

Raman Quantitative Analysis System

ATRMAS

Features

- The software supports modeling, quantitative analysis, and origin classification;
- The software can directly measure the concentration of the sample and supports multiple concentration units;
- Supports qualitative measurements and is compatible with all the company's Raman spectroscopy instruments;
- Cooperating with the company's online Raman instrument, it can perform in-situ and online monitoring;
- The software supports customized design;
- Simple operation and convenient measurement

Description

ATRMAS is a Raman modeling quantitative analysis system that facilitates users to conduct quantitative testing and substance classification analysis according to their actual needs. The software supports multi-variable and single-variable modeling. The software is simple and convenient to operate. It supports quantitative analysis and testing of online Raman instruments and all the company's Raman spectrometers. The software supports customized design.

ATRMAS provides a human-computer interaction interface and measurement results, and provides multiple functions such as data storage and export, further enhancing the application scope and scenarios of the instrument.

Application

- | | | |
|---|---------------------------------|--------------------------|
| ● Substance classification | ● flow chemistry | ● hydrogenation reaction |
| ● Online monitoring for pharmaceutical industry | ● Polymerization | ● synthesis reaction |
| ● Crystallization process | ● biological process monitoring | ● chemical synthesis |
| ● Polymorph identification | ● Cultural relic identification | ● Purification process |



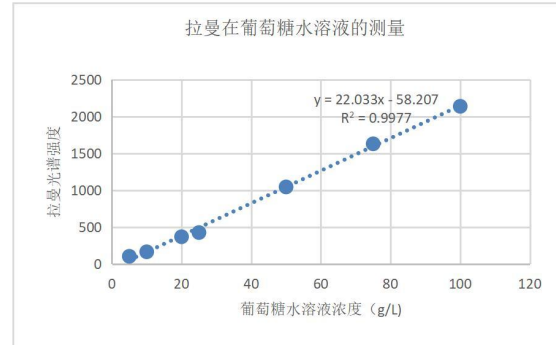
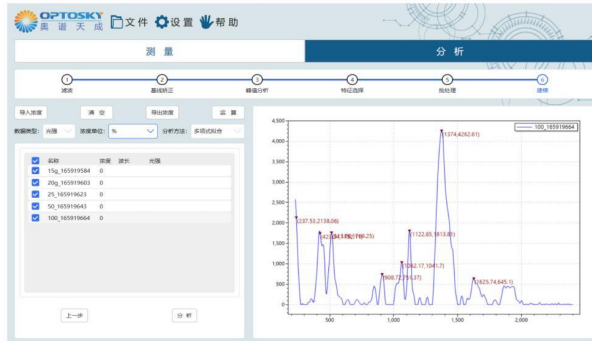
Acquisition: Collect the Raman spectra of substances, and can collect Raman spectra of a series of samples with gradient concentrations.

Quantitative analysis: Import the measured data, conduct analysis and modeling, and then quantitatively measure the concentration of the unknown liquid.

Classification: Classification and identification of classes of substances.

1. Applications of ATRMAS

1.1 Modeling



ATRMAS can support the modeling of a variety of substances. The completed model can be applied to online Raman and all the company's Raman analyzers. The modeled substances can be Qualitative and quantitative analysis.

1.2 Quantitative analysis



样品编号 (葡萄糖)	测量浓度 (g/L)	相对误差
1-1	16.71	-11.41%
1-2	16.17	-7.78%
1-3	16.76	-11.71%
2-1	37.91	5.23%
2-2	38.09	4.78%
2-3	38.45	3.87%

After importing the model, the concentration of the substance can be measured in real time and supports multiple concentration units. As shown in Figure 2 above, the glucose concentration is measured. Created model guide After entering online Raman, the concentration of substances can be monitored in real time, and it can be adapted to all the company's Raman spectrometers.

1.3 Sample classification

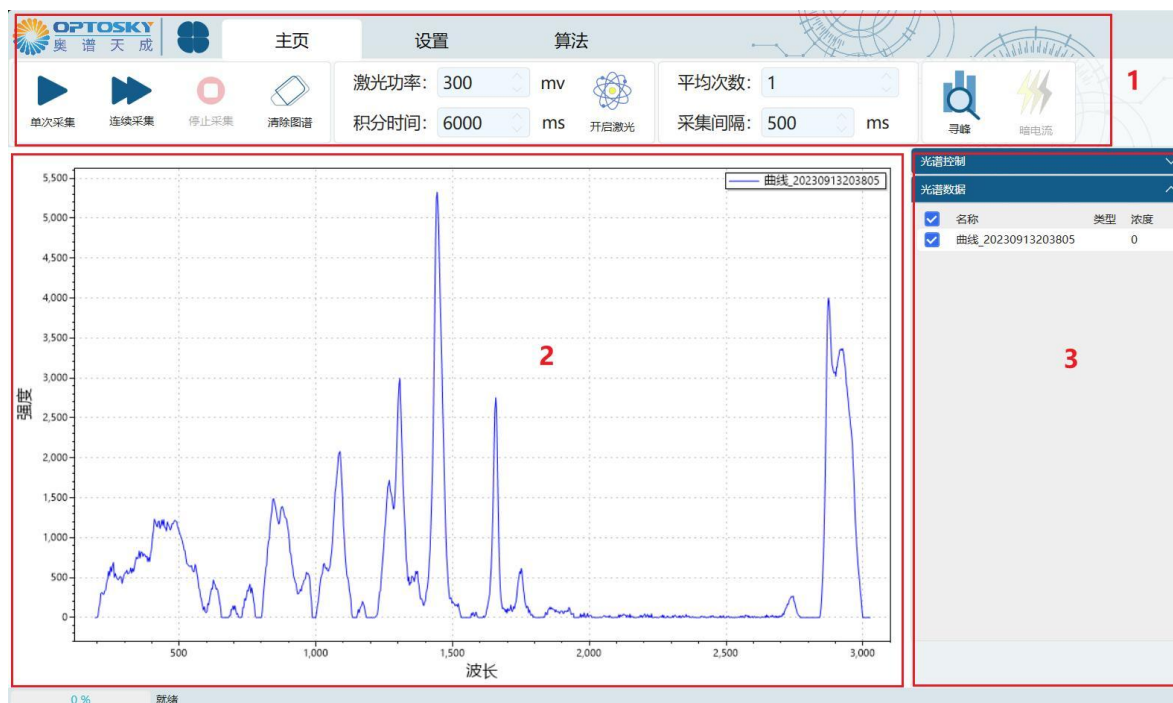


样品编号 (分类)	样品类别
1-1	湖北
1-2	湖北
1-3	湖南
2-1	北京
2-2	福建
2-3	福建

Substances can be modeled and classified, and the categories of substances can be qualitatively identified.

2. ATRMAS Introduction

2.1 Collection main interface



Area 1:

Area 1 is the toolbar of the software

Save: You can save and delete the selected measurement data.

Home page: current measurement interface.

Settings: Set the cooling temperature of our spectroscopic instrument, etc.

Algorithm: Perform derivation, baseline correction, etc. on the measured Raman spectrum curve.

Single acquisition: Click to collect the Raman spectrum of the sample once.

Continuous collection: Click to collect continuous Raman spectra of the sample.

Stop collection: Click to stop the current collection process.

Clear spectrum: clear all spectrum collection data.

Laser power and integration time: You can set the laser power and integration time.

Turn on laser: You can turn on the laser.

Average times: collect Raman spectra of the sample multiple times, and take the average of the multiple acquisitions.

Collection interval: During continuous collection, you can set the time interval for each collection.

Peak search: Query and mark the peaks of the Raman spectrum.

Dark current: The dark bottom of the sample can be collected.

Area 2:

For the measured Raman spectrum, the Raman characteristic peaks can be qualitatively identified. Click the toolbar button to identify the characteristic peaks and identify the substance qualitatively.

Area 3

is the measured Raman spectrum data. If a series of concentration gradient samples are measured, enter the corresponding concentrations. After saving the data and importing it, you can

Perform analytical modeling in quantitative analysis, and then import the model wine to start modeling.

2.2 Quantitative analysis modeling interface



Area 1

File: can be imported for batch processing

Settings: Set the laser power and integration time of the laser

Help: You can view the version information of the software

Measurement: You can switch to the measurement interface of quantitative analysis

Analysis: Perform modeling of the sample.

Area 2

Steps for modeling

Filtering: You can select the data source and select the filtering method. The methods are divided into cyclic median filtering and SG filtering.

Baseline correction: divided into adaptive iterative weighted least squares, asymmetric least squares smoothing, and baseline correction.

Peak analysis: You can select signal-to-noise ratio threshold, intensity threshold, and percentage threshold.

Feature selection: You can select batch processing options such as peak center, peak intensity, peak area, and half-peak width.

Batch processing: Batch processing of data.

Modeling: Select the corresponding data for modeling analysis.

Usually we can click Next after importing the data in the modeling bar. If you want to make adjustments, you can make adjustments as appropriate in each step.

Area 3

Select the corresponding characteristic wave number, import the corresponding concentration, select the corresponding analysis method, select the concentration unit and other operations. If the peak is not found, you can

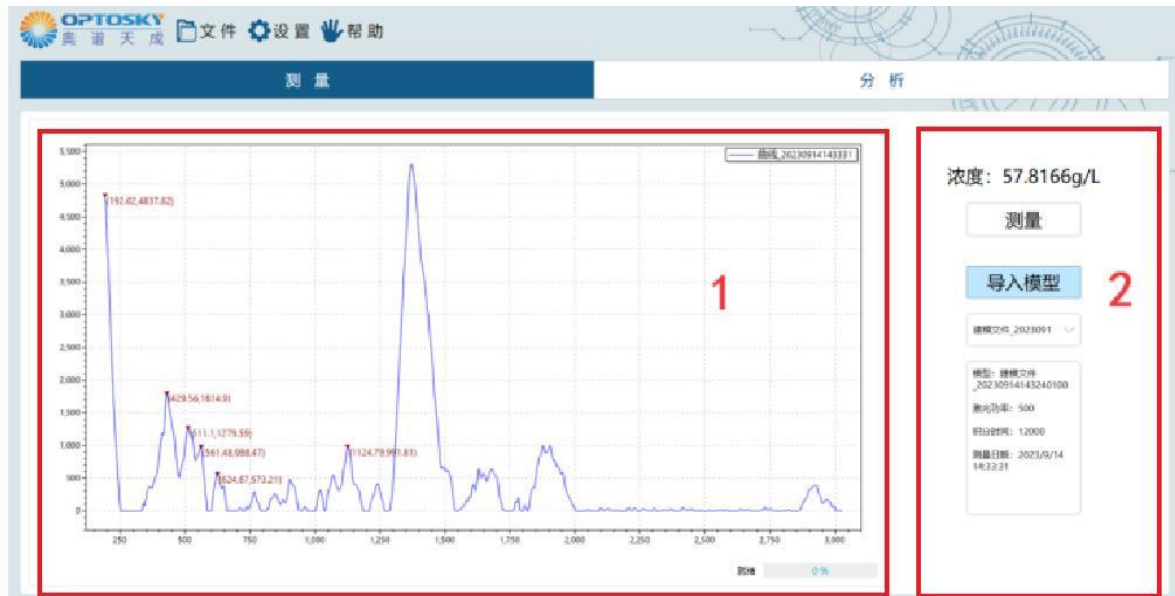
Manually input the wavelength, the instrument will automatically find the corresponding light intensity, check all samples, and then click Analyze, the software can automatically analyze, and then

After exporting the model, you can click measurement. After importing the model and placing the sample, you can start measurement.

Area 4

To find the peak spectrum of the Raman characteristic peak of a substance, you can select the corresponding characteristic peak spectrum.

2.3 Measurement main interface



Area 1

is the Raman spectrum of the substance to be tested.

Area 2

You can click to import the model, and then click Measure to measure the concentration of the substance to be measured.

Information about the laser settings created by the model can be viewed.

interest.

2.4 Classification



Substances can be modeled and classified, and the categories of substances can be identified and analyzed.

The modeling method is similar to quantitative analysis. After establishing the model, import the model and perform classification measurements (the above figure uses edible oil classification as an example).

Area 1

Raman spectra measured for classified oils

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Area 2

These are the measurement results after importing into the model. The results show that the origin of the oil is Hunan.

3. ATRMAS Specifications

Detection Probe		
1	Operating System	Windows10、11
2	Model	Qualitative, modeling, quantitative analysis
3	Equip Instruments	Company Raman spectrometer
4	Other	Support user customization