ATP8900PLUS series Fourier transform infrared spectrometer user 's manual

OPTOSKY
Spectroscopy Solutions

Optosky (Xiamen) Photonics Inc.

catalogue

1. Safety precautions

Electricity safety

There is no rechargeable battery inside the ATP8900PLUS infrared spectrometer, which requires users to connect 220V power supply or 18-24v on-board battery for power supply . ATP8900PLUS has no switch button. Users can switch on the equipment normally by directly inserting the attached power adapter into the rear power port of the instrument. When switching off the instrument, turn off the main power supply directly or disconnect the plug of the power adapter.

Do not put the instrument in water or soak it, so as not to damage the instrument or even cause personal injury.

Laser safety

The laser used in the ATP8900PLUS infrared spectrometer is a 794nm semiconductor

solid-state

laser, which is invisible to the naked eye but harmful to human eyes. Do not open the shell and look directly at the light source outlet to avoid visual damage.

Light source safety

The light source of the spectrometer is a silicon carbide rod with strong light intensity. Do not open the shell and look directly at the light source outlet to avoid visual damage.

The light source is built in the instrument. It is normal that there is a small amount of heat on the instrument panel after a long time of startup.

ATR use safety

When using ATR to test powder, you need to turn the ATR pressure clamp directly above the crystal, and then rotate it to compress the sample for testing. The pressure of the clamp is high, so be careful to clamp your fingers.

Don't try to put your hand on the crystal to test the pressure!

Safe use of diamond crystal

Although the diamond crystal is corrosion-resistant and very hard, it is strictly forbidden to use metal devices, hammers and other tools to directly knock or collide with the crystal. The diamond crystal cannot directly test metal samples.

Safe use of drying tube

The drying tube is installed on the rear panel of the instrument, with built-in desiccant, which is used to absorb water vapor and CO2 in the optical path. After the desiccant is saturated, the instrument software will display the humidity, and the user can regenerate. Users can replace the drying tube by screwing it by hand and then tighten it. Do not screw it with a wrench to avoid cracking.

After drying the desiccant, be sure to wear thick gloves to prevent high temperature scalding

hands and skin.

Safe use of network cable

The data communication between the infrared spectrometer and the computer is through the network cable. Don't fold the network cable to prevent the internal fracture of the network cable, resulting in inability to connect.

Safe use of instrument

It is strictly forbidden to drop the instrument directly from a height, which will cause the shell deformation, seriously affect the built-in optical devices, and even cause the instrument to be unusable.

2. Installation requirements

To ensure that the spectrometer is in the best working condition, please read and meet the requirements of the spectrometer for the working environment and related equipment. If you have any questions, please contact our installation and maintenance engineer.

Ensuring the dry environment inside the instrument is the premise to ensure the normal operation of the instrument. Users should pay more attention to the change of air humidity.

It can't be used in high humidity environment for a long time. After the measurement, it is recommended to check the humidity change inside the instrument and regenerate the molecular sieve desiccant.

If the instrument components are damaged by moisture due to ignoring this information, it is not within the normal warranty period.

The spectrometer itself has certain anti-interference ability of power supply, but try to avoid placing it in high-voltage and high magnetic environment. For high-power electrical appliances that may cause power fluctuations, such as vacuum pumps, motors, etc., it is best to use another circuit system. At the same time, try to stay away from vibration sources, such as air conditioners, elevators, etc.

Environmental requirements

Installation location: indoor (below 2000 meters above sea level)

Ambient temperature: 5°C-35°C

Relative humidity: ≤ 60%

The internal humidity of the spectrometer is ≤ 20% (if it is not used for a long time, it can be turned on regularly, for example, it can be turned on for 2 hours every day, and the state of the instrument can be detected, and the humidity of the instrument can be checked inside the software); If the humidity is more than 20%, the instrument will automatically remind the user to regenerate the desiccant.

The temperature change shall not exceed ± 1 ° C

Power supply 220V ± 10%, 50-60Hz, well grounded

Operating system requirements

The computer operating system is windows 10, English operating system;

Desktop or laptop can be connected, with standard interface of network cable

3. Basic structure and components of spectrometer

ATP8900PLUS infrared spectrometer is mainly composed of three parts, including power, interferometer part and optical cavity. These components are all integrated in the metal shell, and the humidity is monitored by the molecular sieve desiccant.

The power supply chamber is responsible for the power supply of the instrument.

The interferometer part includes interferometer and beam splitter, which is the core part of the instrument. The moving mirror of the interferometer moves continuously to generate interference signals, which are transmitted to the detector to form an interferogram. Finally, the infrared spectrum is obtained after Fourier transformation.

The optical cavity contains a focusing mirrors and related sampling accessories, which is convenient for sample collection in different types.

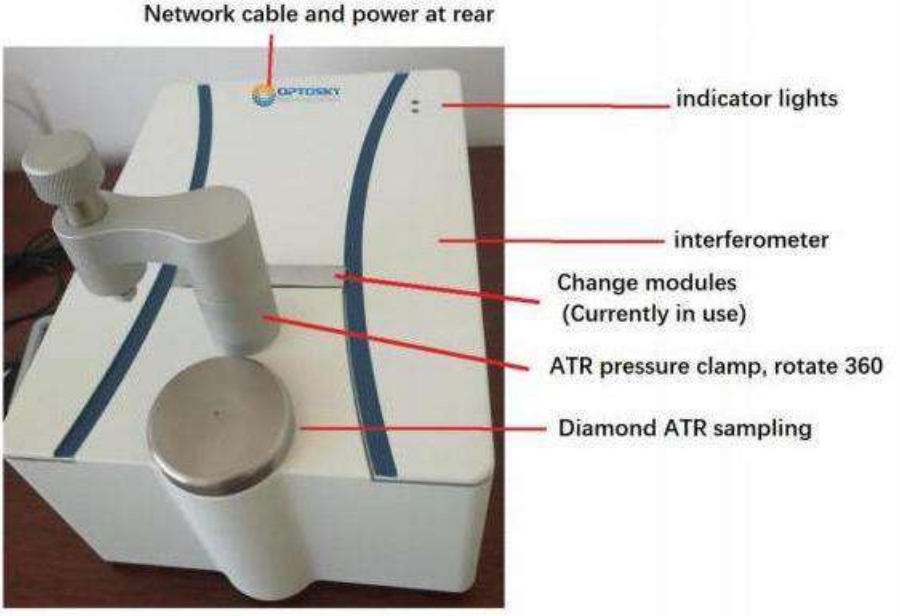
Meaning of status indicator:

1. Initialization:

Please ensure that the instrument is connected to the computer through the network cable, and the IP address of the computer is set correctly. When powered on, the two indicators display yellow, red and blue in turn. After initialization, the indicator will go out and enter the working state.

2. During measurement:

The two indicator lights display green and flash alternately.


Network cable and power at rear
indicator lights
interferometer
Change modules
(Currently in use)
ATR pressure clamp, rotate 360
Diamond ATR sampling

4. Basic operation of spectrometer

Power supply

Connect 220V power supply (well grounded) and it can work normally. If possible, UPS power supply can be connected to avoid the interference caused by voltage fluctuation to the instrument, and the damage caused by sudden power failure to the instrument can also be prevented.

Connect the network cable

The spectrometer communicates with the computer host through the general network cable. Users can configure wireless routes to access and control the instrument through the wireless network, which is more convenient to use.

Connect different sampling accessories

According to different applications of users, the instrument configuration is different. Different sampling accessories can be connected in front of the infrared spectrometer to adapt to different applications. For example, ATR attenuated total reflectance accessories (users can configure different types of single reflection crystals, such as Diamond, ZnSe, Ge, etc., or configure multiple reflection crystals, such as ZnSe crystals), liquid flow cell accessories, transmission accessories, reflection accessories, diffuse reflection accessories, etc.

5. Routine maintenance and fault analysis

5.1 replace desiccant

Before shipment, the instrument has been sealed and dried, but after long-term use, a small amount of water vapor will enter the interior of instrument.

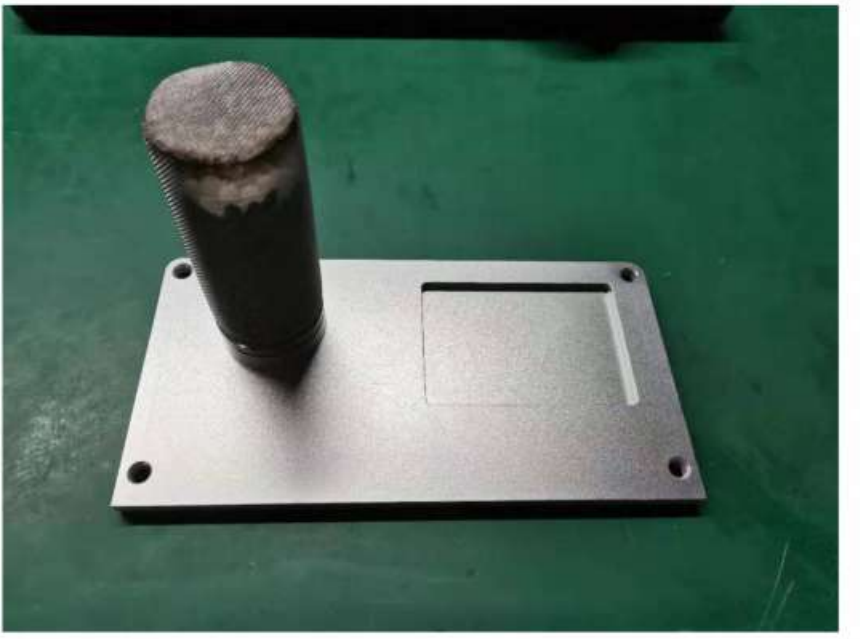
When the internal humidity of the instrument exceeds 20%, it will cause damage to components, such as beam splitter and detector. At this time, it is necessary to take out the built-in drying tube and regenerate the built-in desiccant.

The desiccant after moisture absorption is placed in the oven at 120 ℃ for 24 hours for activation, and can be used again after cooling. Pay attention to high temperature to prevent scalding!

The replacement steps of desiccant are as follows:

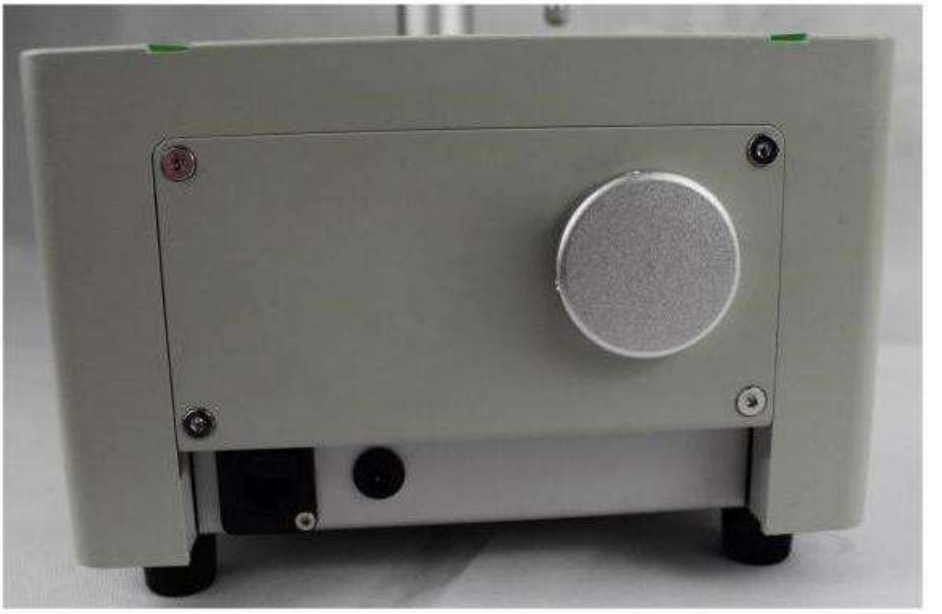
1. Counter-clockwise unscrew the drying tube. As follows:

2. Remove the drying tube, the desiccant pipe is inside the instrument.



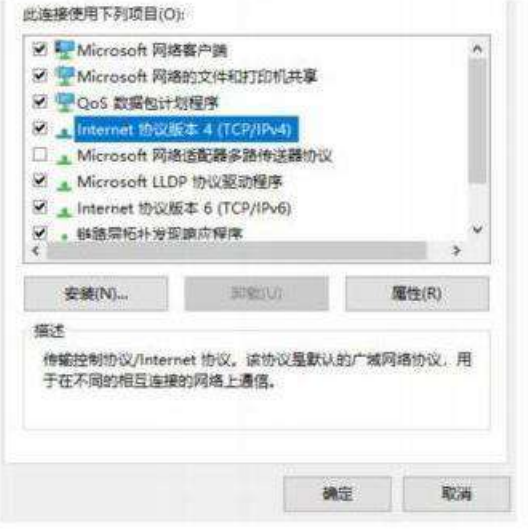
3. Take out the desiccant for regeneration(120 °C and 24 hours)

4. After replacing the new desiccant, install the drying tube back to the rear of the instrument clockwise, and can be use normally.



5.2 Connection of the instrument (the infrared host has been set before shipment, and the IP address of the computer needs to be set on customer's site)

5.2.1 Find "local connection" in the "control panel" of the computer, click "properties", and select "Internet Protocol version 4 (TCP/IPv4)", as shown in the following figure.



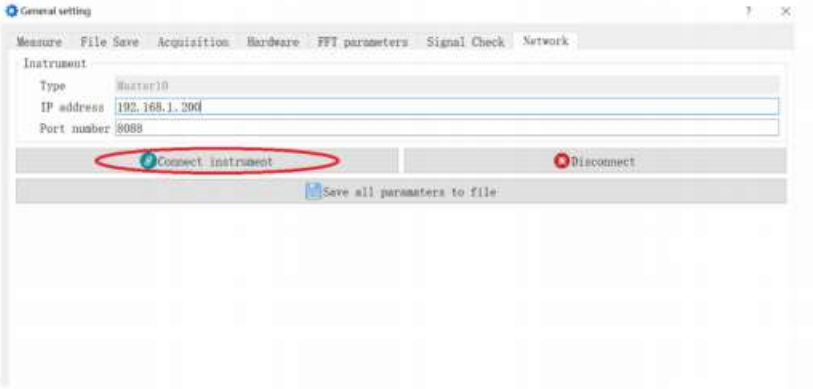
Click "properties" and enter the IP address of the computer in "use the following IP address", as shown below. Finally, click "confirm".

5.2.2 in the software interface of the host, enter the IP address of the infrared host: (the infrared host has been set before shipment)

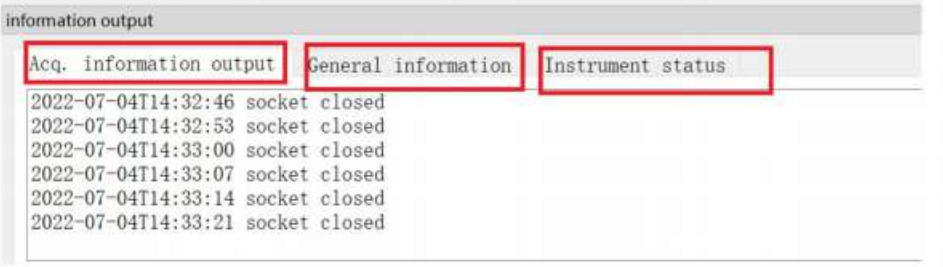
IP address: 192.168.1.200
Port: 8088

Finally, click "connect instrument", as shown below, and the instrument can be successfully connected. After the connection is successful, the indicator light in the lower right corner of the software interface will display green; When there is no connection, red is displayed.

After connection, a green indicator light will be displayed in the lower right corner of the main software, as shown below.



In the lower left corner of the main software, the "information output window" will be displayed to view the real-time change of humidity in the "instrument status". If the host exceeds 20%, the software will alarm and automatically remind the user to replace the regenerated molecular sieve desiccant.



5.3 the instrument cannot be connected

In case of abnormal instrument connection, a red indicator light will be displayed in the lower right corner of the software. 

If the connection is abnormal, you can check in sequence:

5.3.1 check whether the connecting network cable is normal; Sometimes, the cable will be accidentally touched, resulting in looseness. Solution: reconnect.

5.3.2 check whether the instrument power supply is normal; Without power supply, the infrared host cannot be started; Solution: plug in the external power supply.

5.3.3 check whether the network settings are normal. The IP address of the host has been set at the factory. If the IP address of the computer is changed, the host cannot automatically connect with the computer. Solution: enter the correct IP address for the computer.

5.4 the connection is successful, but there is no signal

5.4.1 check whether there is temperature at the light source; Touch the panel of the instrument with your hand to see if there is temperature. If there is a feeling of temperature, it indicates that the light source is working normally.

5.4.2 check whether the accessories are connected normally; ATR crystal is built in the crystal disk, mainly to check whether the crystal is damaged and the optical path is disturbed.

5.4.3 check whether the sampling accessories are normal, mainly to see whether the accessories are locked, whether the ATR crystal surface is polluted or whether the sample remains, and whether the sample transmission holder is blocked.

Other issues

Please contact our after-sales service engineer.

Tel: 0086(0592)6102588
Email：sales@optosky.com

6. Technical parameters

Resolution: better than 2cm^{-1} (upgrade: better than 1cm^{-1})

Spectral range: 5000cm^{-1} - 500cm^{-1} (related to the selected beam splitter type)

Light source: high performance MIR light source

Interferometer: high stability cube corner interferometer

Beam splitter: moisture-proof ZnSe beamsplitter (can select KBr beamsplitter)

Detector: high sensitivity DTGS detector (KBr window, pay attention to moisture prevention)

TE-MCT detector can be selected to improve detection sensitivity

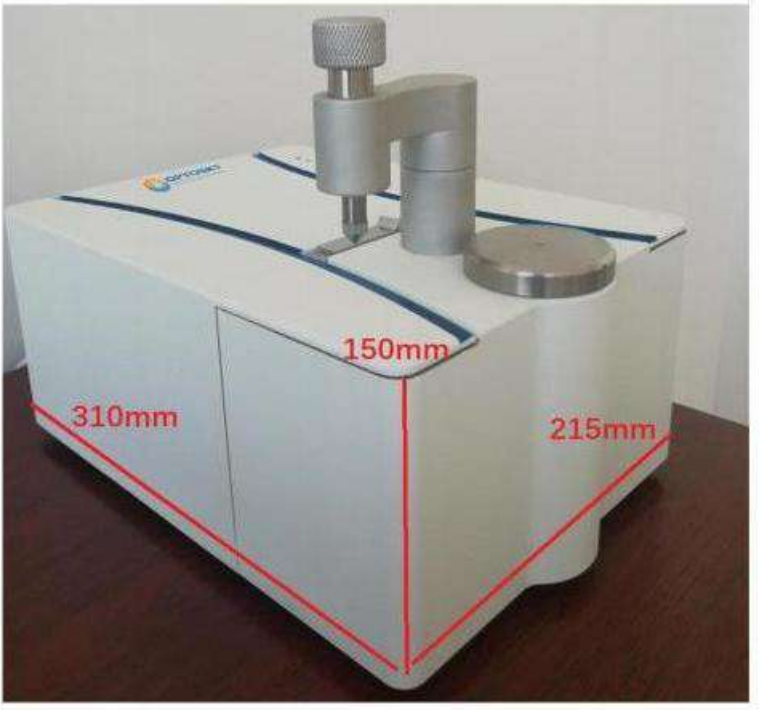
Laser: solid state laser, with a lifetime of 10 years

Scanning speed: 8cm^{-1} resolution, 5 spectra per second

Power supply:100-240 VAC, 50-60 Hz

Computer communication: Ethernet connection

7. Dimension parameters



Length * width * height: 310*215*150 mm

Weight: The host is about 7kg

8. ATR attenuated total reflectance module

Replace the ATR module: slide the locking switch on the instrument panel to the left to replace the ATR module; Slide it to the right to lock the ATR module, which can be used normally. The following figure shows the normal locking state.

Introduction to Diamond ATR accessories

The ATR accessory adopts pure Diamond crystal, high strength, super corrosion resistance, high throughput and excellent sensitivity.

Users can choose other types of crystals, such as zinc selenide crystal, germanium crystal, etc. Different modules can be replaced with each other.

Application market

This accessory has a wide application market and can meet the testing needs of different industries such as organics, polymers, inorganics, minerals, stones, asphalt and various composite materials.

Sampling principle

ATR is the abbreviation of attenuated total reflectance. After the infrared light passes through the interferometer, it forms interference light. When the interference light irradiates the crystal surface, the infrared light will produce attenuation reflection wave on the crystal surface. Therefore, after placing the sample on the crystal surface, the sample and the infrared reflection wave will interact to obtain the infrared information of the sample.

Sampling method

1. For polymer particles, hard materials, inorganic minerals and other samples, it is necessary to rotate the clamp above to make the samples and crystal in close contact;

2. For viscous samples, such as asphalt, colloid, paste and other samples, only need to be smeared on the diamond crystal;
3. For liquid samples, only one drop of the sample is needed on the crystal to measure.

Sampling process

1. Clean the crystal surface and click "acq. background spectrum". The background spectrum is collected with air as the background, so the crystal surface needs to be wiped clean;
2. Take a small amount of sample, smear it on the crystal, and click "acq. sample spectrum" to obtain the spectrum of the sample;
3. After collection, take a suitable solvent (water or organic solvent) and clean the sample on the crystal surface to complete a test;

Sampling diagram:

The surface of the crystal in the figure is smeared with black asphalt samples for measurement. At this time, the clamp can be rotated to the rear to increase the operation space.

9. Temperature controlled ATR attenuation total reflectance module

Replace the ATR module: slide the locking switch on the instrument panel to the left to replace the ATR module; Slide to the right to lock the ATR module, which can be used normally.

Attachment introduction

The ATR accessory adopts pure diamond crystal, which is corrosion-resistant and can be heated and controlled at a temperature of more than 100°C.

Application market

The accessory is suitable for users to measure the infrared spectrum of samples at different temperatures; Study the phase transition of substances.

Sampling principle

ATR is the abbreviation of attenuated total reflection. After the infrared light passes through the interferometer, it forms interference light. When the interference light irradiates the crystal surface, the infrared light will produce attenuation reflection wave on the crystal surface. Therefore, after placing the sample on the surface of the heated crystal, the high-temperature sample and the infrared reflection wave will interact, so as to obtain the infrared information of the sample at different temperatures.

Sampling method

1. For polymer particles, hard materials, inorganic minerals and other samples, it is necessary to rotate the clamp above to make the samples and crystals in close contact;

2. For viscous samples, such as asphalt, colloid, paste and other samples, only need to be smeared on the diamond crystal, without pressing the clamp;
3. For liquid samples, only one drop of the sample is needed on the crystal to measure. If necessary, a liquid flow cell can be configured for measurement.

Sampling process

Clean the crystal surface and click "acq. background spectrum". Collect the background spectra at different temperatures and take the air as the background. Then place the sample, and click "collect sample spectrum" after the temperature is stable.

10. Multiple reflection ATR module

Attachment introduction

The multiple reflection ATR accessory, using ZnSe crystal, can realize 5 times reflection measurement.

Application market

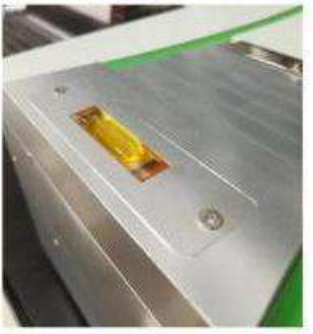
This accessory is suitable for users to study low concentration liquid samples, and can obtain a stronger infrared spectrum than a single reflection ATR.

Sampling principle

ATR is the abbreviation of attenuated total reflection. After the infrared light passes through the interferometer, it forms interference light. When the interference light irradiates the crystal surface, the infrared light will produce multiple attenuated reflection waves on the crystal surface. Therefore, when the sample contacts the reflection waves at different points, it will interact with the infrared reflection waves, so as to obtain the superimposed infrared signal of multiple reflections of the sample.

Sampling method

1. For viscous samples, such as asphalt, colloid, paste and other samples, you only need to apply them on the surface of the crystal without pressing the clamp;
2. For liquid samples, the measurement can be carried out only by dripping the sample all over the crystal surface.



11. Infrared transmission module

Replace the transmission module: slide the locking switch on the instrument panel to the left to replace the transmission module; Slide to the right to lock the transmission module, which can be used normally.

Attachment introduction

The transmission attachment is the most traditional infrared sampling method. Infrared light passes through the sample to be tested in a direct transmission or multiple reflection mode.

High throughput and excellent sensitivity.

Application market

The application market of this accessory is very wide, and it can meet the testing needs of different industries such as conventional solid pellets pressing, film, liquid film coating, liquid cell quantitative measurement, short path gas cell measurement, long path gas cell measurement, and so on. Just configure the corresponding sampling accessories.

Sampling principle

After the infrared light passes through the interferometer, it forms interference light. When the interference light irradiates the sample, the infrared light will interact with the sample, and then focus on the detector to obtain the infrared information of the sample.

Sampling method

1. For solid particles, powders, fibers and other samples that can be pressed into pellets, it is necessary to cooperate with the tablet press and KBr powder to press the pellets, and then place the pellets on the holder of the transmission chamber for transmission measurement;
2. For viscous samples, such as colloids, pastes and other samples, just apply a small amount on the infrared window;
3. For liquid samples, just drop a drop of the sample on the window to form a film or put the liquid into the liquid cell for qualitative and quantitative analysis.

Sampling process

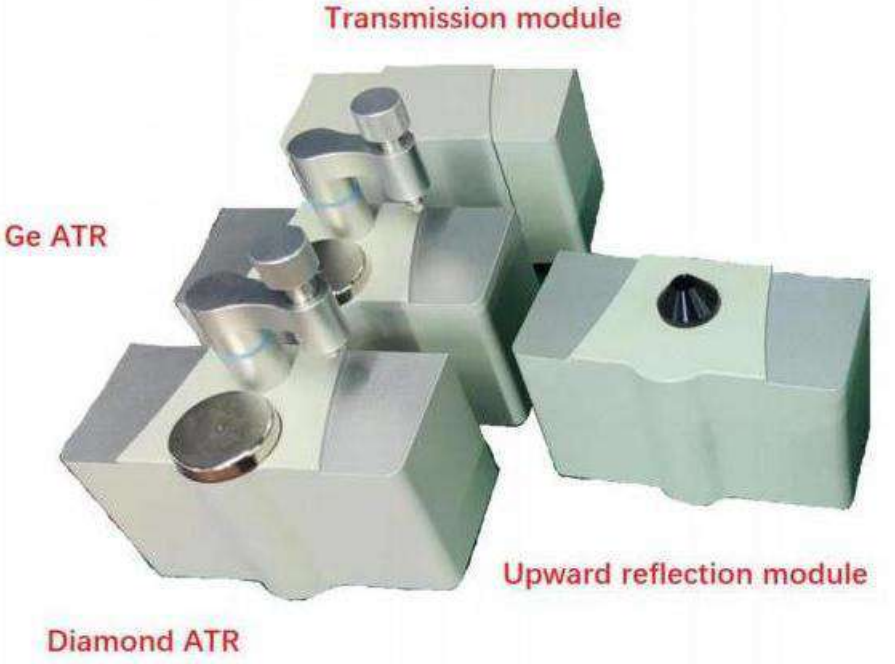
First, click "acq. background spectrum". The background spectrum is generally based on air. After collection, place the prepared solid pellet or liquid window on the support of the transmission chamber, and then click "acq. sample spectrum".

Gas cell: straight through gas cell, which can continuously collect the infrared spectrum of gas for online analysis.

Gas cell: multiple reflection gas cell, users can choose different optical paths, which can

improve the detection limit, even to ppm level.

12. Upward (forward) reflection module



Attachment introduction

The upward (forward) reflection module adopts the non-contact measurement mode, which can realize the non-destructive reflection measurement.

Application market

This accessory is suitable for users to measure jewelry, emerald, bracelet, minerals and other samples, with high reflection signal and non-destructive measurement.

Sampling principle

After the infrared light passes through the interferometer, it forms interference light. When the interference light irradiates the sample surface, the infrared light will reflect on the sample surface. Therefore, the infrared reflection signal interacts with the sample to obtain the reflected infrared signal of the sample.

Sampling method

1. For small samples, such as diamonds and trinkets, a disc with a small aperture can be used as a support, which can be placed flat on the support, so that the surface of the sample in contact with infrared light is as flat as possible;
2. For large samples, the forward reflection module can be used for measurement, and the forward reflection module can be placed in front of the large sample for measurement.

13. Software installation

1. Window 10 operating system.
2. Open the software and run FTIRDasAnalyzer.exe software program for testing.

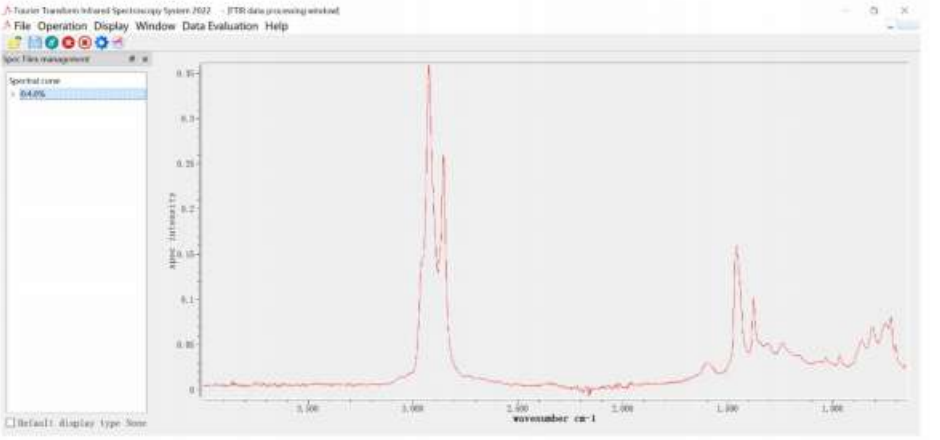
The next chapter will introduce in detail. FTIRDasAnalyzer.exe

3. Tablet network settings:

4. After connection, the light in the lower right corner of the software turns green. Green progress bar and test progress percentage will be displayed during measurement.

14. Introduction to main software interface

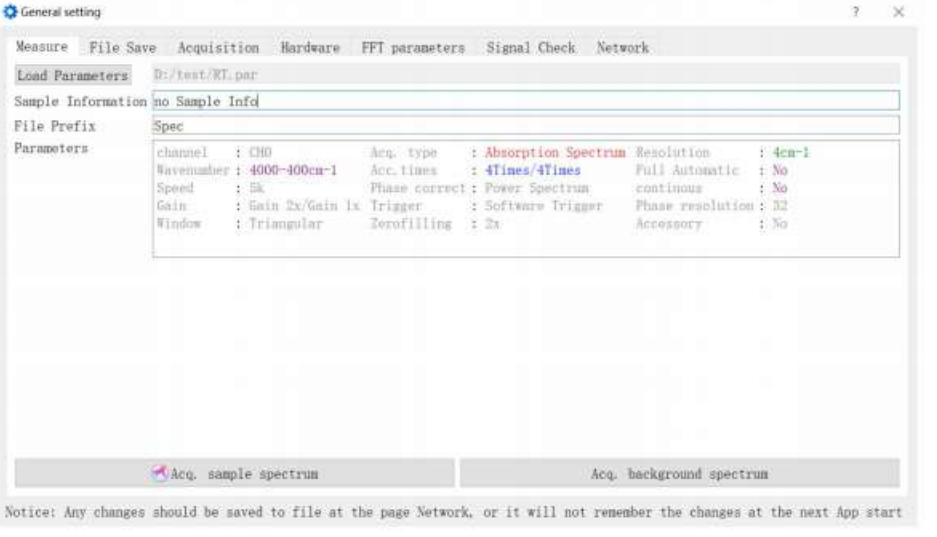
Click the "General setting" button  to enter the parameter setting and sample measurement. This icon is often used.



➢ **General setting and Measure process**

The interface is divided into seven pages, which are "Measure", "File Save", "Acquisition", "Hardware", "FFT parameters", "Signal Check" and "Network", as shown in the following figure.

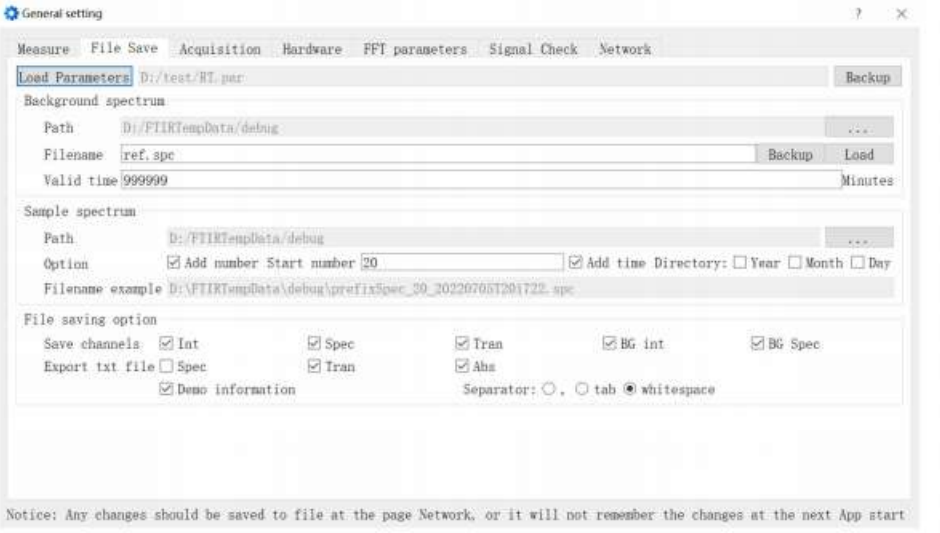
1. Measure page:



- "Load parameters" column: users can load the saved parameter file and use it directly.
- "Sample information": enter the relevant information and description of the sample.

- "File prefix": enter the name of the sample. You can enter English, such as sample 2020. In order to distinguish the sample name from the test time automatically generated by the system, it is recommended to add a connector "-" after the sample name.
- "Parameters":The basic information of the currently selected parameters is displayed in the acquisition parameter box and cannot be changed. If you need to change it, you can change it in the next settings pages.
- "Acq. sample spectrum" and "Acq. background spectrum": when all parameters are set, click " Acq. background spectrum" first, and the software will display the collection progress bar; Then place the sample on the ATR crystal for example and click " Acq. sample spectrum" button to scan the sample.

2. File Save:



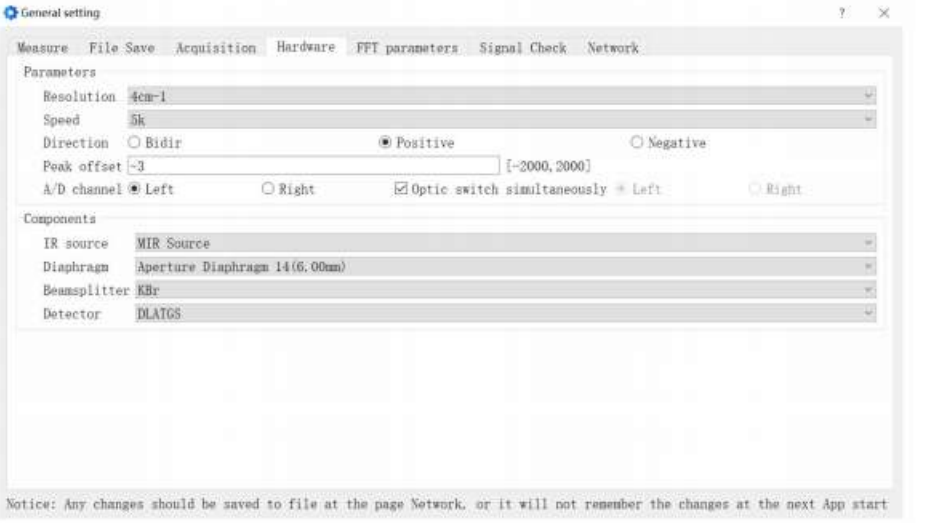
- "Load parameters" column: users can load the saved parameter file and use it directly;
- "Backup " button: when all parameters are set, click this button to back up these parameters, which can be loaded and used directly next time;
- "Background spectrum" column: you can set the storage path of the background spectrum, name the background spectrum and set the effective time of the background spectrum. The default is 999999 minutes. You can also back up the background, and click the "Backup" button to save as; "Path" can select different folders of background files for storage, or load the existing background, and click the "Load" button to load in.
- "Sample spectrum" column: "Path" you can select different folders of spectrum files for storage; Check the storage "Option" to add a number to the file. When "Add time" is checked, the measured time can be automatically formed after the file name, such as 20_202200705T201722.After the "Directory" grouping is checked, the folder can be automatically established according to the year, month and day. This function is very convenient for users who need to measure every day.

- "File saving option" column: the user can check the channel spectrum to be saved. "Export txt file": depends on the" Acq. type "in the" Acquisition" setting, and the checked content is consistent with the acquisition type.
- "Demo information": when checked, the exported txt file will contain the basic information of the instrument, such as humidity.
- "Separator": the default is comma, and tab or whitespace is optional.

3. Acquisition

- "Measurement" column: mainly displays parameter files and addresses under different channels. The default channel parameter is: CH0; "Accessories", select none; Software trigger; Gain 1X is selected for sample gain and background gain. None filter;
- "Acquisition settings" includes different type of spectrum "original interferogram", "interferogram", "interferogram + spectrum", "spectrum", "transmission spectrum", "absorption spectrum", "reflectance spectrum", "diffuse reflectance spectrum", "Radiation calibration spectrum" and other options. Usually, "absorption spectrum" is selected, and the peak is upward; At this time, if you want to export txt files, remember to check "abs" in "File saving option".
- "Debug mode": when checked, the spectrum of each frame is displayed in the acquisition process. When not checked, only the last synthesized spectrum is displayed;
- "For sample spec" and "For background spec" columns: display the acquisition time of the current sample and background. You can choose how many times to repeat the measurement, or set it to how many seconds to measure; Generally, the acquisition time of sample and background is set to 16 or 32 times.
- When "Continuous" is checked, the software will finish scanning after continuous acquisition according to the number of groups set for continuous acquisition.
- When "Full automatic" is checked, the software will collect data at intervals according to the set time interval until the user ends the scanning **manually.**

4、Hardware



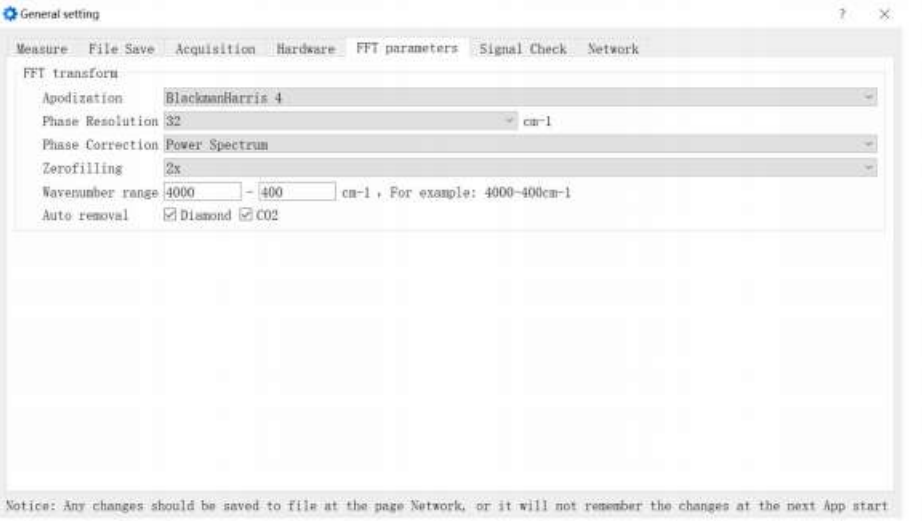
Parameters:

- "Resolution" column: the corresponding resolution can be selected from the drop-down menu. Currently, the selectable resolutions are 2cm-1, 4cm-1, 8cm-1, 16cm-1; Usually choose 4cm-1.
- "Speed": the sampling speed of the interferometer, which can be 10K, 7.5K and 5K; Usually choose 5K.
- "Direction": including bidirectional, positive and negative. At present, select the "positive" sampling method.
- "Peak offset": the parameters set before shipment, and the peak position should be corrected, and the user should not change it;
- A/D channel: default transmission cavity detector.

Components:

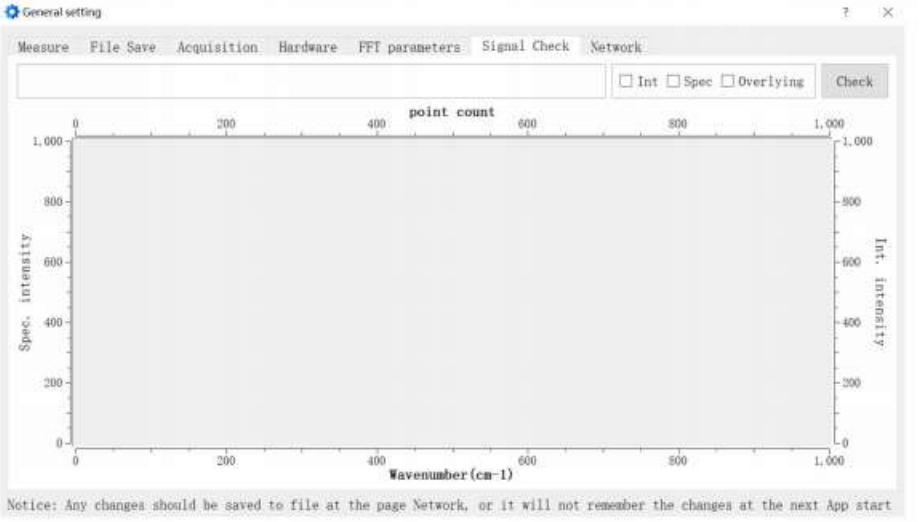
- For MIR infrared spectrometer: selection of devices: MIR source(carbon silicon rod), aperture, KBr beamsplitter, DLATGS detector

5. FFT parameters



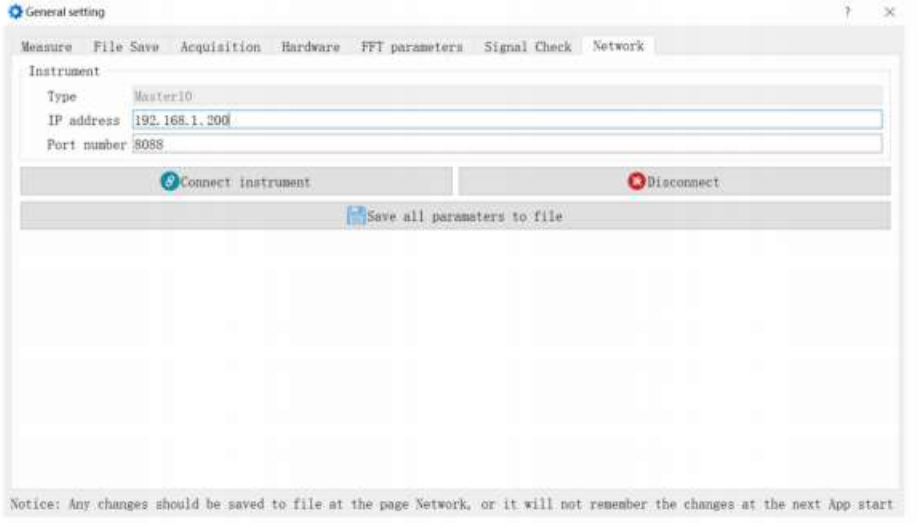
- "Apodization": this function is used to eliminate negative peaks. There are multiple functions to choose from, such as triangular functions, rectangular functions, etc., usually select BlackmanHarris4.
- "Phase Resolution": select 32cm-1.
- "Phase Correction": mainly used to calculate the phase of the spectrum, usually select "Power Spectrum".
- "Zerofilling": the larger the zero factor, the more data points. For example, selecting 1x means filling in 2 times zero.
- "Wavenumber range": enter the left and right boundaries of the spectrum, such as 4000-400cm-1.
- "Auto removal": by default, diamond and CO2 are checked, and the software automatically removes the interference peak of Diamond and CO2 when using ATR accessory with diamond crystal.

6. Signal Check



- Click the "Check" button, and after a while, the "interferogram" signal will appear automatically. and user can check the "Spec" to show the spectrum, which is to check whether the instrument is connected normally.
- "Overlying": when checked, the new spectrum will be continuously superimposed on the previous spectrum in green colors.

7. Network

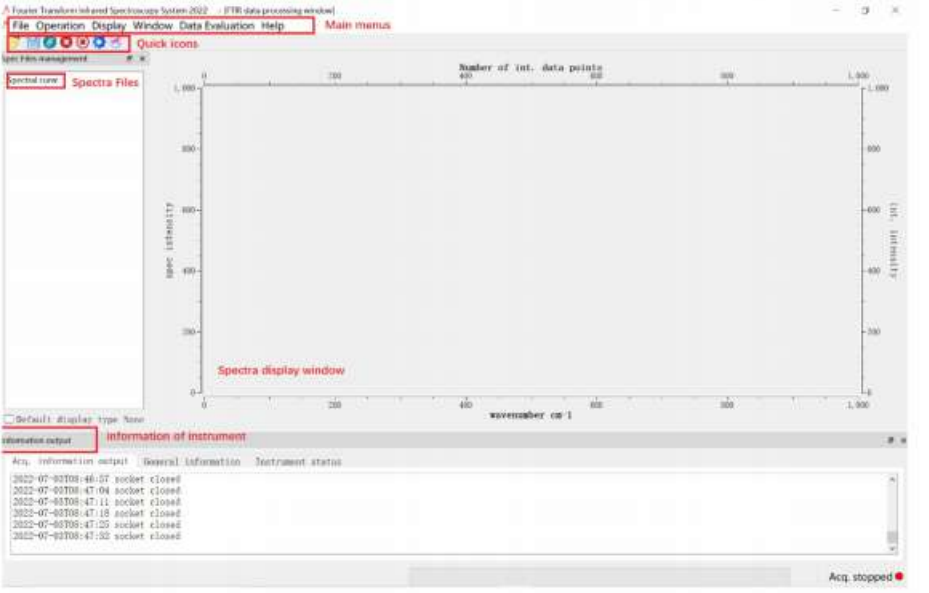


- "IP address": the IP address of infrared spectrometer is 192.168.1.200; Please refer to the previous IP settings for the IP address of the computer;
- "Port number" defaults to 8088;
- "Connect instrument" and "Disconnect": connect and disconnect spectrometer

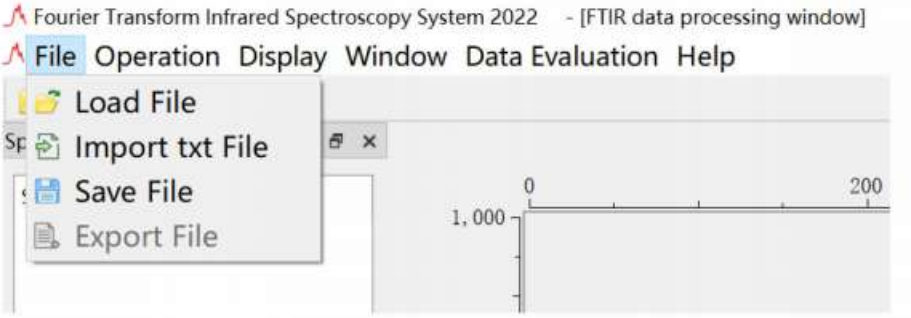
buttons respectively; After clicking, a green / red display light will be displayed in the lower right corner of the software, indicating that the computer and the infrared spectrometer have been successfully connected / disconnected.

- "Save all parameters to file": when all parameters are set and the connection is normal, the user can click this button to save all the previously set parameters as the default. In this way, even if the software is closed and then opened, the software will automatically call in the saved parameter settings.

Fourier transform infrared spectroscopy system 2022 main software interface

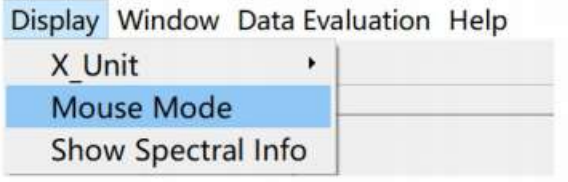


1. The software can import the txt file from "File" menus and can load .spc files by "Load Files" function.



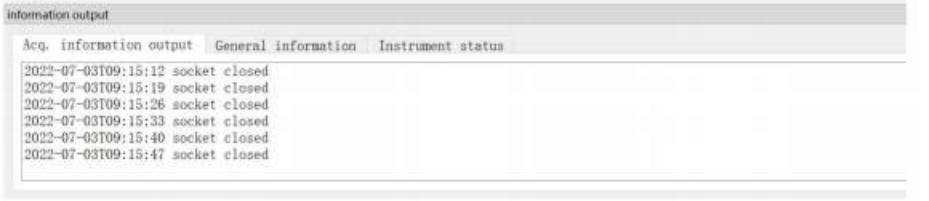
2. When importing the corresponding txt file, select the format as "absorption spectrum" or other format, and click OK.

3. Reading spectrum data position by selecting the function or double click the middle mouse button on the spectrum, the position of the date point will show. If you want to cancel the function, click the right button of your mouse once.



4. Information output window:

At the bottom of the main interface, there is an information output window, including "acquisition information output", "general information" and "instrument status", where users can see the changes of humidity and temperature of the instrument; Details of each acquisition, etc.



5. Other functions of mouse on software interface:

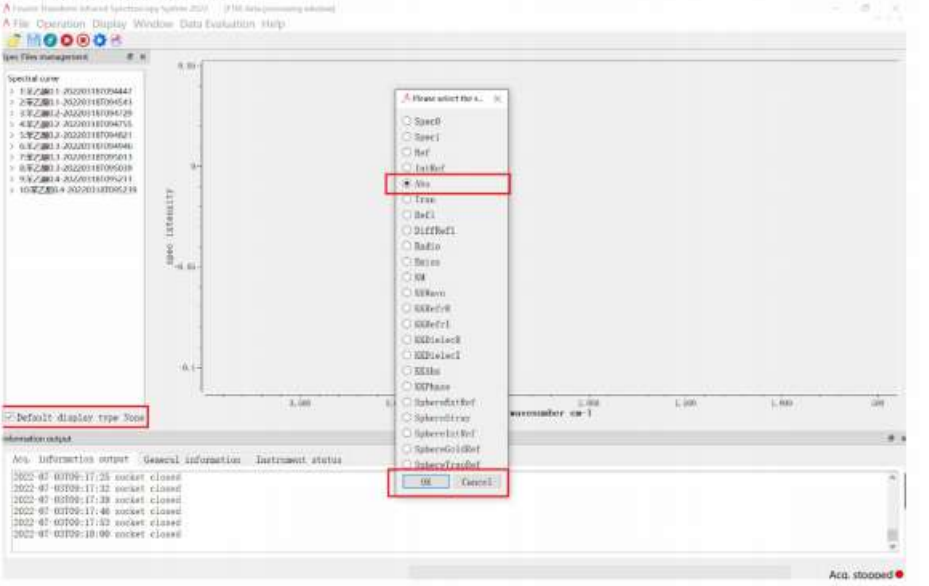
- Zoom in area: press and hold the left mouse button to drag. No matter which direction

you drag, it is zoom in;

- Double click with the right mouse button: the size will be restored to 1:1 and you can also exit the mouse reading function;
- Double click the middle mouse button: open the mouse reading function;
- Remove the spectra file from display: Click the right mouse button on the spectra file.
- Middle mouse button spectrum movement: press and hold the middle mouse button to drag;
- Mouse scrolling: the mouse wheel can move the spectrum up and down, and pressing and holding the Ctrl key to scroll the mouse can realize the left and right movement of the spectrum.

6. Batch display function:

The software can batch display the spectra of the same spectrum channel of different files without selecting one by one with the mouse. Method: open multiple files, as shown in the figure. After checking "default display type", the dialog box pops up. Users can select the spectrum channel they want to view, as shown in the following figure. Select the absorption spectral channel and click the "OK" button. All spectra will show the Absorption format.




File Operation Display Window Data Evaluation Help
Spectral curve
spec_intensity
wavenumber cm-1

15. Quick Identification of spectra

Steps to setup identification method:

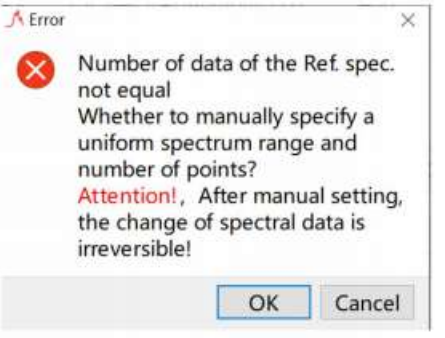
1. Open the function of "Setup Identification method" under "Quick Identification" in "Data Evaluation" menus.

2. If a method has been established, directly open the "Load method"; If it is a new method, click "Load reference spectrum", select one or more spectra that will be used to establish a quick identification method, and click "Open". The spectra format is txt file.

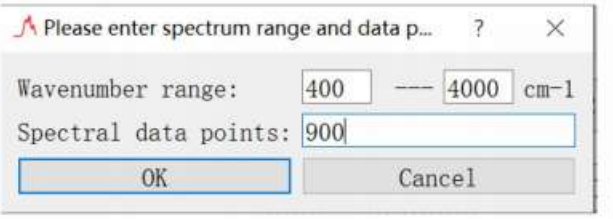
3. Sometimes, users collect multiple spectra of the same sample many times, or multiple spectra of different manufacturers and batches of the same type of sample, which are very similar. Then, if multiple similar spectra are selected as reference and the "Use Average spectrum as reference" check box is checked, the average spectrum of these samples will be used as the reference spectrum for quick comparison.

4. If multiple different standard spectra are selected and the " Use Average spectrum as reference " check box is not checked, the tested sample spectrum will be compared with each standard spectrogram one by one during quick comparison, and the correlation coefficient will be displayed respectively, with the highest correlation coefficient ranking first.

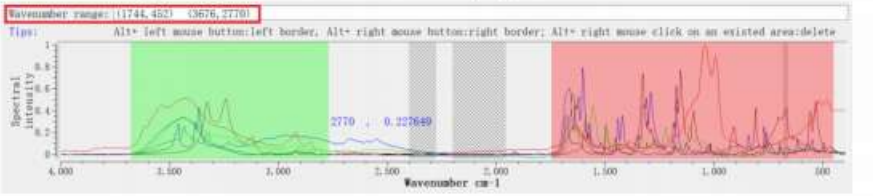
5. Load reference spectrum: The software can load spectra with different spectra range, different resolutions and different number of spectral data points. Click the "validity check" button, and the software will automatically judge and inform the user, as shown in the following figure. Users can input the spectra range and number of spectral data points, and "normalize" these spectra to the same condition for comparison. Click the "Reload reference spectrum" button to return to the spectra range and number of spectral data points of the original spectrum.



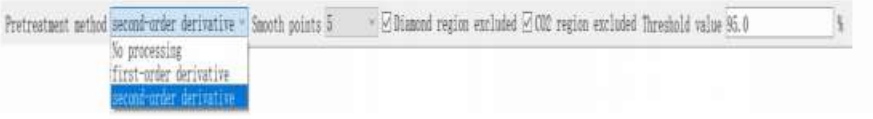
Press"OK", enter the spectra range and number of spectral data points you wanted.



6. Select range for comparison: After all standard spectra are showed in the window, user can select range for comparison. Press and hold Alt key and the left / right mouse button respectively to determine the left / right range. At this time, the spectral curve at the bottom will show the selected different color areas. Press and hold Alt and the right mouse button to delete the selected range (different color areas) and select the range again. At the same time, users can select multiple ranges, and there are selected ranges showed at the "Wavenumber range" area, as shown in the following figure.



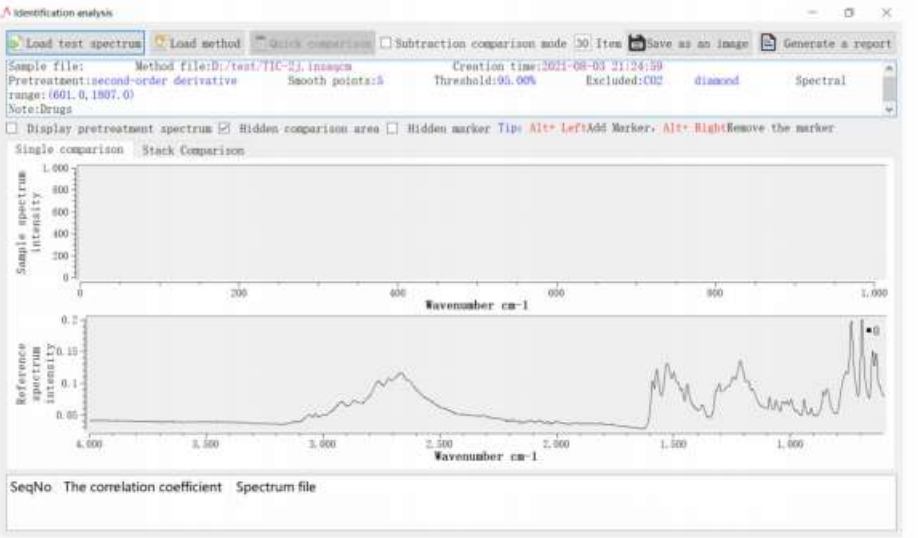
7. Select "no processing" in "pretreatment method" or process the spectrum with "first-order derivative" and "second-order derivative"; Select the smoothing method of different points in "smooth points"; Enter an appropriate threshold in "Threshold value", such as 95%; If there is interference peak of diamond, you can check " Diamond region excluded". If there is interference peak of CO2, you can check "CO2 region excluded ". or you can check both.



8. Finally, after adding "Note" to the method, click "Save method" at the top to complete the establishment of a quick comparison method.

Identification Analysis

1. Open the function of "Identification Analysis" under "Quick Identification" in "Data Evaluation" menus.



2. Click the "Load test spectrum" button and select a spectrum for comparison.

3. Click the "Load method" button to load the established method. The software will remember this method, and the next time you open this function, you don't need to load the method again.

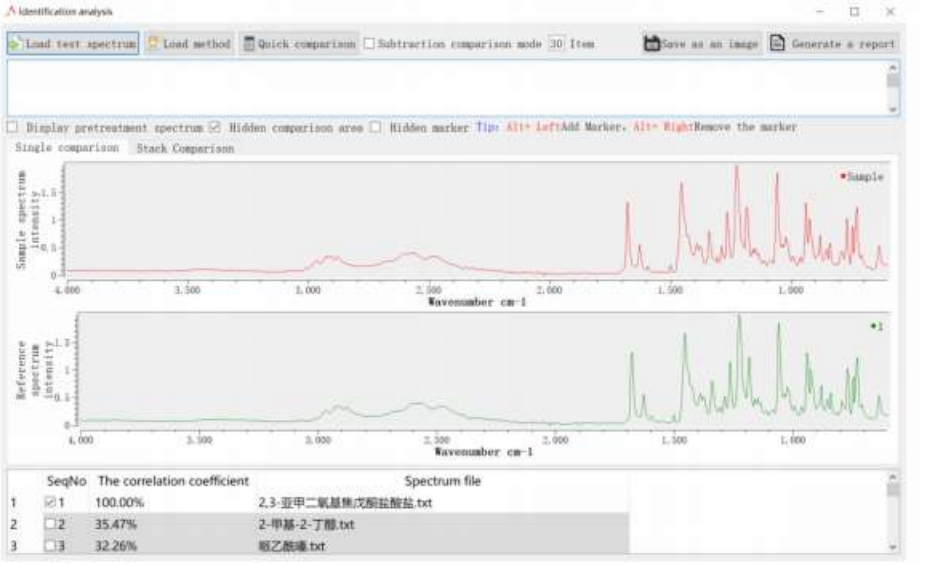
4. Finally, click the "Quick comparison" button, and the software will automatically compare the correlation coefficient of the spectrum, and the correlation coefficient of the spectrum and the name of the compound will be displayed at the bottom.

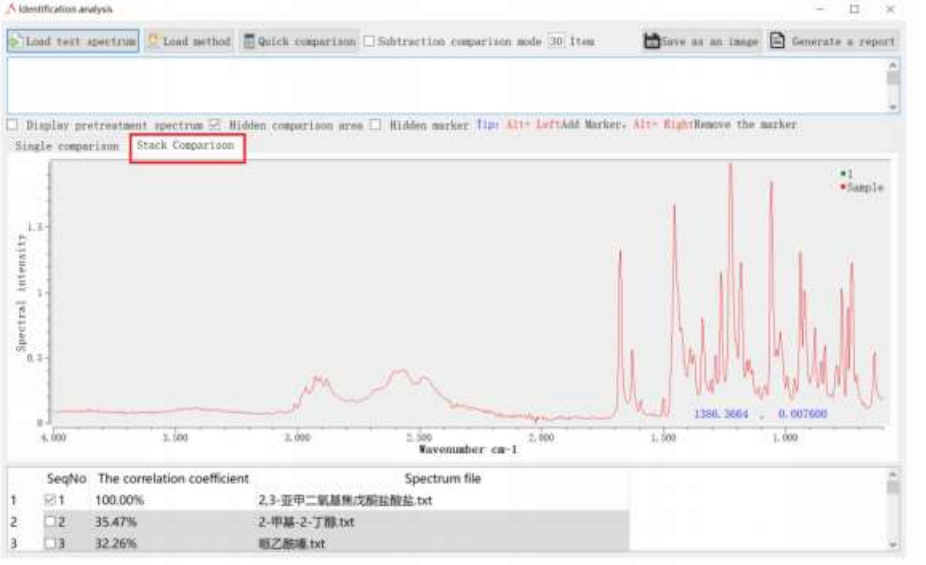
The features of the quick identification software is that different peak positions can be added for comparison, which makes the comparison more intuitive.

- If you want to show the pretreatment spectrum, click "Display pretreatment spectrum" to show.
- If you want to hide the comparison area, click "Hidden comparison area" to eliminate the comparison area.
- If you want to hide the mark, click "Hidden marker" to eliminate the peak position.
- If the correlation coefficient of quick comparison is higher than the threshold, the results will be displayed on a white background, indicating that the compound is

very similar; If the correlation coefficient is lower than the threshold, the results will be displayed on a gray background, indicating that the results of the compound are not necessarily similar and need to be noted.

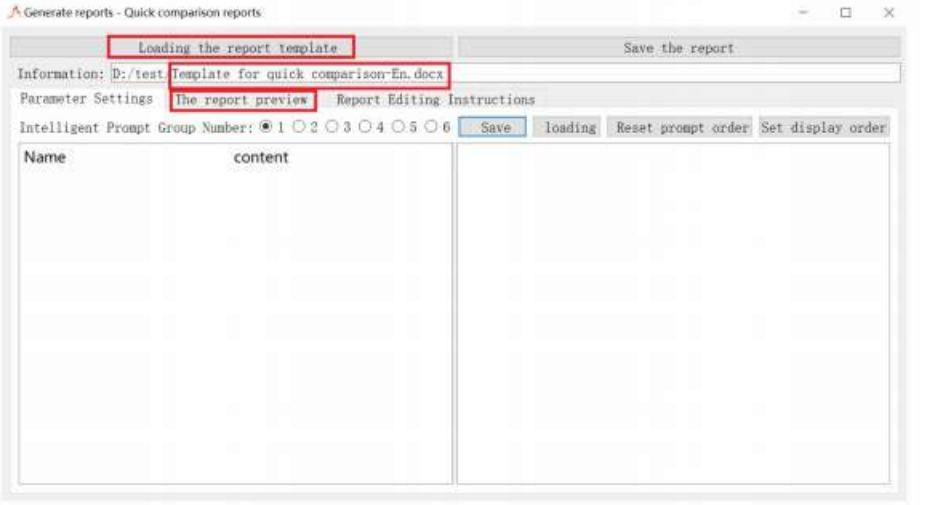
- The results of quick comparison can be compared separately or stacked, as shown in the following figure.



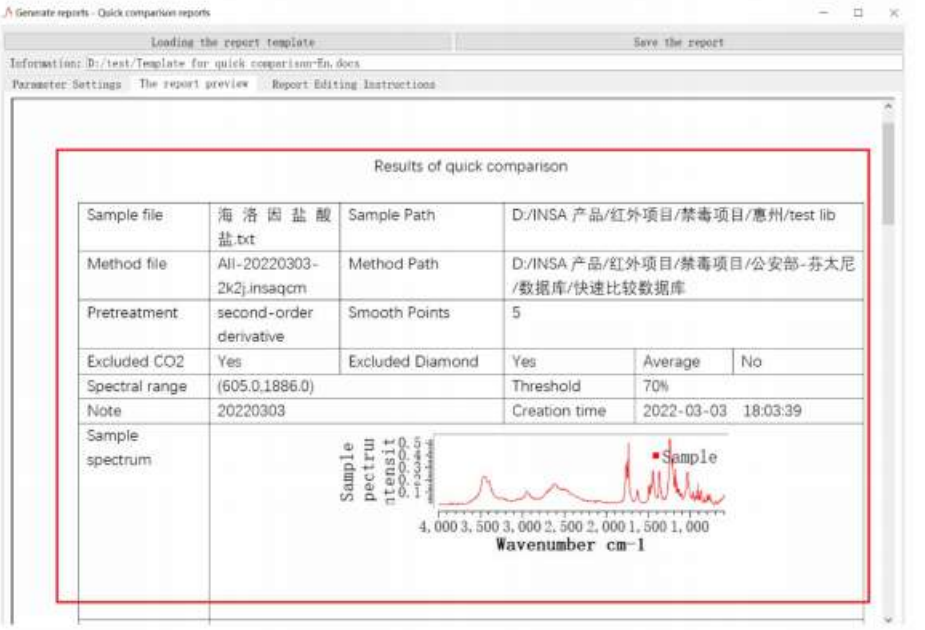


5. Users can click the "save as an image" button to directly save the comparison results as image files for convenient storage or printing.

6. Or click the "generate a report" button to directly output the comparison results to the report format and print them as PDF documents for storage and printing. First you should install the PDF reader software and then use the function.

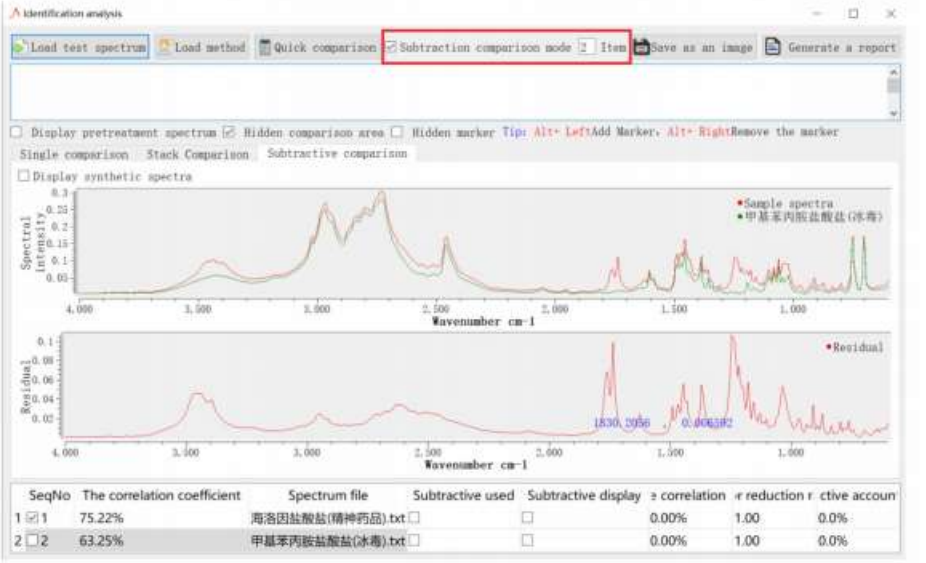


You can preview the report in real time, and save the report.

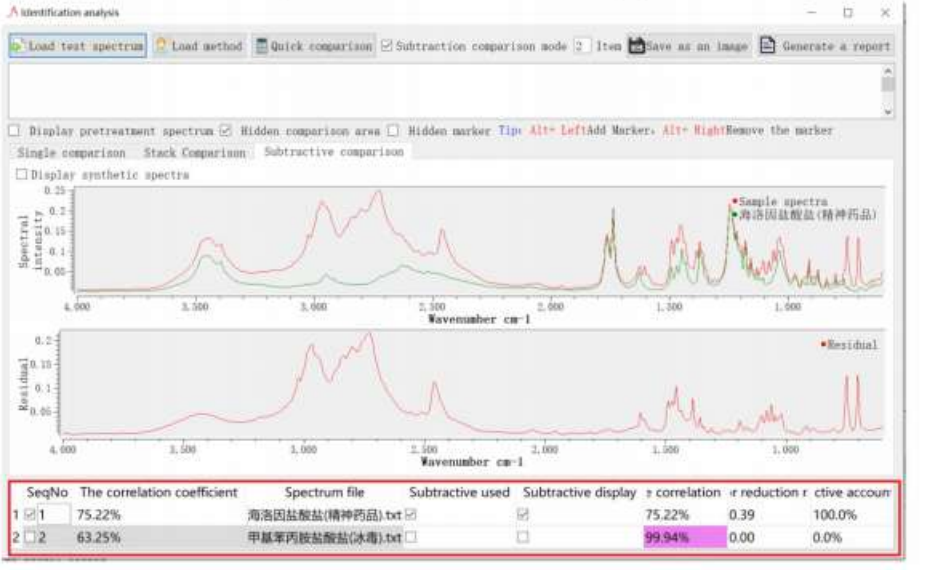


16 Analysis of mixed drugs

1. It is the same as the analysis steps of single component. First, load the spectrum and method. Check the "Subtraction comparison mode" check box, and the following number can be selected as 2, indicating that the mixed drug is composed of 2 components. Then click the "Quick comparison" button to get the following figure.



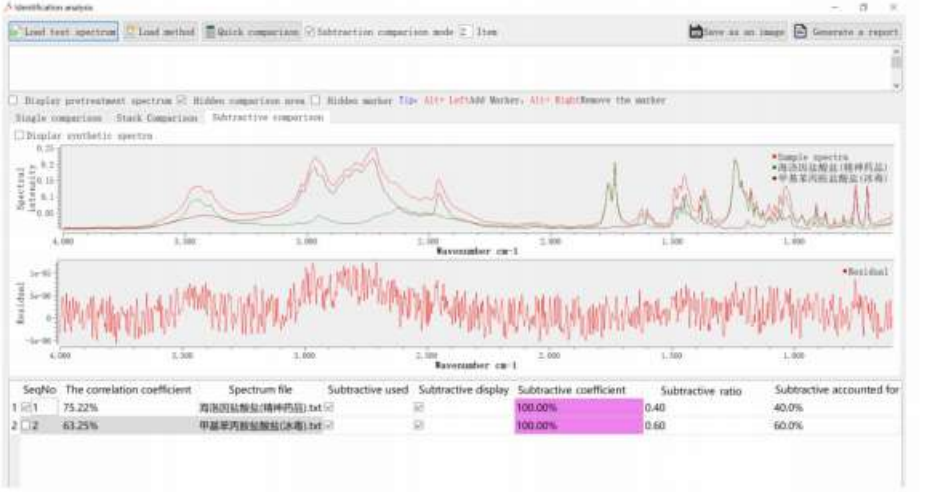
2. The software first determines that the mixture contains "heroin hydrochloride". The user can click the "Subtractive use" check box in the line of heroin hydrochloride, subtract this spectrum from the mixture spectrum. as shown in the following figure.



3. It can be seen that after the subtraction, the software will automatically make a second comparison and get a new correlation coefficient of the second component. In the figure above, the correlation coefficient of methamphetamine hydrochloride has changed from 63.25% to 99.94%, indicating that the second component in the mixture is indeed methamphetamine hydrochloride.

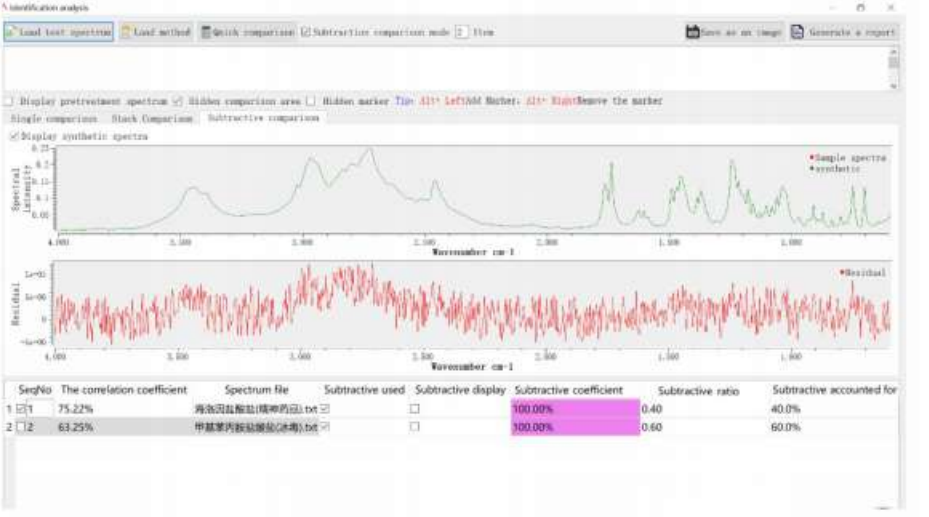
4. The user can continue to subtract, check the "Subtractive use" check box in the second line,

and get the picture below. "Subtraction ratio" refers to the proportion of two pure component spectra in the mixed spectrum, which is different from the actual quantitative relationship.



SeqNo	The correlation coefficient	Spectrum file	Subtractive used	Subtractive display	Subtractive coefficient	Subtractive ratio	Subtractive accounted for
1 ☑1	75.22%	海洛因盐酸盐(精神药品).txt	☑	☑	100.00%	0.40	40.0%
2 ☐2	63.25%	甲基苯丙胺盐酸盐(冰毒).txt	☑	☑	100.00%	0.60	60.0%

As you can see, the resulting residual spectrum is very small, indicating that the mixture is made up of these two drugs. The user can display a comparison of the synthetic and actual spectra.

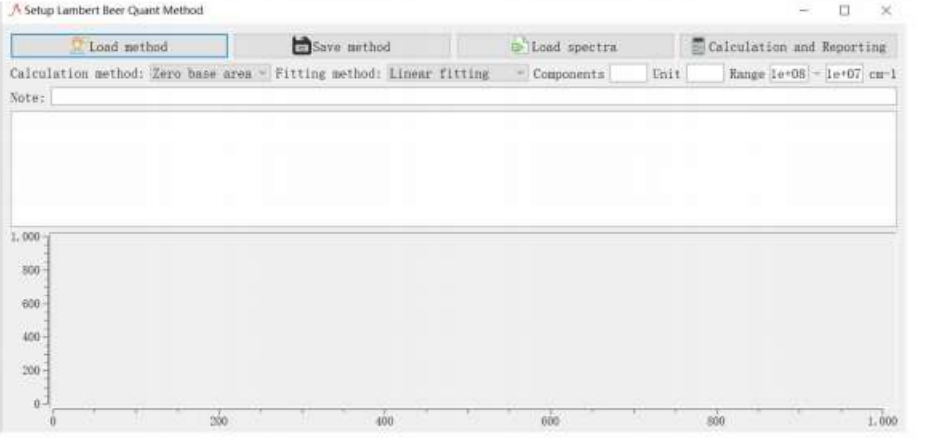


SeqNo	The correlation coefficient	Spectrum file	Subtractive used	Subtractive display	Subtractive coefficient	Subtractive ratio	Subtractive accounted for
1 ☑1	75.22%	海洛因盐酸盐(精神药品).txt	☑	☐	100.00%	0.40	40.0%
2 ☐2	63.25%	甲基苯丙胺盐酸盐(冰毒).txt	☑	☐	100.00%	0.60	60.0%

17. Quantitative Analysis

Steps for setup Lambert Beer Quant method

1.Open the function of " Setup Lambert Beer Quant method " under "Quantification" in "Data Evaluation" menus.



2. If a method has been established, click"Load method" directly. If it is a new method, click "Load spectra", select the multiple infrared spectra to be used, then click "Open".

3. Enter the name of the component in "Components"; Enter the concentration unit of the component in the Unit column. In the range, the left and right boundaries of the quantitative spectrum peak are input respectively. At this time, the bottom spectral curve will show the selected region and indicate different colors.

4. Select "End base Area" in "Calculation method"; In Fitting method, select Linear fitting. The fitting method can also choose "Quadratic fitting" and "cubic fitting".

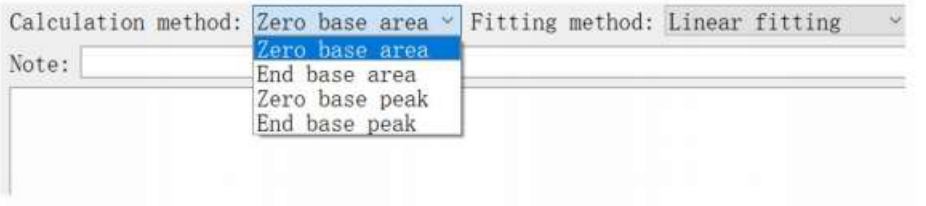
Note:

"Zero base area" means the integral area based on 0;

"End base area" refers to the integral area based on the left and right ends;

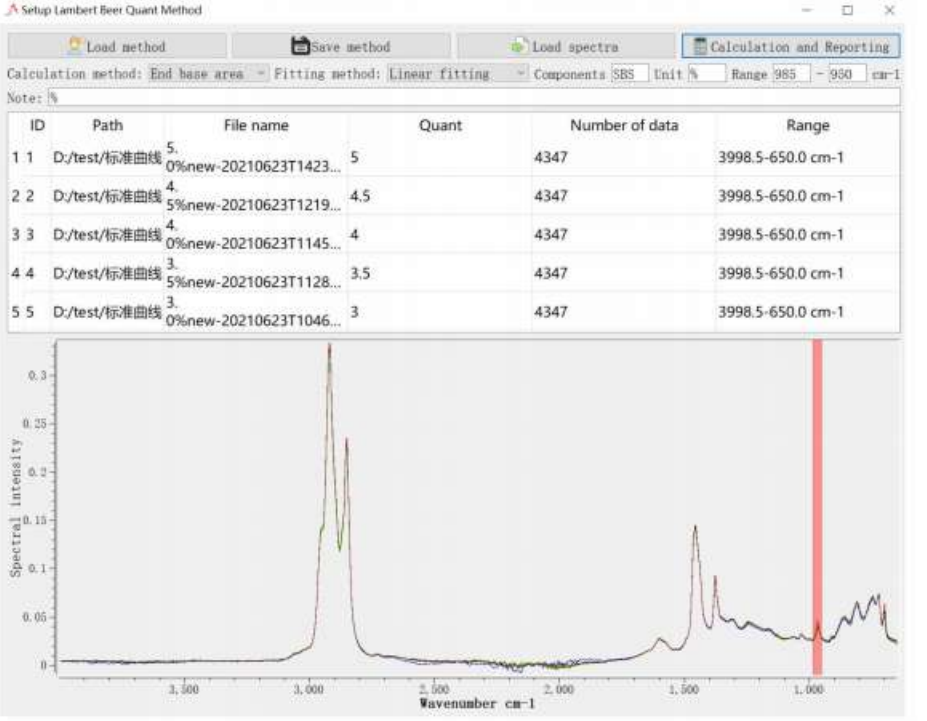
"Zero base peak" refers to the peak height value based on 0;

"End base peak" means the peak height value based on the left and right ends;

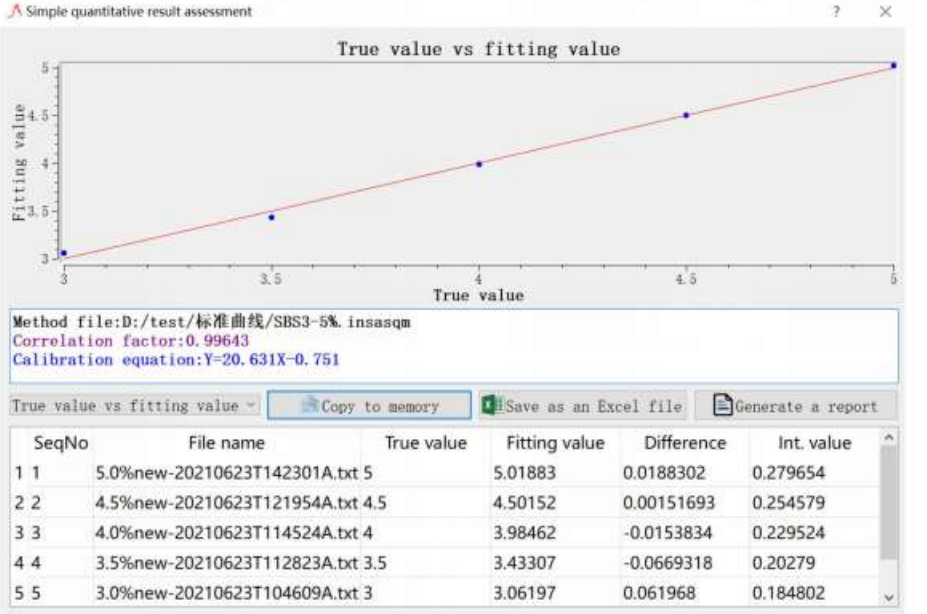


5. In the "content" column of the middle table, enter the true values of different

concentrations of the components.

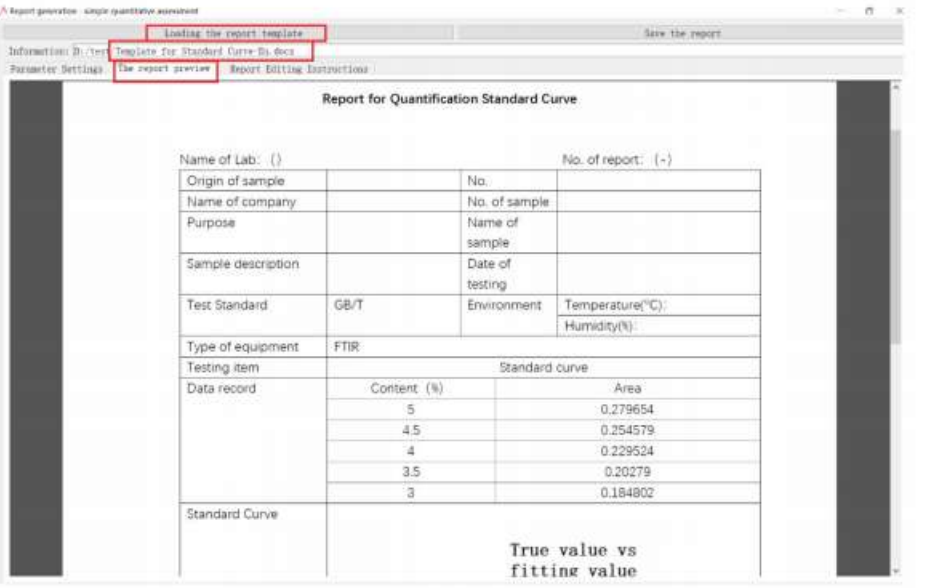


6. Click "Save method", name the quantitative method, and "save" the result. At this time, "Calculation and Reporting" changes from gray to black. Click the button to view the result.



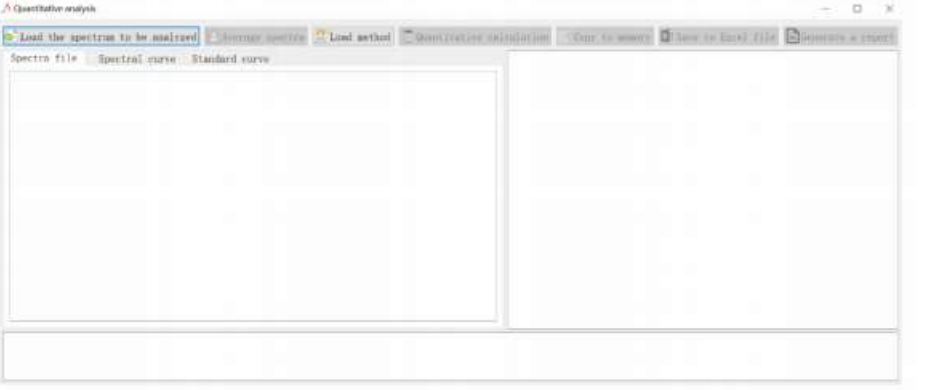
7. In the interface of "Simple quantitative result assessment", the working curve is displayed at the top; The correlation factor and calibration method of the curve are shown in the middle. Below are detailed data results. Users can click the drop-down menu to display different evaluation results and curves: true value vs fitting value; True value vs error; Integral vs true value.

8. Click "Save as an Excel file" to save the result; or click "Generate a report" to print a detailed report. First you should install the PDF reader software and then use the function.



Quantitative analysis

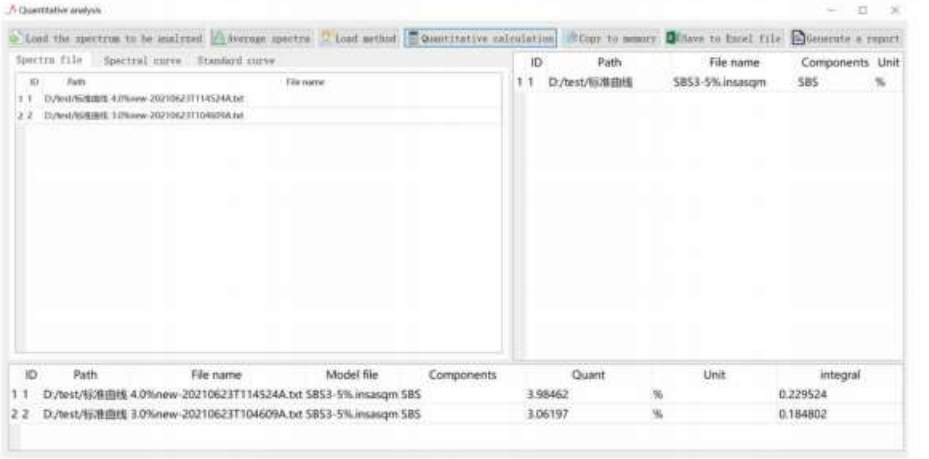
1. Open the function of " Quant Analysis" under "Quantification" in "Data Evaluation" menus.



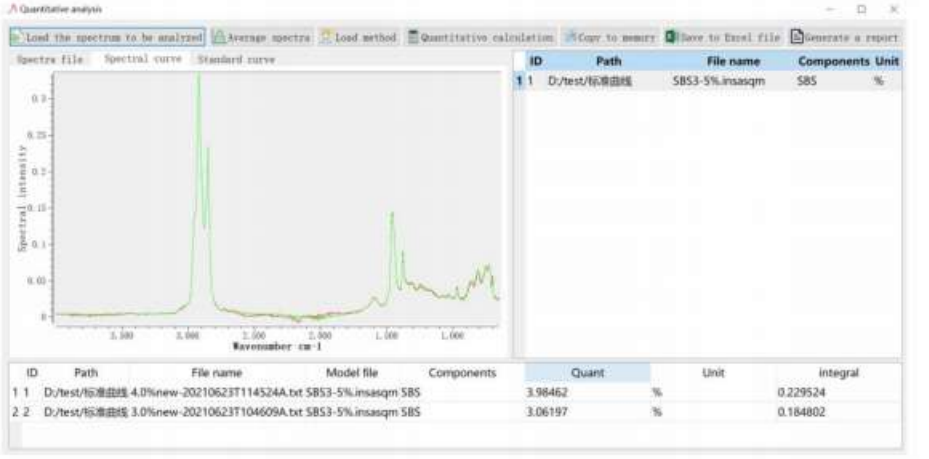
2. Click "Load the spectrum to be analyzed" button and select one or more spectra for analysis. If more than 2 spectra are selected, the button of "Average spectra" will be displayed. Click the button and the software will average these spectra before quantitative analysis. This function is suitable for testing the same sample for several times to predict the results.

3. click "Load method" button, load the established method, you can select one or more methods, quantitative analysis at the same time.

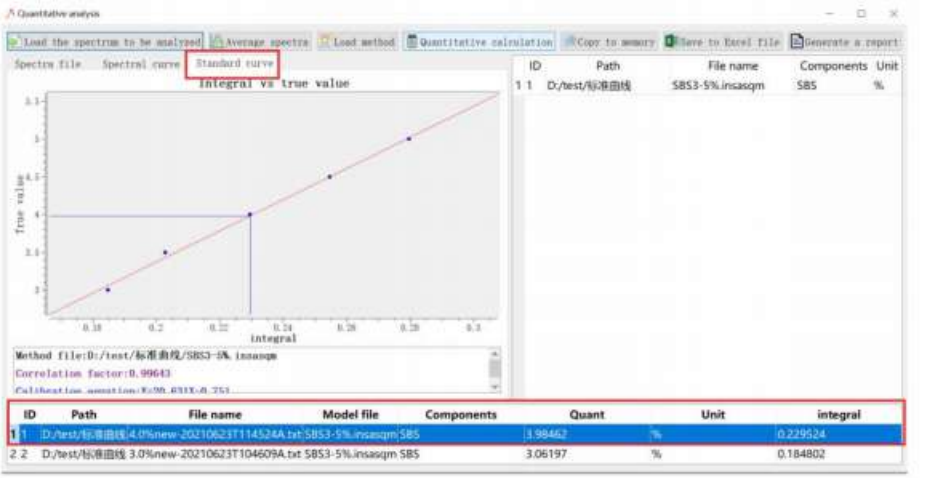
4. Finally, click the "Quantitative calculation" button, and the software will automatically calculate the quantitative result.



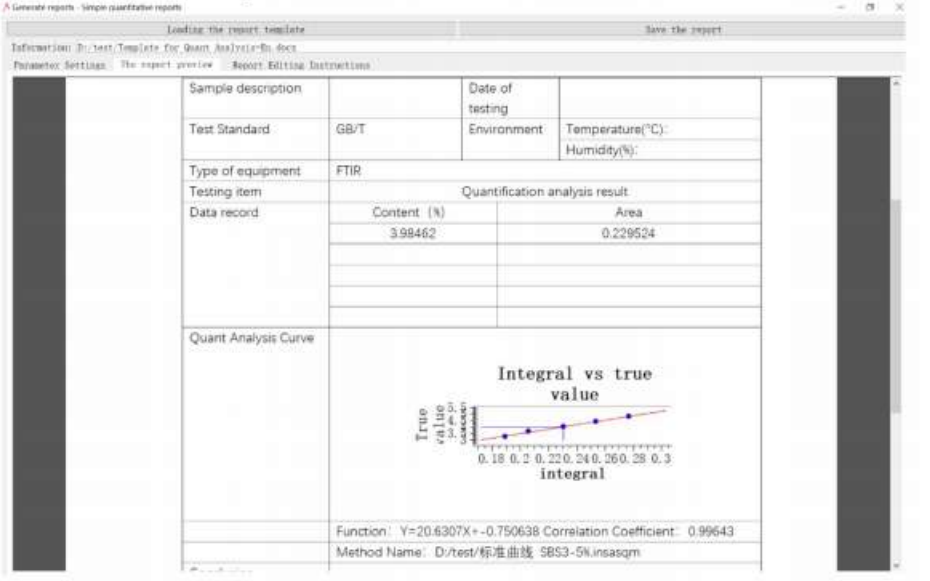
At the same time, the user can also view the spectral curve of the file and the standard curve page used, very intuitive.



Display of standard curve:



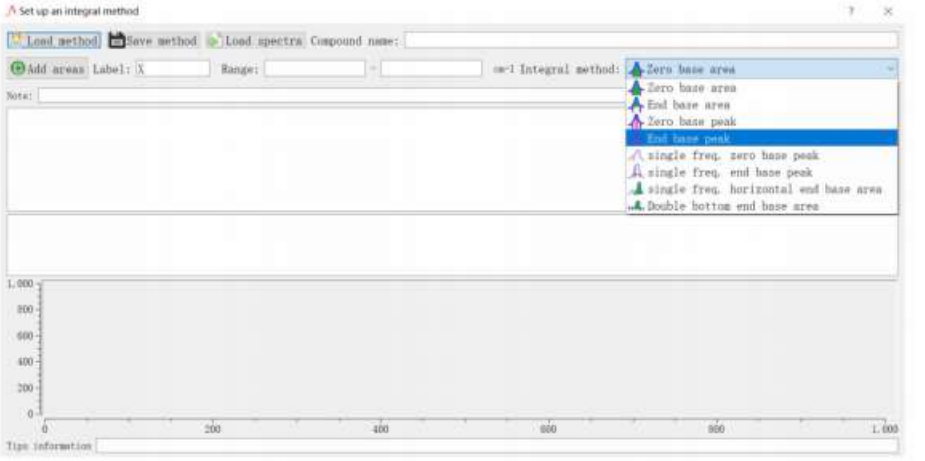
5. Users can directly click "Save to Excel file" or "Copy to memory". If you need to print a report, you can click the "Generate a report" button to print a detailed report for easy archiving and viewing.



18. Integral calculation

Setup Integration Method

1. Open the function of " Setup Integration Method" under "Quantification" in "Data Evaluation" menus.



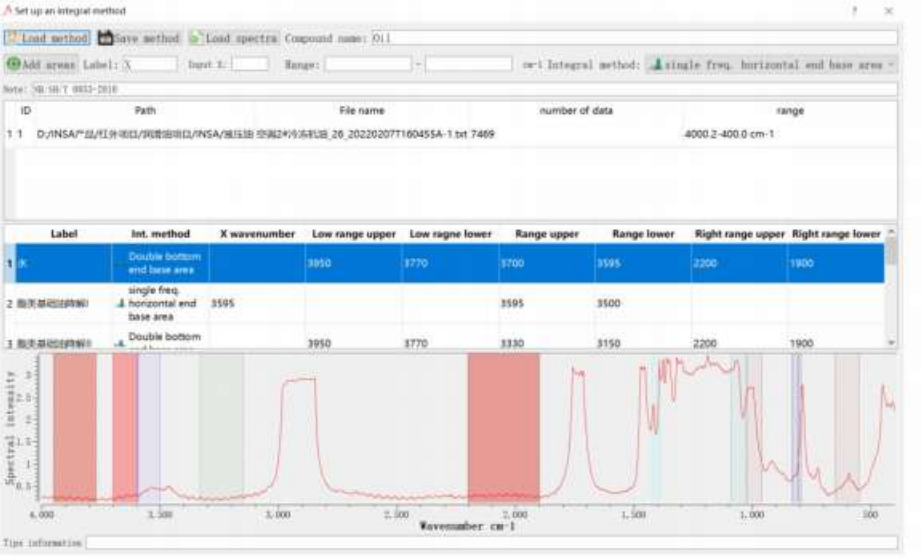
2. If the integral method has been established, click "Load method" button directly; If it is a new method, click "Load spectra", select the infrared spectrum to be integrated, and click "Open".

3. Enter the name of the compound in "Compound Name". Fill the labels for the different components in the label column. In the range, the left and right boundaries of the integral spectrum peak are input respectively.

4. Select the appropriate integration method in the integral method. Specific instructions are as follows:

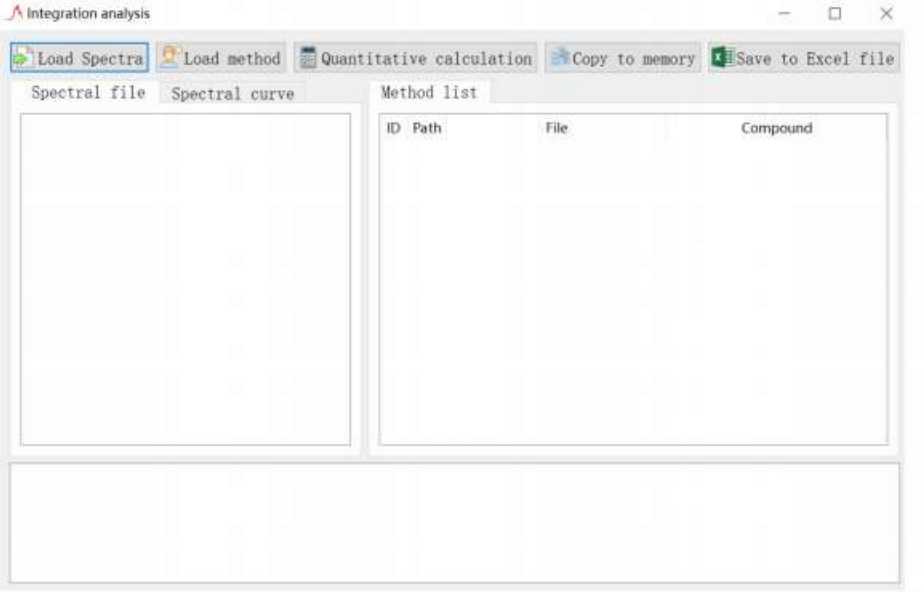
- "Zero base area" means the integral area based on 0;
- "End base area" refers to the integral area based on the left and right ends;
- "Zero base peak" refers to the peak height value based on 0;
- "End base peak" means the peak height value based on the left and right ends;
- "Single freq. zero base peak" refers to the peak height value based on 0 at a specified frequency;
- "Single freq. end base peak" refers to the peak height value based on the left and right ends at a specified frequency;
- "Single freq. horizontal end base area" refers to refers to the calculation of peak area under two given frequency ranges, but the baseline is the horizontal line corresponding to a certain frequency;
- "Double bottom end base area" refers to refers to the calculation of peak area under two given frequency ranges, but the two ends of the baseline depend on the valley bottom of two optional spectra ranges.

5. Click the "Add Areas" button, and different colored areas will be displayed in the spectrum below to represent different components.
6. Finally click "Save method" to save the integral method.

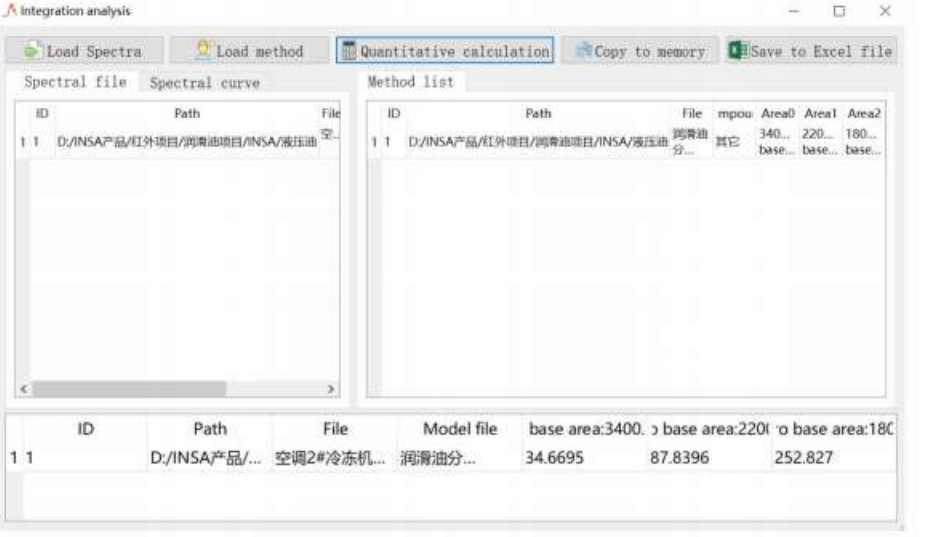


Integral quantitative calculation

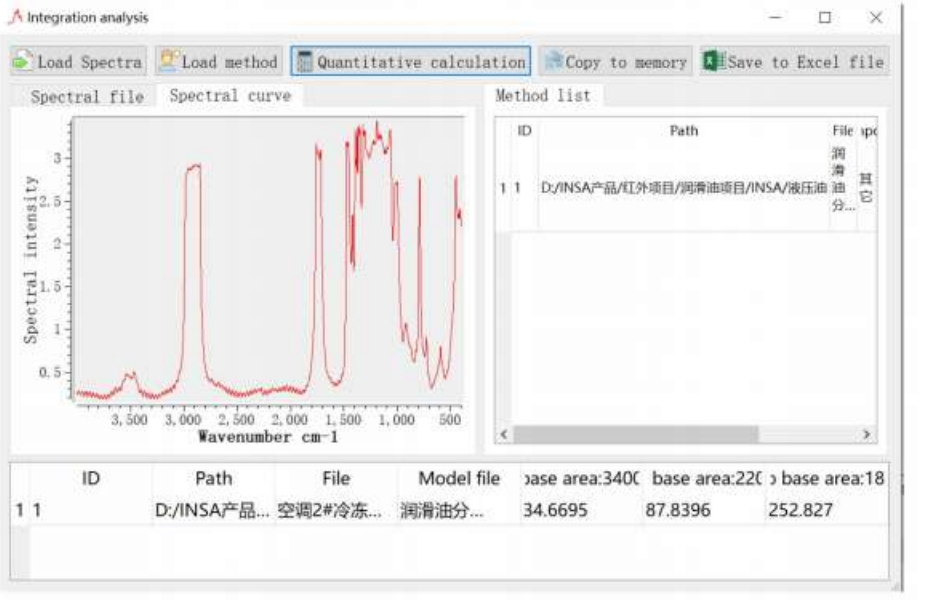
1. Open the function of " Integration Analysis" under "Quantification" in "Data Evaluation" menus.



2. Click "Load Spectra" button and select one or more spectra for analysis.
3. Click the button of "Load method" to load the established integral method, select one or more integral methods, and perform integral quantification analysis at the same time.
4. Finally, click the "Quantitative calculation" button, and the software will automatically calculate the integral quantitative result corresponding to each spectrum.
5. Users can directly click "Save to Excel file" or "Copy to memory" to save the results.



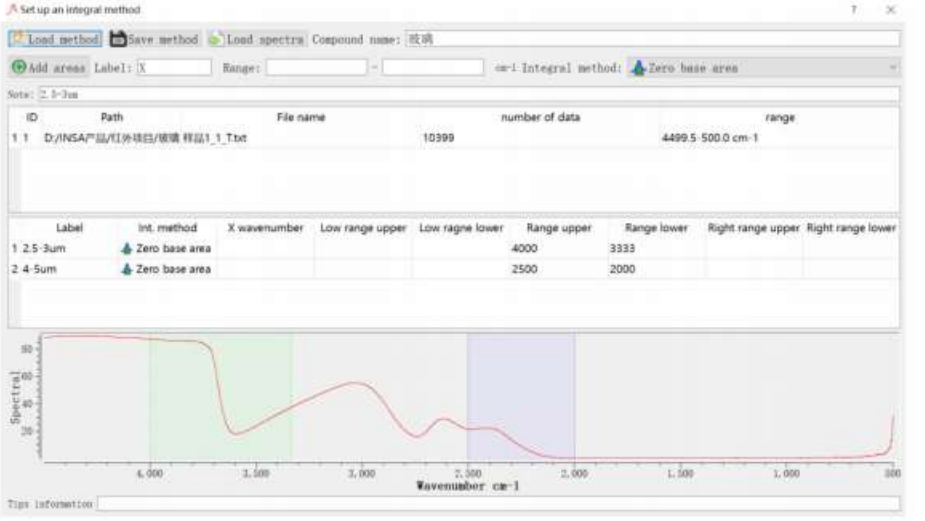
At the same time, users can view the imported infrared spectrum, as shown in the following figure.



19. Calculation of average transmittance

Set up an integral method

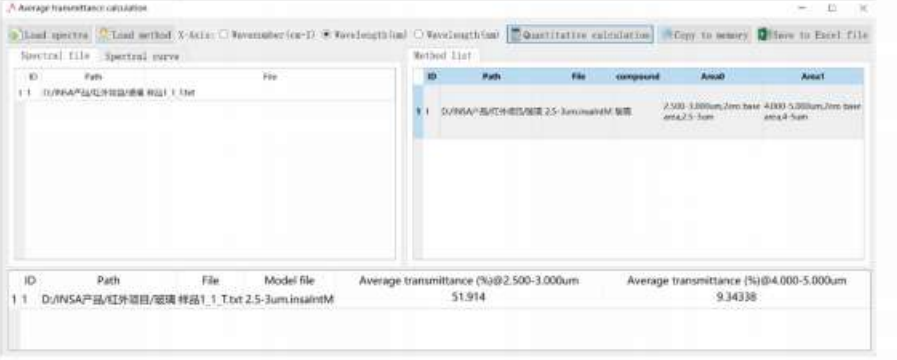
First, the integral method of average transmittance is established. The integral method under different wavebands can be established according to the description of previous chapter - Integral Calculation.



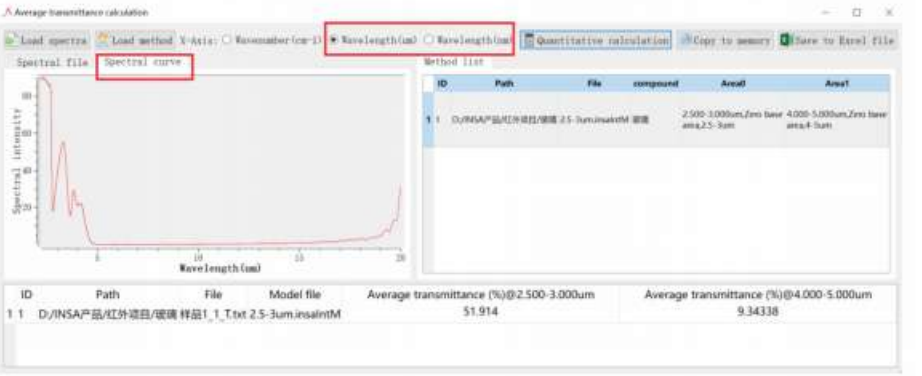
Calculate the average transmittance

1. Open the function of "Average Transmittance " under "Quantification" in "Data Evaluation" menus.

2. Click the button "Load spectra" and the button"Load method", then click "Quantitative calculation", the software can automatically calculate the average transmittance.



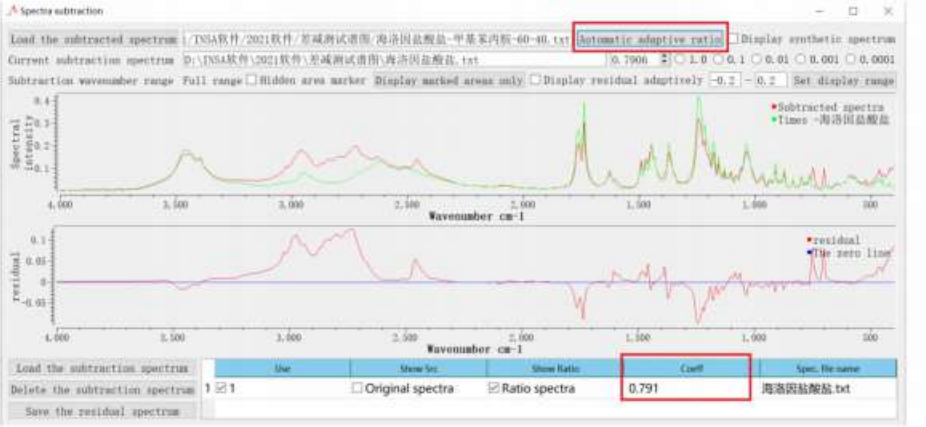
3. The coordinates of the X axis can be replaced by the wavelength, and the spectrum can be viewed in the "Spectral curve" column. Users can directly click "Save to Excel file" or "Copy to memory" to save the results.



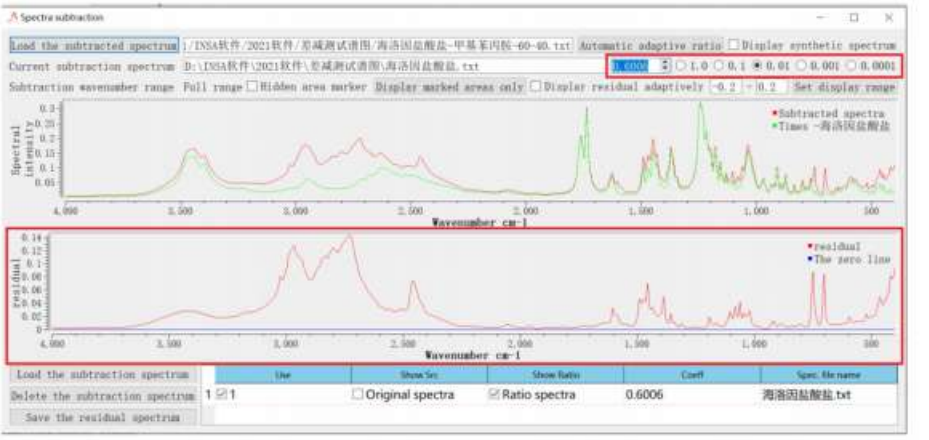
20. Spectra Subtraction

1. Open the function of " Spectra Subtraction" under "Quick Identification" in "Data Evaluation" menus. Click the "Load the subtracted spectrum" button. This is the mixture spectrum, as shown red color in the box below. Click the "Load the subtraction spectrum" button. This is the spectrum of a pure compound, as shown in green in the box below .If checked, the spectrum is to be subtracted. The box below shows the result of the 1-fold subtraction. Users can also select a variety of spectra for subtraction, which can be selected separately.

2. Users can first click the "Automatic adaptive ratio" button in the upper right to roughly subtract, and the effect is shown in the picture below.

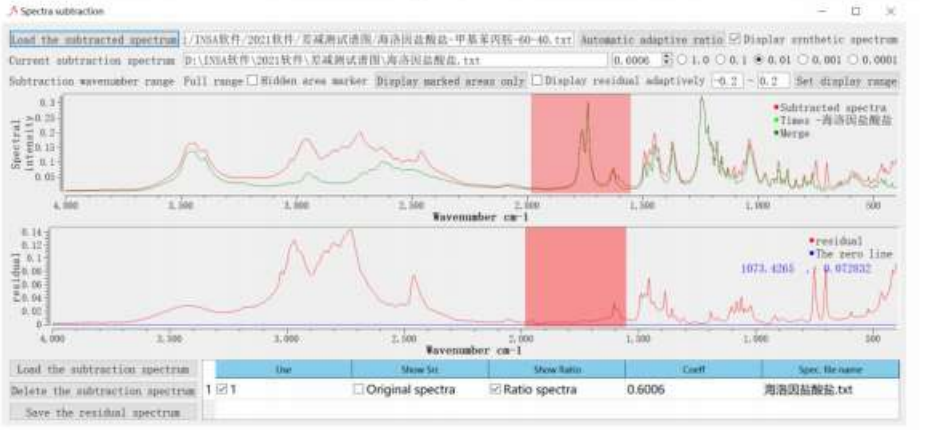


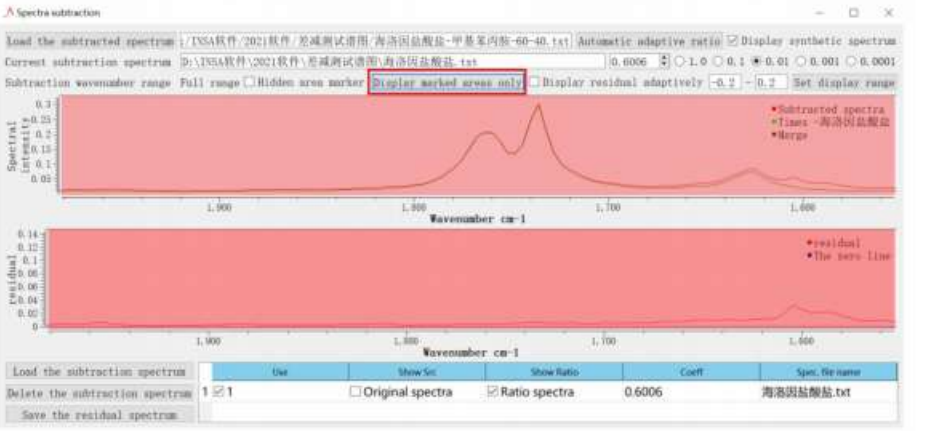
3. In the manual selection multiplier box, the user can finely adjust the multiplier of the subtraction. The minimum 0.0001 fold can be selected for subtle subtraction. At the same time, observe whether the red residual spectrum in the box has no negative peak, and the blue line indicates the reference of zero reference line.



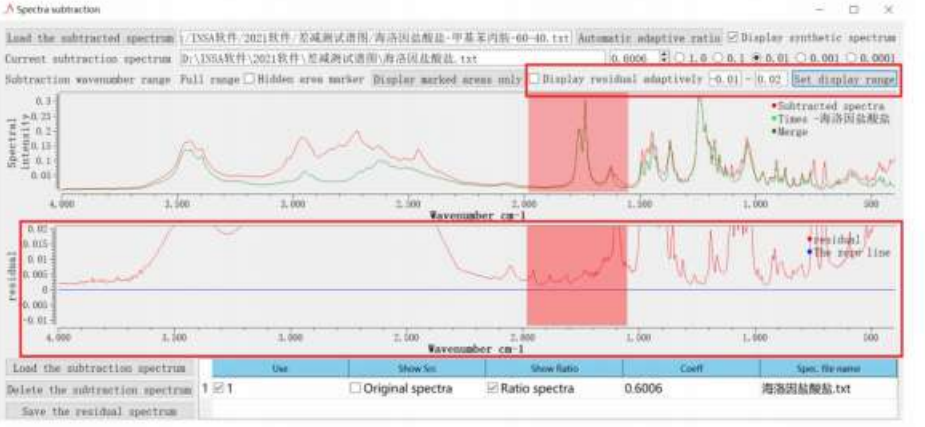
4. After the fine subtraction is completed, users can click the button of "Save the residual spectrum" in the lower left to save the subtraction result for use.

5. User can choose some of the range to subtraction, Press Alt key and click the left / right mouse button respectively to determine the left / right range. User can click "Display marked area only"button to show the selected range, and can restore the whole range by double click right mouse button. User can hide the range by check the "Hidden area marker"check box.



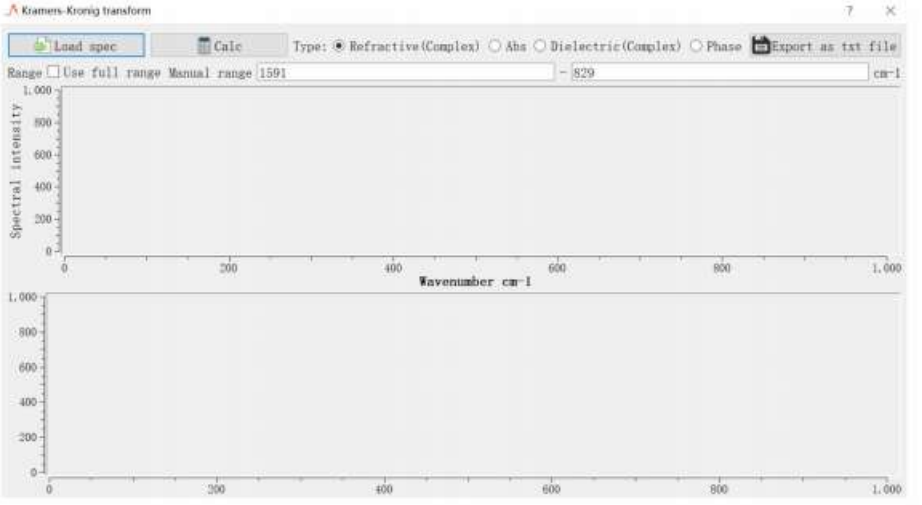


User can set the display range of residual spectrum by clicking "Display residual adaptively" button and enter the corresponding numbers, for example:-0.01 to 0.02.

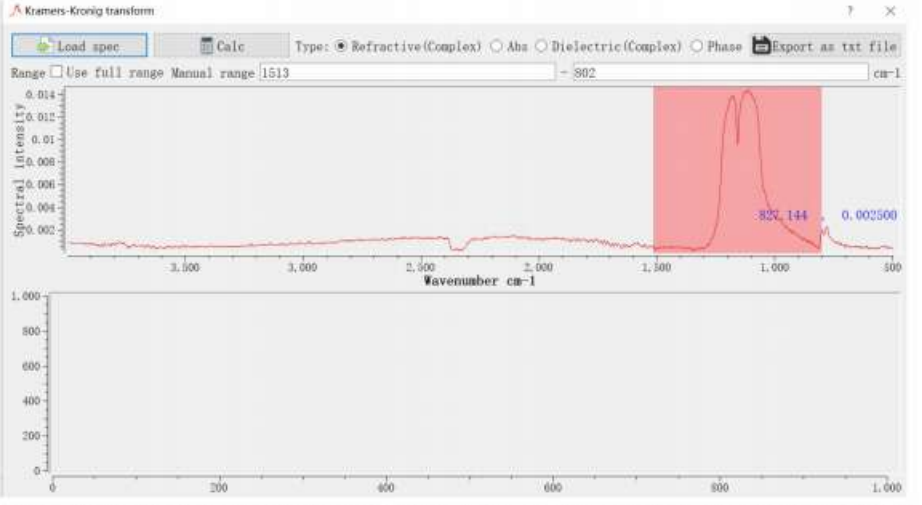


21. Kramers-Kronig transform (KK transform)

1.Open the function of "KK transform " in "Data Evaluation" menus. Click the "Load Spec" button. This function suit for the specular reflection spectrum at nearly normal incidence to the sample surface, such as a 10 degree or 12 degree specular reflection measurement.



2. Select the range of KK transformation. If "Use file range" is checked, the full range of the spectrum is used. If not selected, you can manually enter the left boundary (high wavenumber) and right boundary (low wave number). Or you can press Alt key and click the left / right mouse button respectively to determine the left / right range. To remove the range, use Alt+ right mouse button to cancel.



3. Select "Type" for calculation. User can obtain the real and imaginary parts of refractive index, real and imaginary parts of dielectric constant, absorption spectra and phase spectra in one

transformation. The transformed spectra can be exported by clicking the "Export as txt file" button.