port.**



Figure 3.1 Power Port & Power Switch

2. The instrument may be powered up by switching on the Power Switch located in the upper left corner of the back panel. When the instrument is powered on, the green “System Power” on the front panel illuminates.

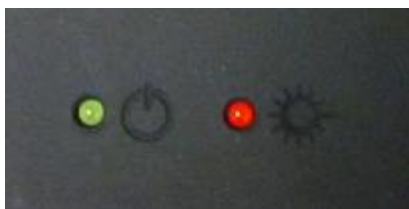


Figure 3.2 Status Indicator LEDs

3. The interlock is an additional safety feature with a connector on the back panel. It is a 4 CONTACT PLUG W/PIN INSERT. One of the mating plugs supplied with each instrument has pins 1 and 2 shorted internally to operate the laser. The other, blank plug can be wired to a safety switch is desired. Connector pins 1 and 2 need to be crossed for the laser to operate.



Figure 3.3 Interlock & Ignition Switch

4. Insert the Laser key into the ignition switch on the back and turn the key to “Laser On” position. The red LED labeled “Laser Power” will not turn on at this time. Because this is a safety control, the laser is kept Always-Off until the software command is initiated to collect a spectrum. After collecting the dark scan during a sample measurement, the red status LED will illuminate when the laser beam is active.

3.3 Operate RSIQ Software

3.3.1 Start the software

Locate the RSIQ icon on the desktop of the computer connected to the instrument and double click to start the software.

3.3.2 Main Screen

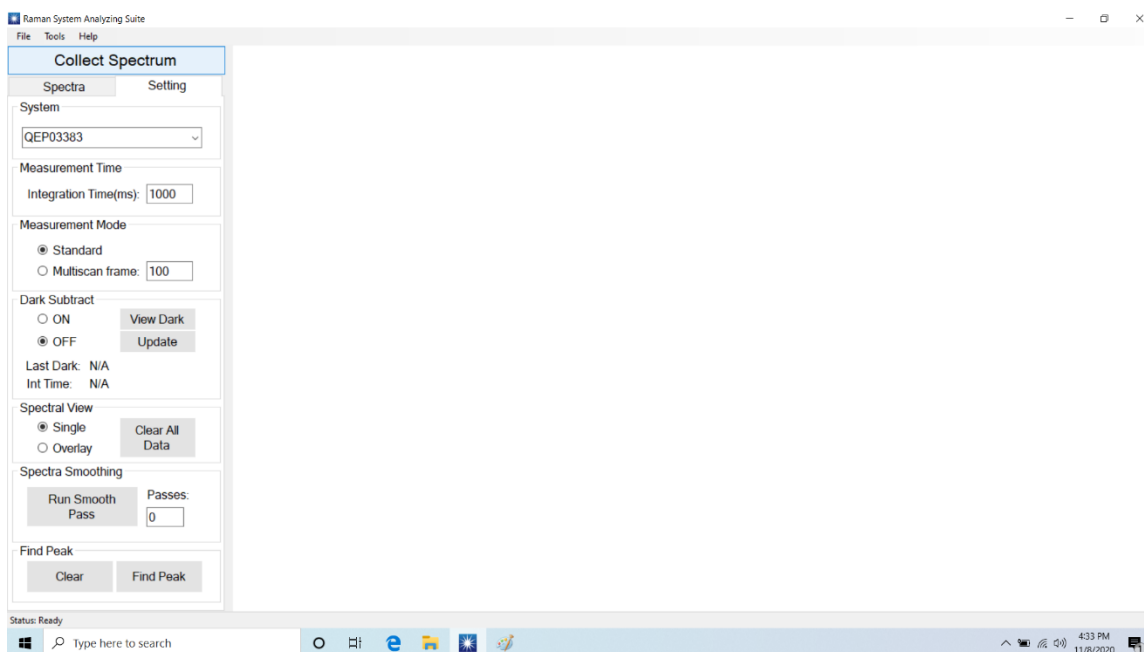


Figure 3.4 Main Screen

1. Menu Bar

- a. File: Allows user to open, save and print files.
- b. Tools: Brings up the options menu.
- c. Help: System documentation

2. Collect Spectrum – Takes a scan.

3. **Settings/Data Display**

Spectra Tab- Displays the currently loaded spectra and associated file data.

Settings Tab- This section is used for setting parameters for data collection.

4. **Status Bar**- Displays the current state of the system.

5. **Plot Area**- Displays the spectral plot of the active spectrum.

3.3.3 Settings Tab

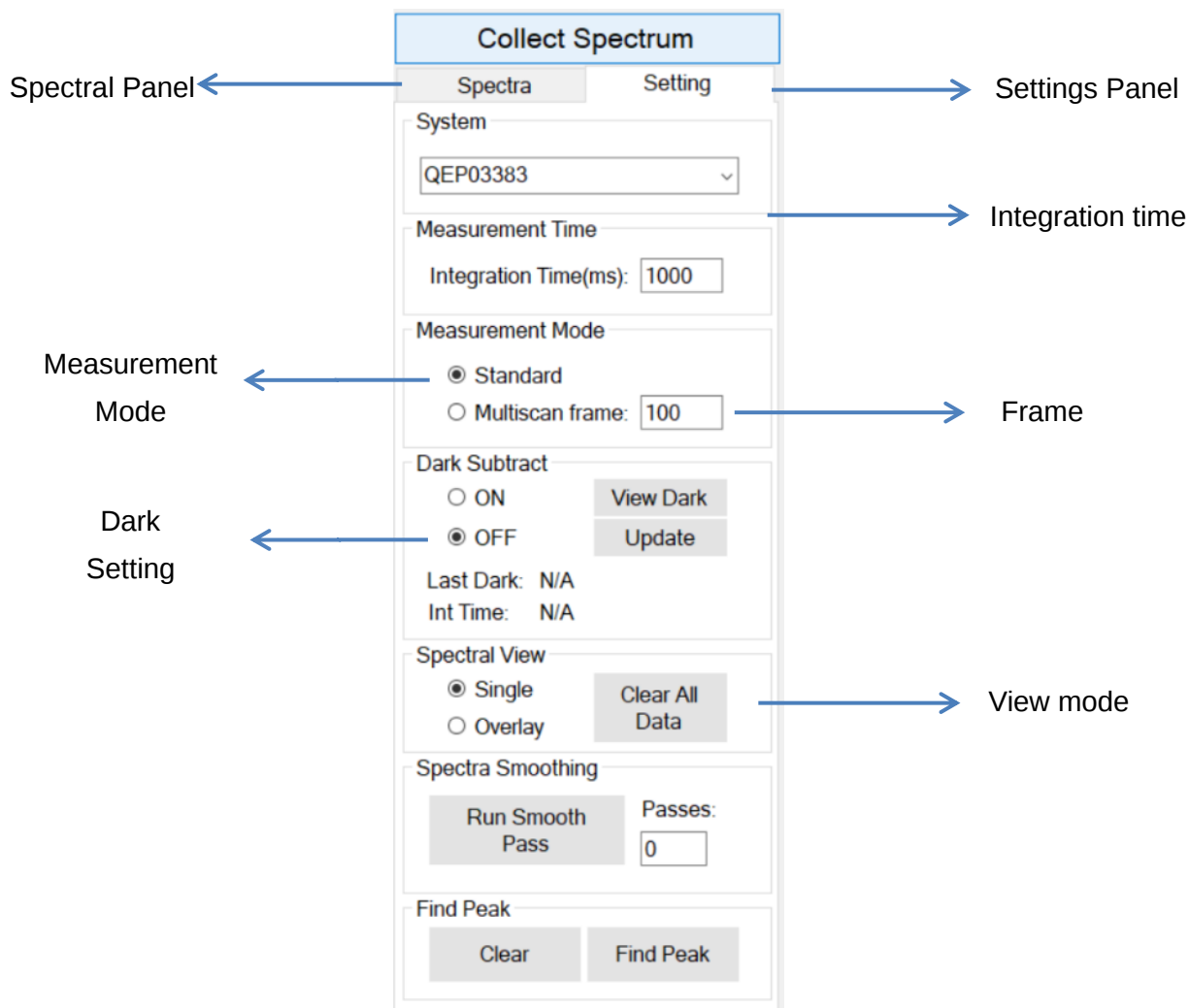


Figure 3.5 Settings Tab

Integration Time- This setting is used to determine the length of time (seconds) for the measurement.

PeakSeeker: 3 ms to 30 sec

PeakSeeker Pro: 8 ms to 15 min

Measurement Mode

Standard – This mode takes a single spectrum at the given integration time and displays it on the plot area. A dark subtract is taken if the option is turned on.

MultiScan – This mode allows the user to take spectra at a given interval. The start time of each spectrum is based on the frame setting.

Frame – This setting determines the integration time from start to end of a single spectrum.

Ex: If the frame is 30, a spectrum will start every 30 sec. The total scan time is determined by the integration time.

Ex: If the integration time is 310 sec., and the frame size is 30, there will be 11 scans - 10 scans at 30 sec. and 1 scan at 10 sec.

Dark Setting

A dark scan is a measurement of the dark signal on the CCD array at the set integration time. It adds a baseline bias to sample scans if not subtracted.

On/Off – This turns the dark scan subtraction on and off. A new dark scan will automatically be performed before any sample scan when the integration time is changed or if more than one hour of time has passed at the same integration time.

View Dark – Click this button to display the dark spectrum on the plot area.

Update Dark – Click this button to update the dark. A dark is immediately taken and updated in memory by the system.

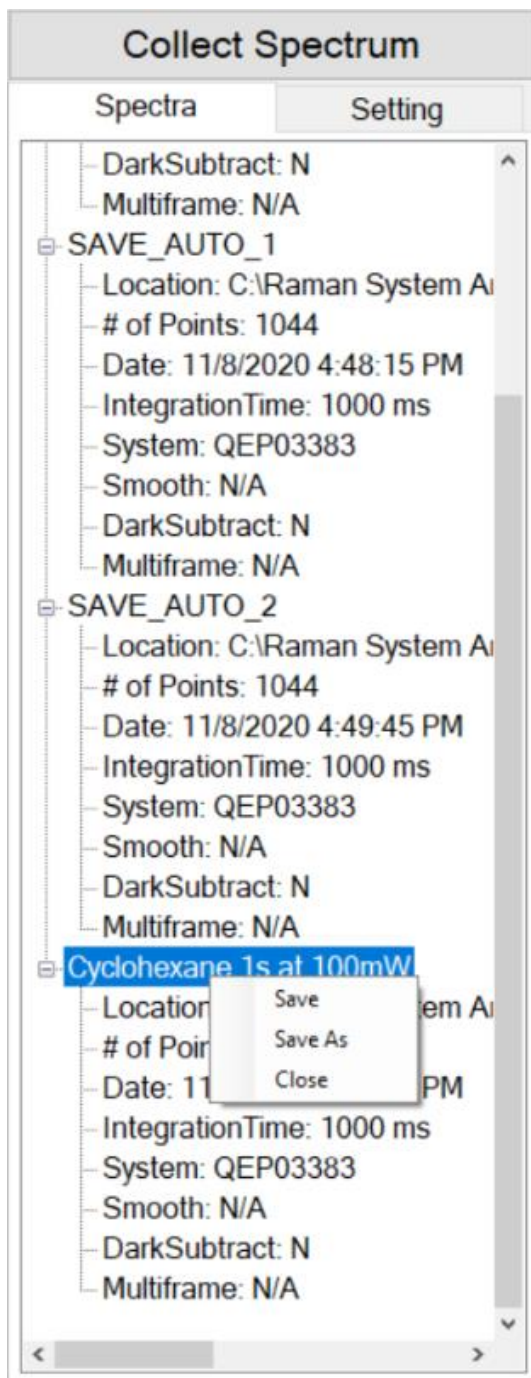
Last Dark Taken/Integration Time – Displays the time the last dark scan was recorded, and the integration time used.

Spectral View – Toggles the plot area between overlay and single display.

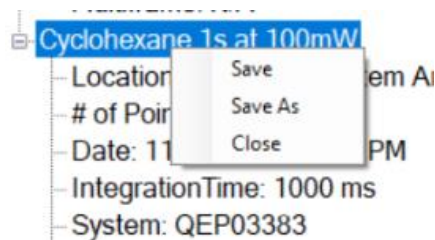
Clear All – This setting erases all spectra recorded.

Smooth – This setting will smooth the displayed spectrum. The number of smoothing 'passes' accumulates for each time the 'Run' button is pressed.

3.3.4 Spectral Data



The Spectral Data panel displays all of the currently loaded spectra. To view the data associated with a spectrum or to make a spectrum the active spectrum simply click on the  sign. In the Spectral Data panel, you can also right click to view a context menu for commands associated with each spectrum.



1. Location: The path that the spectrum is saved.
2. # of points: The length of the spectrum.
3. Date: Date and time when the spectrum is taken.
4. Integration time: The integration time of the spectrum.
5. Smooth: The passes of the spectrum if smoothed.
6. Dark Subtract: Y/N, indicate whether or not the dark was subtracted.
7. Multiframe: Indicate if this is a standard spectrum of multiframe.
8. Save: Save an unsaved spectrum, there is a '*' to indicate if the spectrum is not saved.
9. Save As: Save the current spectrum to another file or format
10. Close: Close the current spectrum

Figure 3.6 Spectral Data

3.3.5 Spectrum Display

The display for a Single Spectral View is shown below.

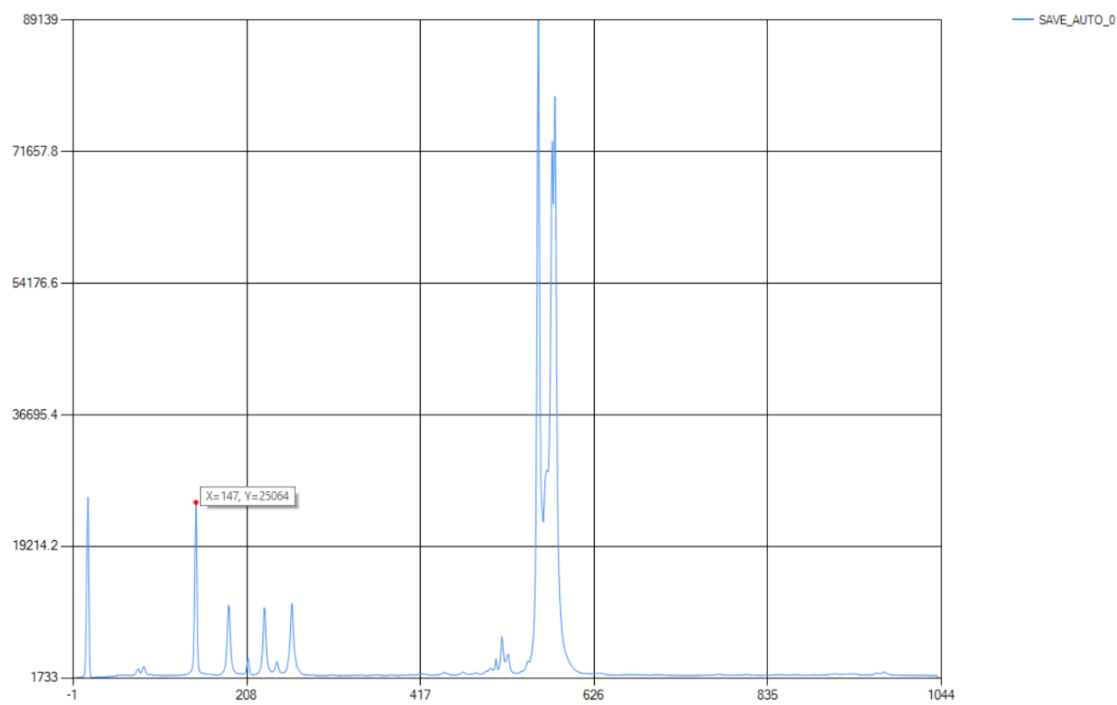


Figure 3.7 Display

Placing the mouse on the spectrum will bring up the X/Y coordinates while X is the position---pixel number or wavenumber, Y is the intensity.

4. Advanced Operations

4.1 Options

Select the pull down menu for “Tools” and click on “Options”

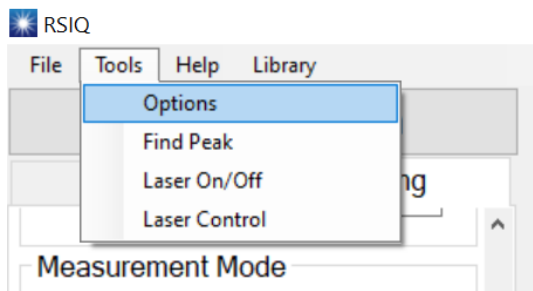


Figure 4.1 Tools Menu

The Options screen is divided into 2 sections. Each section is accessible by clicking a tab.

4.1.1 Settings Panel

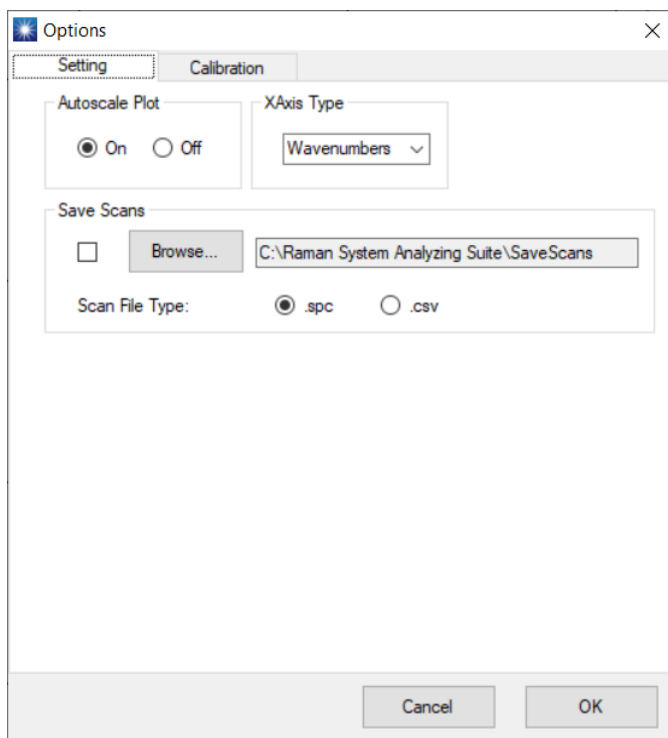


Figure 4.2 Settings

1. **Auto Scale Plot**- This option turns on and off the automatic scaling when a spectrum is displayed.
2. **X axis**- Allows the user to select the units they want for the X-axis plotted. There are 2 units: Pixels and Wavenumbers. If the system X-axis is not calibrated, only pixels is displayed even when other units are selected to label the X-axis. Units of Wavenumbers use the X-axis calibration to display a calibrated Raman spectrum. The unit used is a matter of user preference for the X-axis label as plotted.
3. **Save Scans**- the default path for saving test data. Change the folder path if desired and select check box to enable this function. The default setting is disabled.
4. **Scan File Type**- Allows the user to specify a format to save the spectrum, spc file or csv format.

4.1.2 Calibration

Each system shipped by Raman Systems is calibrated by recording the Raman spectrum of a substance whose peak locations are specified in the standard ASTM E1840. The calibration consists of determining a function that transforms the measured peak locations from pixel locations to the peak locations in Raman shifted wavenumbers specified by the ASTM standard while minimizing the sum of the squared errors.

Options

Setting Calibration

Calibration Setting

Integration Time(ms): 3000

Collect Standard Spectrum

Calibration Points

1	76	=	378.5
2	100	=	521
3	144	=	786.5
4	168	=	919
5	182	=	1003.6
6	187	=	1030.6
7	219	=	1211.4
8	293	=	1605.1
9	425	=	2253.7
10	580	=	2940.8
11	608	=	3057.1

Calibration Result

Smooth

Find Peak

Run Polynomial Fitting

Degree: ☒ 3 ☐ 5

a0: -106.42840501778

a1: 6.55335516489583

a2: -0.00264424368739

a3: 6.95975263631643

a4: N/A

a5: N/A

Cancel OK

Figure 4.3 Calibration

1. **Integration Time(ms)** The time for collecting a spectrum to calibrate.
2. **Collect Standard Spectrum** To collect a spectrum of the standard material for calibrating.
3. **Calibration Points:** The left side is the pixel position the right side is the standard wavenumbers.
4. **Calibration results:**

- a. **Smooth:** If the spectrum has too much noise, use this button to smooth it.
- b. **Find peak:** manually find each peak
- c. **Run Polynomial Fitting:** Click this button to finish the calibration
- d. **Degree:** Choose the degree of polynomial fitting, default is 3
- e. **a0~a5:** Calibration result

4.2 How to Perform Calibration

1. Ensure that the calibration module is inside the sample compartment, and that the probe with the right Cap attached is set up against the glass vial. Close the lid of the sample compartment and click 'Collect Standard Spectrum' to continue.

Figure 4.4 Collect Standard Spectrum

- a. PeakSeeker PEK-785, PeakSeeker PRO-785E, PeakSeeker PRO-532 use L Cap and 50/50 (v/v) mixture of Toluene and Acetonitrile liquid in a glass vial as the calibration module. (ASTM E1840)
- b. PeakSeeker PRO-785 use S Cap and an acetaminophen tablet as calibration module.

2. The software will then get the spectrum. By default, it takes 3~5 seconds depends on the laser power and sample.
3. Once the collecting has successfully completed, use 'Find Peak' to get the pixel position according to the standard spectrum.

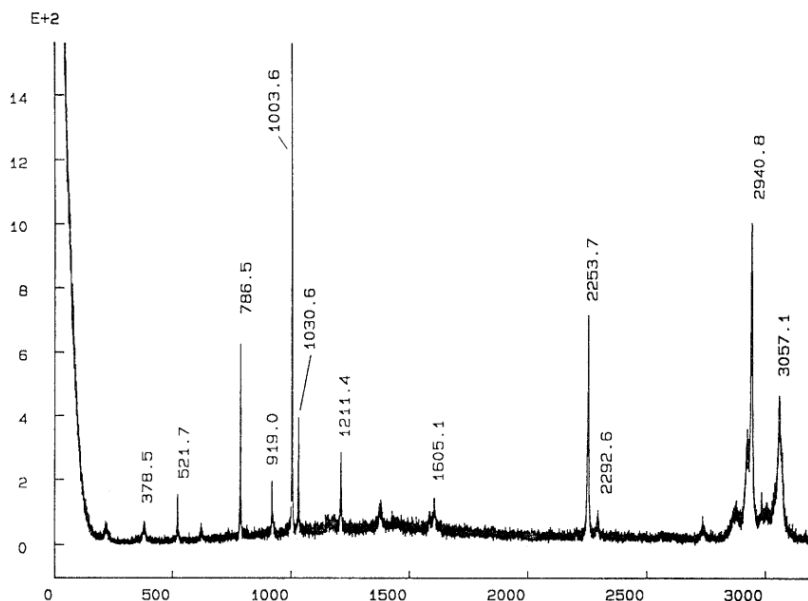


Figure 4.5 Standard Spectrum (50/50 Toluene/Acetonitrile)

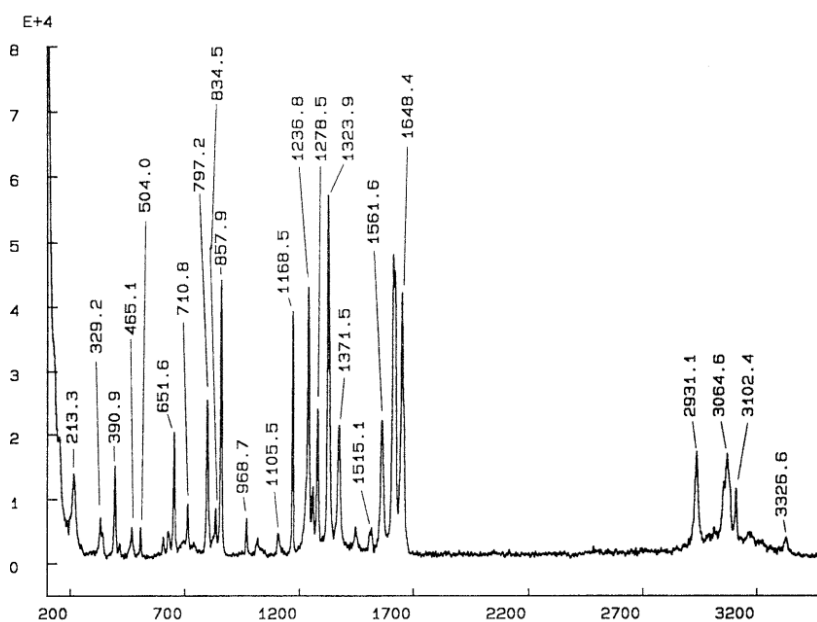


Figure 4.6 Standard Spectrum (Acetaminophen)

4. Use the Peak Find to look for the peak:

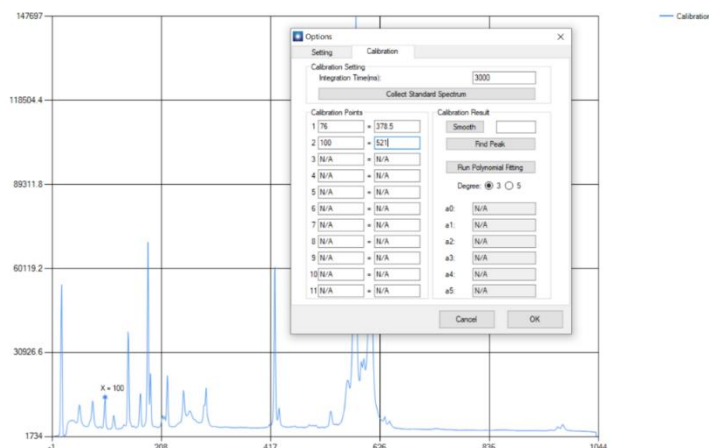


Figure 4.7 Peak Find

- After all the peaks are find, click 'Run Polynomial Fitting' to finish the calibration. After calibration, the a0~a5 will show the parameters.

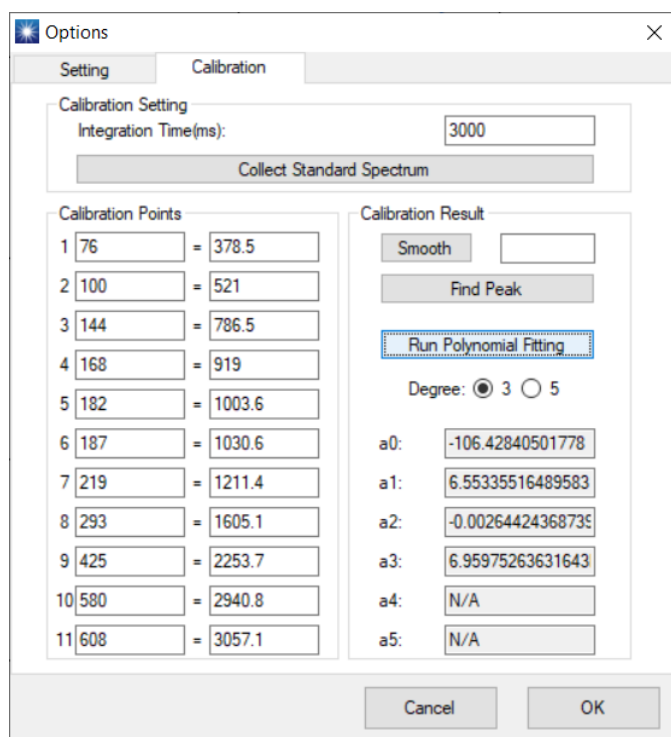


Figure 4.8 Calibrated

- After Calibration, change the X-Axis type to wavenumbers.

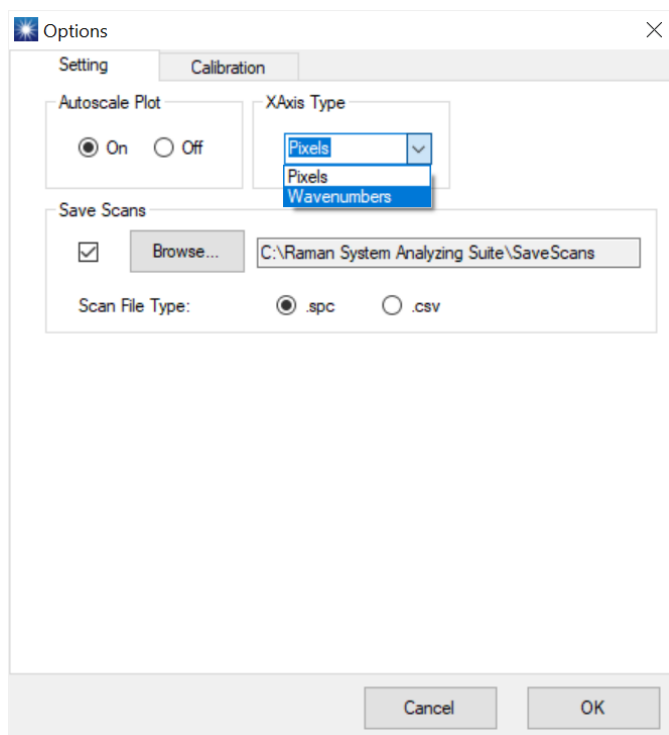


Figure 4.9 Change to Wavenumbers

4.3 Laser Power Calibration

The laser power needs to be calibrated to control by the software, enter the laser control page by clicking 'Laser Control' menu under 'Tools'.

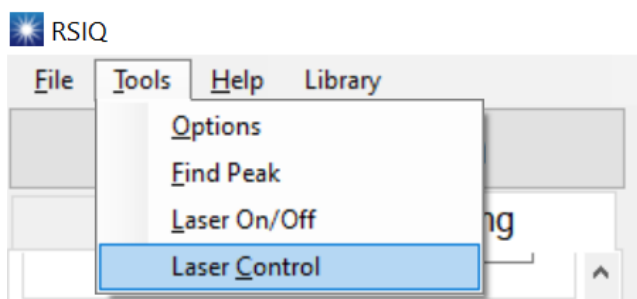
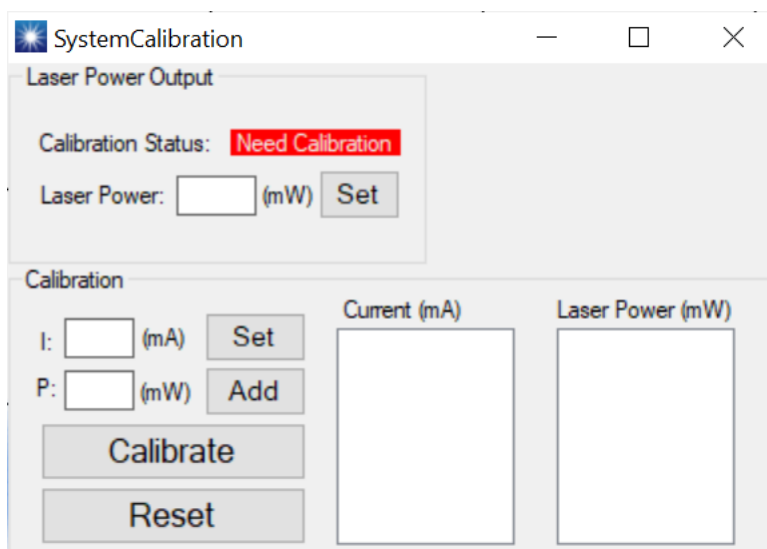


Figure 4.10 Enter Laser Control

The window will show 'Need Calibration' if the laser power is not calibrated.



SystemCalibration

Laser Power Output

Calibration Status: **Need Calibration**

Laser Power: (mW)

Calibration

I: (mA)

P: (mW)

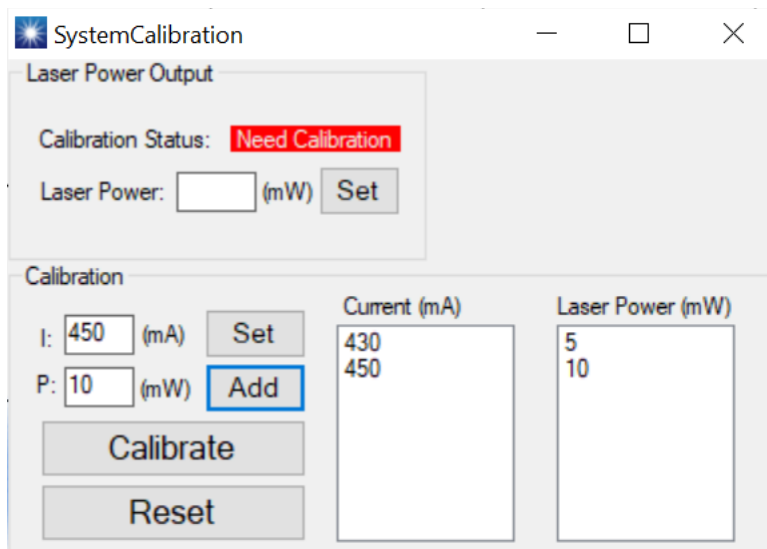
Current (mA)

Laser Power (mW)

Figure 4.11 Not Calibrated System

Enter a current value in the text box in front (mA), the threshold is around 400mA for a typical 785nm system. Measure the real power by using a power meter, input the measured power in the text box in front of (mW). **DO NOT** exceed 1500mA, otherwise it will damage the laser.

*****The recommended power level needed is 5mW, 10mW, 15mW, 25mW, 50mW, 100mW, 150mW, 200mW, 250mW and 300mW.*****



SystemCalibration

Laser Power Output

Calibration Status: **Need Calibration**

Laser Power: (mW)

Calibration

I: (mA)

P: (mW)

Current (mA)

Laser Power (mW)

430
450

5
10

Figure 4.12 Add optical power and laser current to calibrate the system

After input all the power and current, click calibrate to finalize the calibration. Close the window and re-enter, it will show 'Ready to use'. Input any power between the maximum and minimum calibrated in last step and click 'set' to set the laser power:

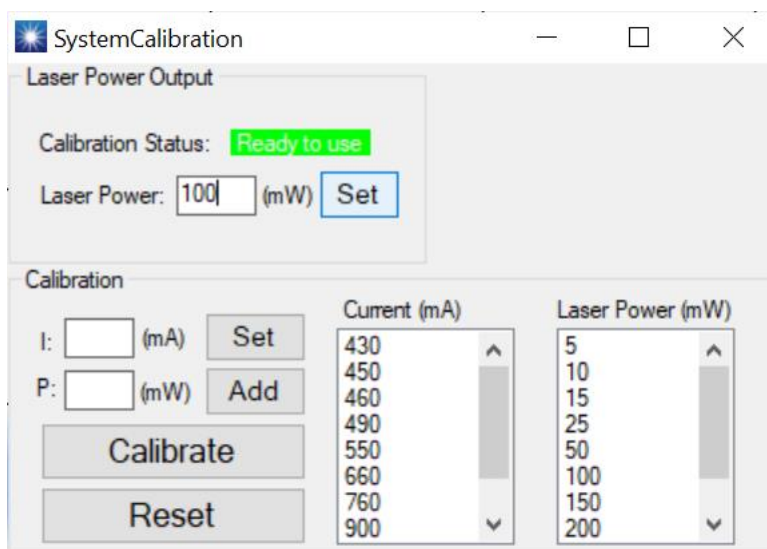


Figure 4.13 Calibration finished

4.4 Library

The library function is to create/edit a spectra database, identify already know samples. To access the library, click the library menu:

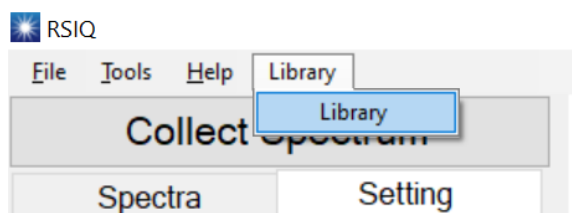


Figure 4.14 Library

4.4.1 Create new library

You can create your own library based on your test results by clicking 'New Library' button on the left size panel:

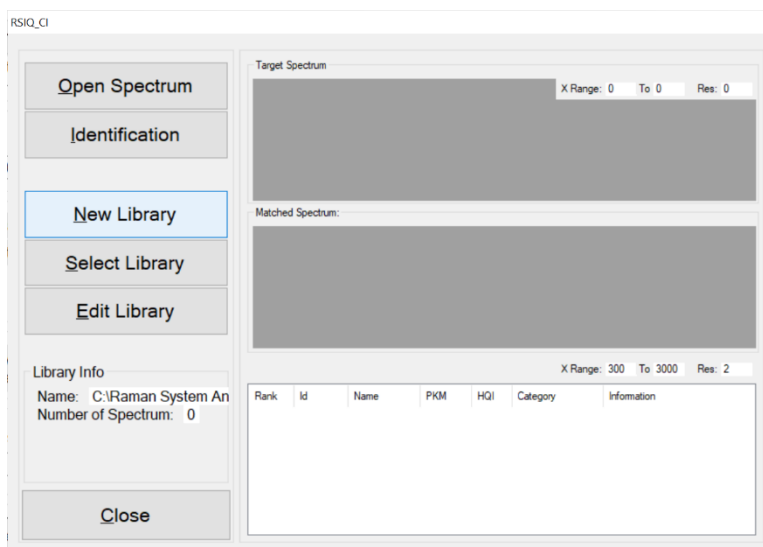


Figure 4.15 Create a new library

The create new library interface is like this, it contains the basic information of the new library, including the data range, resolution and library name:

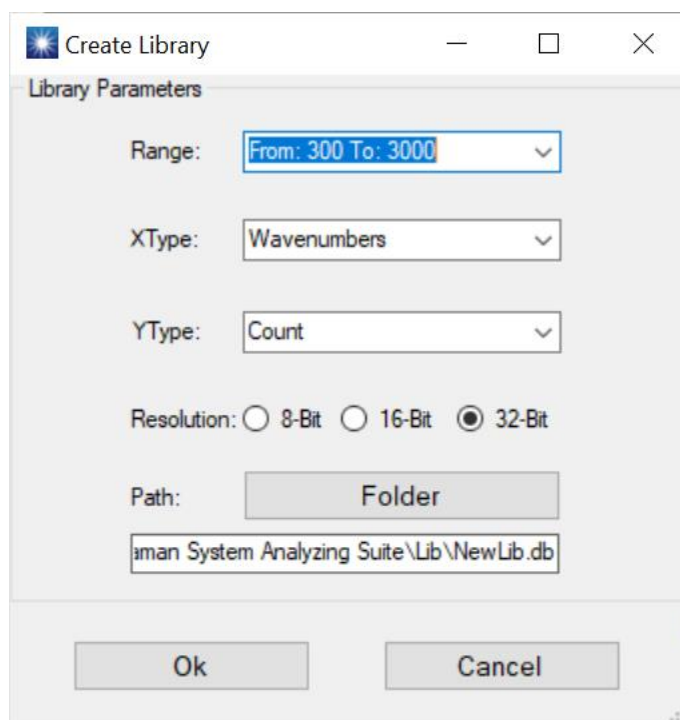


Figure 4.16 New library information

4.4.2 Select library

If you purchased the commercial library, you could visit it by using 'Select Library':

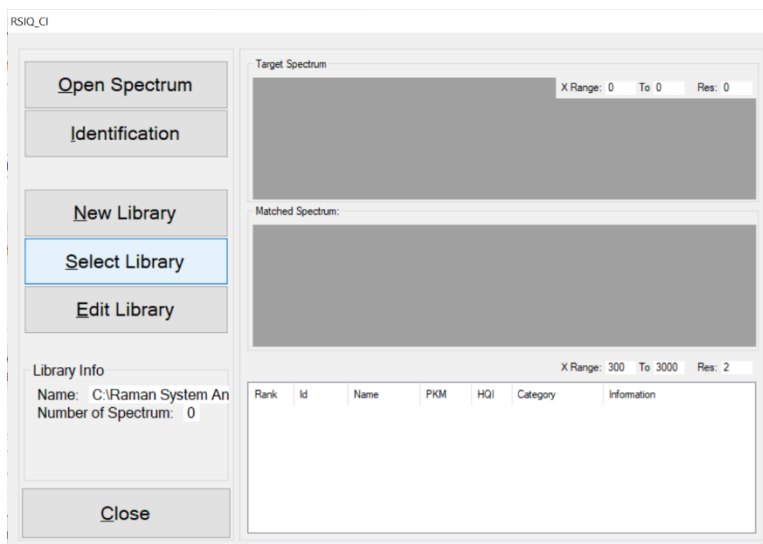


Figure 4.17 Select a new library

Choose the library and click 'Open', by default it's saved in C:\Raman Systems Analyzing Suite\Lib

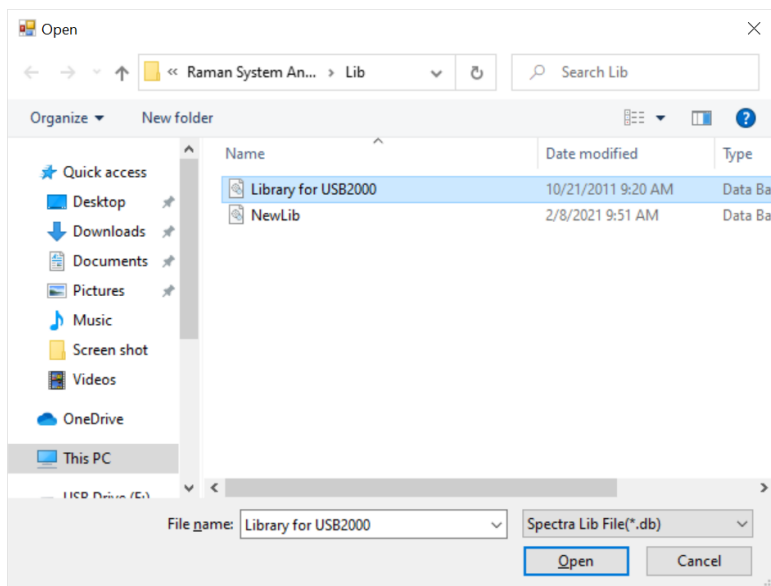


Figure 4.18 Choose the library

After selecting it, the library info on the left panel is changed to show the new library. In this case it shows the library contains 3519 spectra:

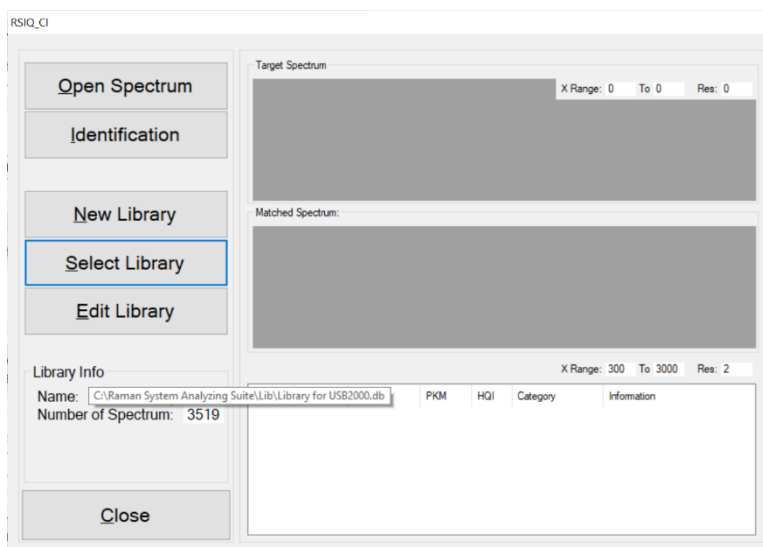


Figure 4.19 Library Info

4.4.3 Edit library

You can visit the spectrum in the library by clicking 'Edit Library', changing the name, adding information, adding more spectrum, checking the spectrum.

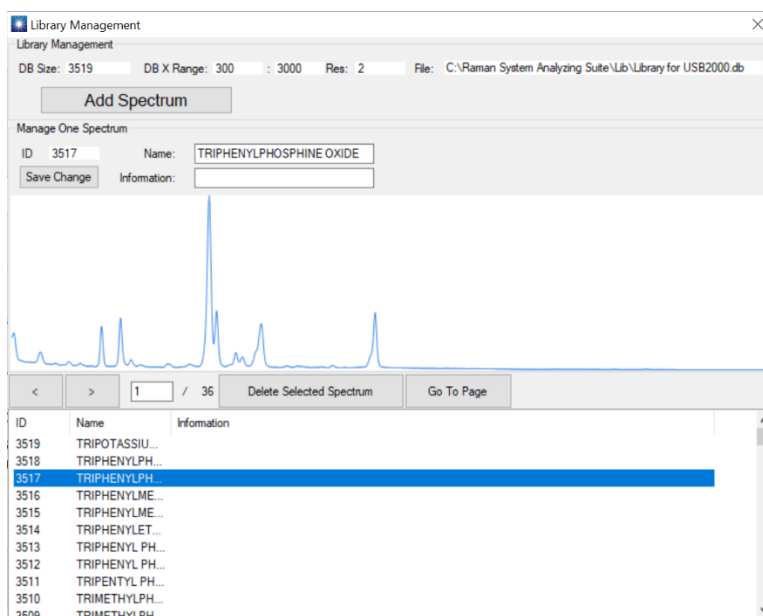


Figure 4.20 Edit Library

4.4.4 Identify a spectrum

First, load the spectrum to be identified by clicking 'Open Spectrum':

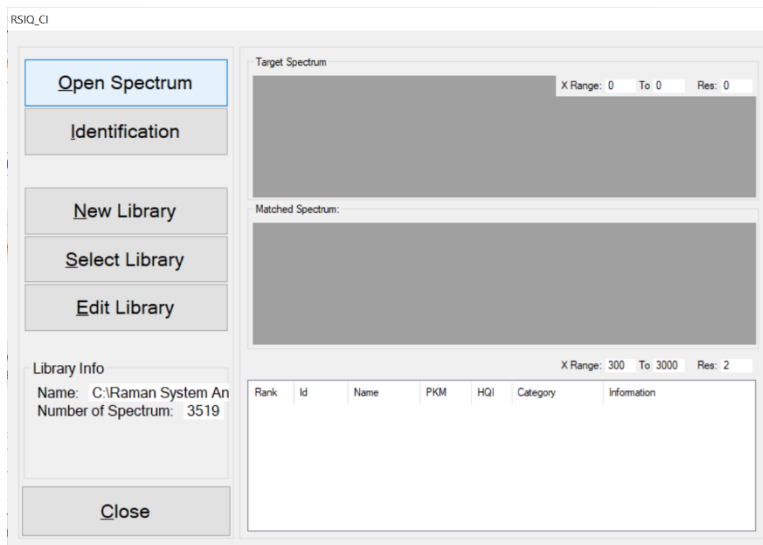


Figure 4.21 Load spectrum

After the spectrum is loaded, it will show up in the target spectrum area, the sample here is a 50/50 mixture of Toluene and Acetonitrile liquid:

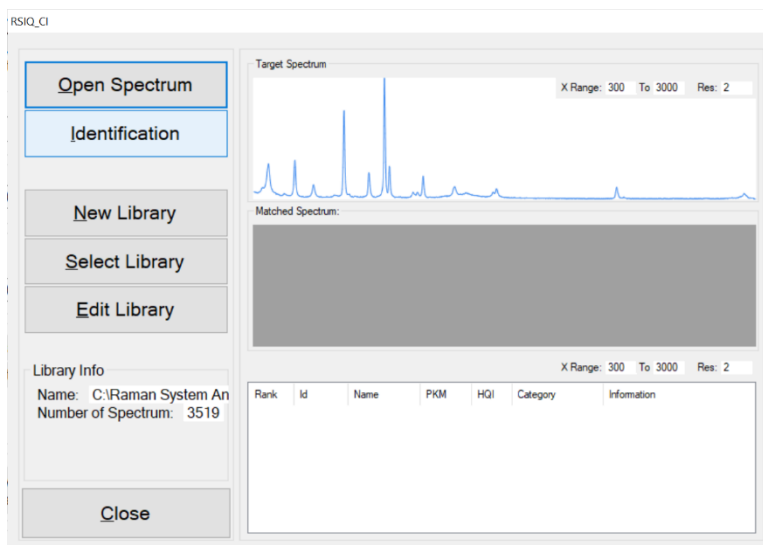


Figure 4.22 Identify spectrum

Then click 'Identification', the software will look for the mostly matched spectrum and show it in the matched spectrum area. It find the toluene peaks:

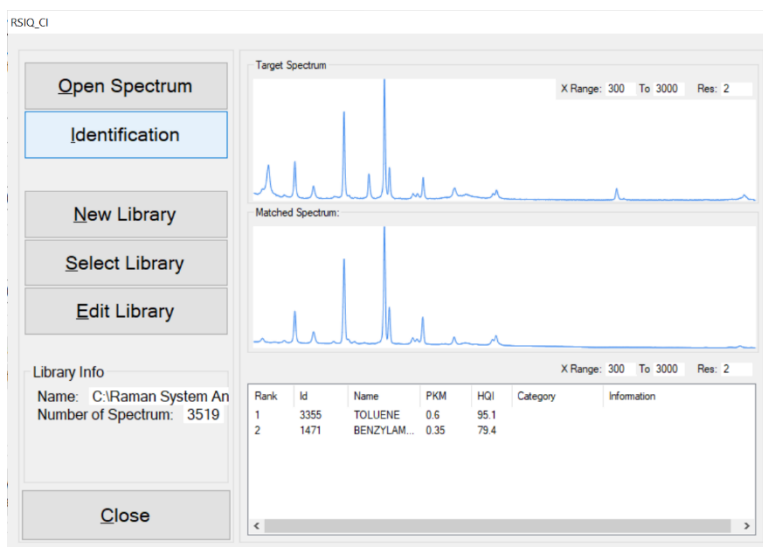


Figure 4.23 Matching result

If there are more than one similar spectrum, it will show multiple results, but only display the one with highest similarity. You can still check other similar spectrum by clicking the name or id.

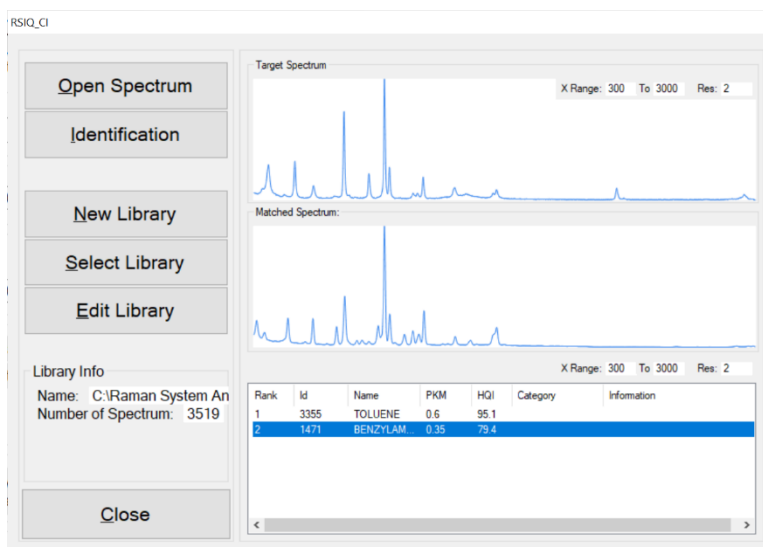


Figure 4.24 Show another spectrum

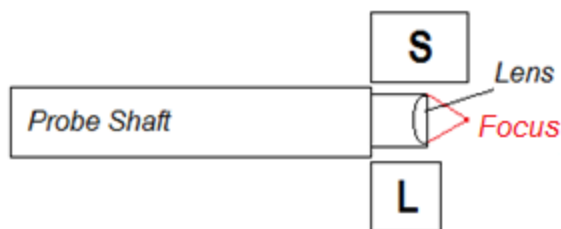
5. Sample Measurements

A sample compartment that accepts the probe shaft ensures eye safety when the laser is on and blocks potential background noise from room light. When the sample is either a liquid or a powder in a small bottle or vial, the sample holder can be used. The combination of electronic laser control and the sample compartment makes it so the user is not exposed to the laser light. The laser is off until a scan is activated through the software. The cover of the sample compartment blocks the laser light. Placing a sample in the compartment and setting the cover in place, prevents user exposure to the laser beam.

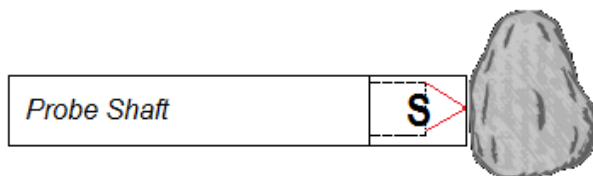


Figure 5.1 Sample compartment and cabled probe

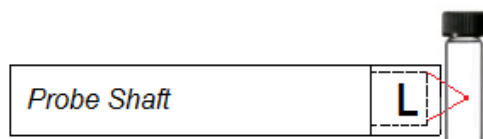
Each instrument is supplied with measurement caps for the end of the probe shaft to aid with placing the focus of the laser beam onto the sample. The default focal point is 8 mm out from the end of the sample tube. The spot size is roughly 100 μm in diameter at that point. Focusing involves positioning the point onto the sample to be measured.



The **cap labeled S** is long enough that the spot is focused on the surface of soft solids when the cap is pressed against the surface. Some solids may require a probe holder with vertical translation to correctly focus the spot on the surface.



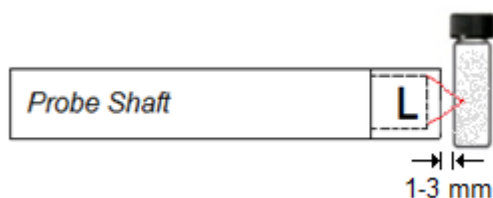
For liquid inside containers with walls less than 2 mm thick, the **cap labeled L** is short enough that the focal point will be inside the container.



Either measurement cap is placed in contact with the sample or container to set the focus.

IMPORTANT NOTE:

For turbid liquids, powders or solids inside a container, the probe with **L cap** may have to be withdrawn slightly (1-3 mm) from contact with the container to place the probe focal point at an optimum position within the highly scattering sample medium. This will improve the scan results.



6. Trouble Shooting

SYMPTOM	ADVICE
WARNING BOX No systems detected!	1) Check that power is on 2) Unplug the USB cable and plug-in again 3) Use another USB port on the computer 4) Try another USB cable. 5) Does spectrometer appear in Device Manager? See Fig 1.19 <i>NOTE: The RSIQ software will operate without a spectrometer. Saved data files can be opened and displayed.</i>
No laser output	1) Check that power is on 2) Check the Key is turned to 'ON' 3) Check the correct male Interlock is totally inserted into the female panel connector 4) Check Device Manager. On 'Ports (COM & LPT)', the communication port number must be less than 16. If it's larger than 16, right click and select 'Properties\Port settings\Advance' to change it to a value less than 16 <i>NOTE: The laser is emitted only during a sample scan. The red panel LED illuminates.</i>

6.1 FAQ

How do I use the blank interlock male connector?

The blank interlock is used for a remote control safety switch if necessary. Pins 1 and 2 must be crossed for the laser to operate.

Why is there a question mark on the 'Ocean Optics' device in Device Manager?

The driver may work unusually, unplug the USB cable or change the USB port or cable and try again. If the problem remains, uninstall the RSIQ software and reinstall.

Why is there a question mark on the 'Ports (COM&LPT)' in Device Manager?

The driver of the PCB controller may work unusually, try to uninstall or update the driver. The driver is found on the CD or USB flash drive shipped with the Raman spectrometer.