

Fourier Transform Infrared Spectrophotometer

# IRAffinity-1S





**IRAffinity-1S**  
INTEGRATED REFLECTANCE ACCESSORY

SHIMADZU



# IRAffinity-1S

## Fourier Transform Infrared Spectrophotometer

Surpassing General-Purpose Instruments in  
Sensitivity and Performance

Easy-to-Use, Advanced Software: LabSolutions IR

Broader Range of Applications

The IRAffinity-1S is a compact Fourier transform infrared spectrophotometer that is housed within an elegant form.

The interferometer is continuously optimized by a dynamic alignment mechanism, and a built-in auto dryer helps ensure ease of maintenance. The IRAffinity-1S offers the high  $S/N$  ratio (30,000:1, 1-minute accumulation, neighborhood of  $2,100\text{ cm}^{-1}$ , peak-to-peak), a maximum resolution of  $0.5\text{ cm}^{-1}$ , and compact dimensions. Furthermore, the high-performance LabSolutions IR software, which emphasizes operability, and analysis support programs make it easier to perform data processing and analysis.

Applicable to Various Fields

# IRAffinity-1S: Meeting the Needs of a Wide Range of Analyses

Fourier transform infrared spectrophotometers are used in numerous fields and applications; some of the most common ones are listed below. The IRAffinity-1S is a highly effective tool for these types of analyses\*.

\* Appropriate accessories and software for analysis are required in addition to the IRAffinity-1S.

## Automobiles

- Material identification tests
- Analysis of contaminant
- Failure analysis

## Chemicals and Polymers

- Raw material identification tests
- Qualitative analysis of plastics and rubber
- Identification of functional groups of synthetic products
- Analysis of surface preparation agents
- Analysis and thickness measurement of thin films
- Analysis of catalysts
- Analysis of paints and coatings
- Analysis of contaminant
- Quantitative analysis

## Construction

- Material identification tests
- Degradation analysis of coatings

## Food Products

- Raw material identification tests
- Packaging material identification tests
- Analysis of contaminant

## Medicine

- Raw material identification tests
- Identification of functional groups of synthetic products
- Identification of functional groups of natural products
- Analysis of contaminant

## Metals

- Qualitative analysis of thin films on metal plates
- Analysis and thickness measurement of thin films
- Analysis of contaminant

## Electricity, Electronics, and Semiconductors

- Thickness measurement of epitaxial films
- Quantitative analysis of interstitial oxygen and substituted carbon
- Quantitative analysis of phosphorus and boron in BPGS
- Quantitative analysis of hydrogen concentration in nitride film
- Quantitative analysis of hydrogen concentration in amorphous silicon
- Detection of brominated flame retardants
- Analysis of thin films
- Analysis of contaminant
- Failure analysis
- Analysis of semiconductor gases

## Cosmetics

- Material identification tests
- Analysis of contaminant
- Failure analysis

Realizing High Performance

## Surpassing General-Purpose Instruments in Sensitivity and Performance

The IRAffinity-1S incorporates a high-throughput optical element and a dynamic alignment mechanism. These features allow the user to experience a level of performance that surpasses that of general-purpose instruments.

### Highest S/N Ratio in Its Class: 30,000:1

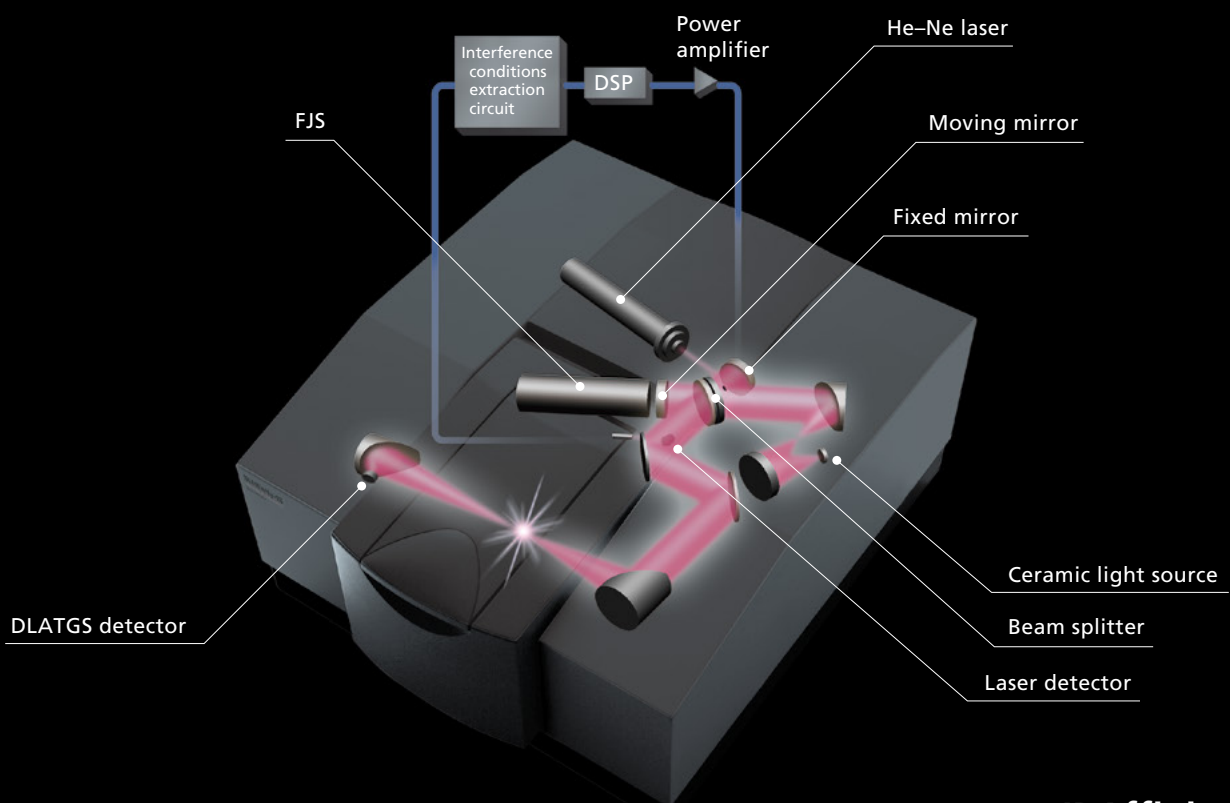
Through the incorporation of a high-energy ceramic light source, a temperature-controlled, high-sensitivity DLATGS detector, a high-throughput optical element, and the optimization of the electrical system and optical system, the IRAffinity-1S achieves the highest S/N ratio in its class.

### Highly Stable Interferometer Achieved with Dynamic Alignment Mechanism

The state of interference in an FTIR instrument is extremely delicate, and the interferometer must be controlled with high precision. With the IRAffinity-1S, the moving mirror is run very smoothly and precisely by a flexible joint system (FJS), and the interferometer is optimized and stabilized by an improved dynamic alignment mechanism. This makes it possible to perform measurement in a stable state with a short warming-up time.

### Dynamic Alignment Mechanism (JPN patent No. 3613171)

The state of interference of the He-Ne laser used for sampling by the interferometer is continuously monitored and compared with the state under the optimum conditions previously recorded by the system. The difference between these states is calculated by an advanced digital signal processor, and the inclination of the fixed mirror is changed continuously in order to eliminate any difference. This feedback is even provided during sample measurement. There is also an automatic adjustment for the interferometer that performs this operation.



**IRAffinity-1S**

Fourier Transform Infrared Spectrophotometer

## Easier Maintenance

# Ease of Maintenance Ensured by Built-in Auto Dryer

(JPN registration of utility model No. 3116465)

Beam splitters in the interferometers of FTIR instruments are susceptible to humidity. In order to maintain the long-term stability of the interferometer, the beam splitter must be protected. In the IRAffinity-1S, the interferometer is airtight and incorporates a unique internal auto dryer.

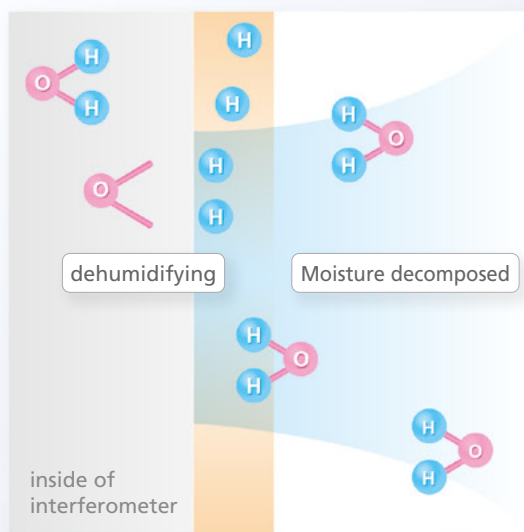
## Measures Taken to Protect the Optical Element in the Interferometer

- The interferometer has an airtight structure.
- Moisture inside the interferometer is continuously removed by an auto dryer.
- The beam splitter is coated with a moisture-resistant protective film.

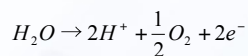
## Principle of the Auto Dryer

The IRAffinity-1S incorporates an auto dryer that electrolytically removes the moisture inside the interferometer using a solid polymer electrolyte membrane.

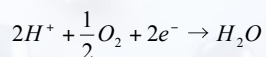
- When porous electrodes are attached to a solid polymer electrolyte membrane and direct current is applied, moisture on the anode side (i.e., the desiccation side) dissociates into hydrogen ions and oxygen.
- The hydrogen ions travel through the solid polymer electrolyte membrane and reach the cathode side (i.e., the moisture discharge side).
- At the cathode, the hydrogen ions react with oxygen in the air to form (gaseous) water vapor, which is released outside the interferometer.



Anode (desiccation side)



Cathode (moisture discharge side)



# Increased Reliability Achieved by Instrument Monitoring

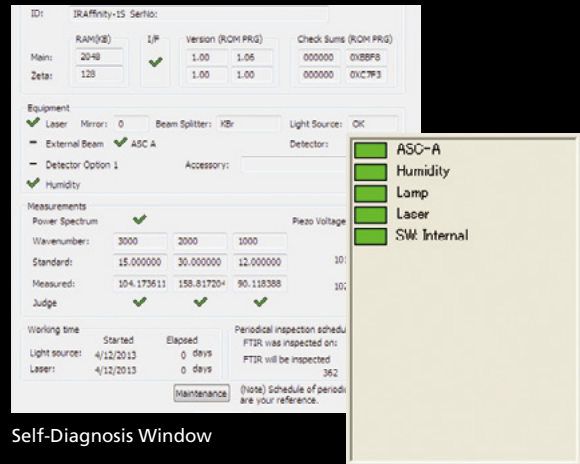
In order to increase reliability, not only does the IRAffinity-1S execute self-diagnosis at initialization, it also monitors the state of the instrument during operation. It is also possible to check basic performance using a validation program that is incorporated as a standard feature.

## Sequential Display of Diagnostic Results

The IRAffinity-1S executes self-diagnosis at instrument initialization, in which it checks the electrical, signalling, and optical systems. If the interference conditions are poor, they are adjusted and optimized using the dynamic alignment mechanism. Additionally, the light source, the He-Ne laser, humidity, information related to accessories, and the auto sample changer settings are continuously monitored by the status monitor function. If accessories are installed, they are automatically identified, and the optimum measurement conditions are set\*.

These diagnostic and monitor results are recorded in logs.

\* Only when QuickStart accessories are installed.



Self-Diagnosis Window

Status Monitor Window

## Validation Program

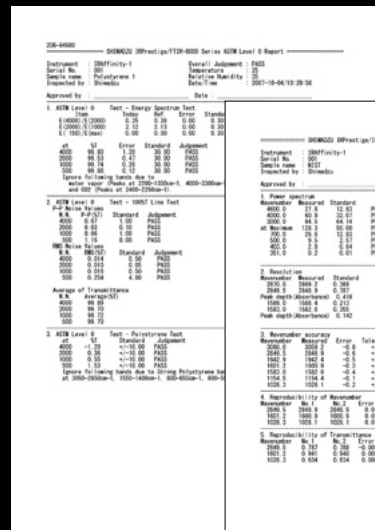
The IRAffinity-1S is equipped with a validation program that complies with the European and Japanese Pharmacopoeias and with ASTM (American Society for Testing and Materials). This validation program checks the basic performance of the instrument using a polystyrene film, and creates reports of the results.

• Test Items Complying with the European and Japanese Pharmacopoeias

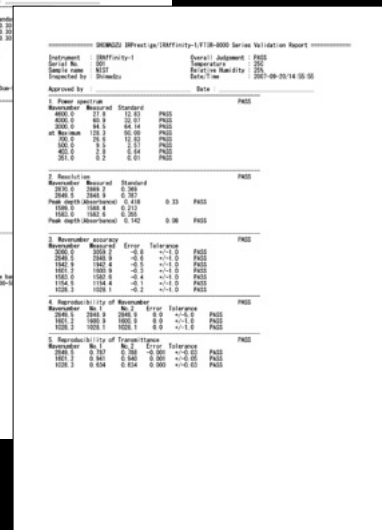
- Shape and intensity of a power spectrum
- The following items for a polystyrene spectrum:
  - Resolution
  - Wavenumber accuracy
  - Wavenumber reproducibility
  - Transmittance (absorbance) reproducibility

• Test items for ASTM (ASTM 1421 Level Zero)

- Energy intensity test based on power spectrum
- Noise test based on 100% transmittance spectrum
- Reproducibility test based on polystyrene spectrum



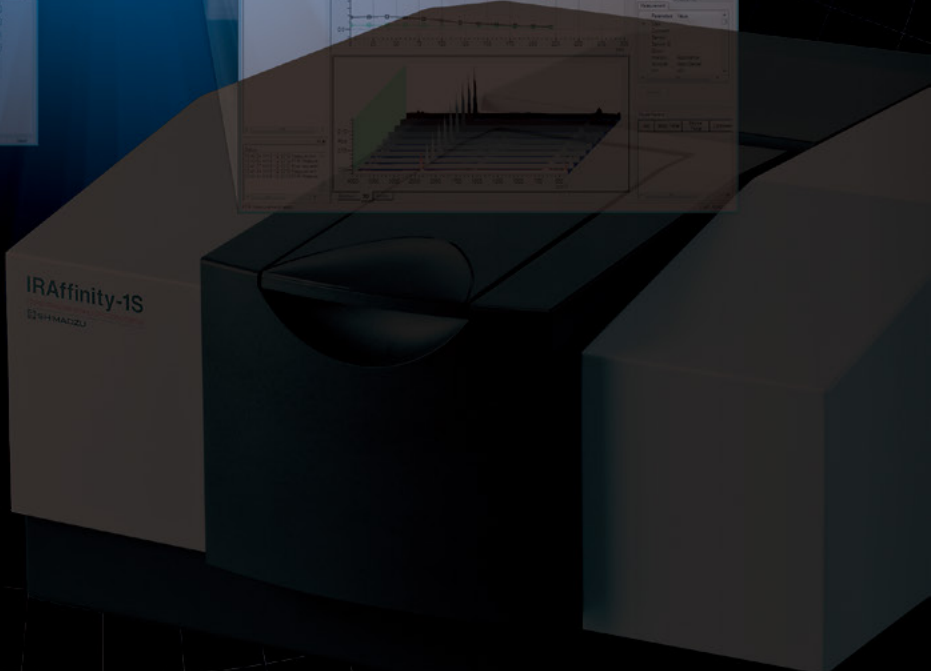
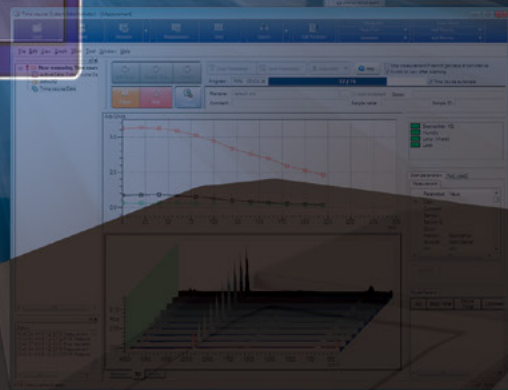
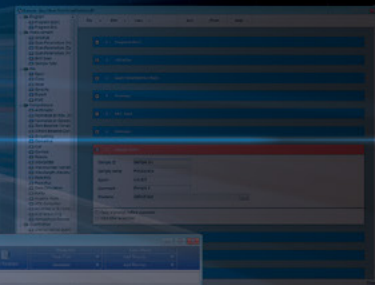
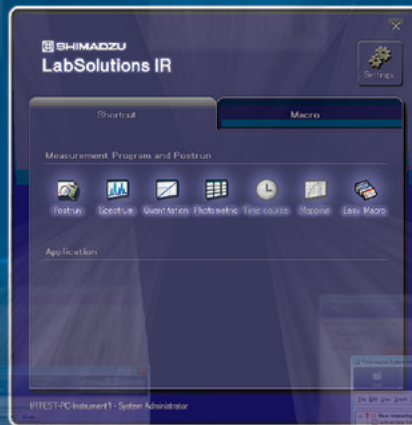
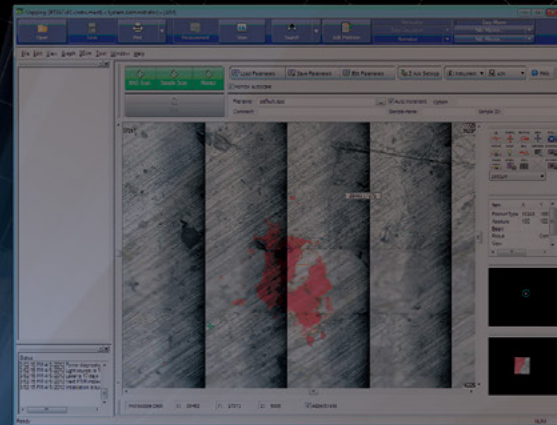
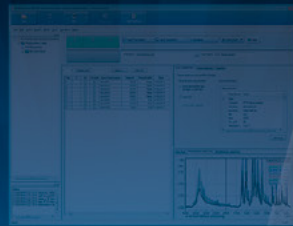
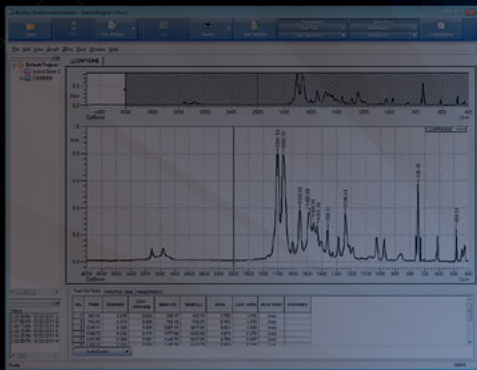
Example of ASTM report output



Example of Japanese Pharmacopoeia report output

# New Generation of Workstation

LabSolutions IR, a member of the LabSolutions family, has been optimized for network applications, includes an extensive library of spectra, and features a high-performance search function. In addition, Macro functions provide automation and labor savings.





# Fast, Easy-to-Use LabSolutions IR Series Software

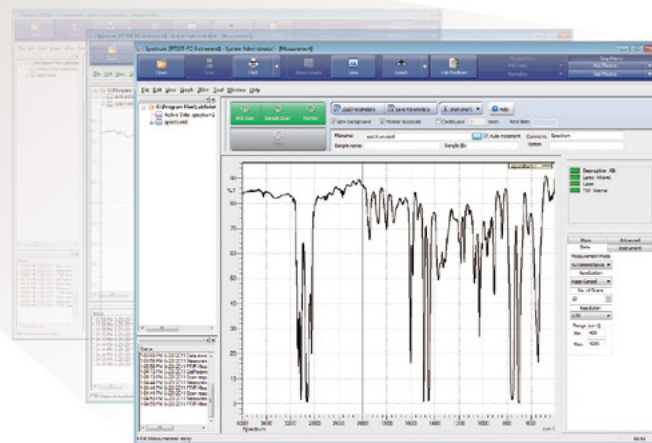
LabSolutions IR easily executes FTIR operations such as scanning, data manipulation, quantitation, reporting, saving, user administration, and more. High-level administrative functions and a variety of data manipulation functions provide for an easier, more user-friendly analysis environment. In addition, numerous optional programs are available to address all modern laboratory needs.



Launcher

## Run Dedicated LabSolutions IR Programs or Windows Applications Easily with the Dedicated LabSolutions IR Launcher.

LabSolutions IR includes a number of dedicated programs, including Postrun, Spectrum, and Quantitation, which are easily launched using the LabSolutions IR Launcher. In addition, macro programs and Windows applications can be registered with the LabSolutions IR Launcher for quick and easy start-up.



## Excellent Features of LabSolutions IR Series

### Network Features

- ▶ High-level security and user administration functions.
- ▶ Suitable for ER/ES regulations such as FDA 21 CFR Part 11, PIC/S, and more.
- ▶ Management of FTIR as well as LC and GC data by the server on a network. With terminal service, LabSolutions IR can be controlled from a client PC without installing LabSolutions IR on it.

### Extensive Spectra Library and High-Performance Search Function

- ▶ Features a library containing approximately 12,000 spectra.
- ▶ Enables high-quality searching with standard libraries.
- ▶ High-performance search methods, including Spectral, Text, Combination, and Peak searches.
- ▶ Shimadzu's unique search algorithm provides precise search results.

### Macro Program Functions Provide Automation and Labor-Savings

- ▶ Simply align steps to create a Macro program.
- ▶ Automated identification tests and contaminants analysis.

### Programs

- ▶ Postrun, Spectrum, Quantitation, Photometric, Time course (option), Mapping (option)
- ▶ All of the Postrun and measurement programs have a common Main toolbar, Menu, Measurement toolbar, Tree view, and Log window. The operation of each program is also similar, providing a familiar feel no matter what task you are working.

### Reporting

- ▶ Easy printing using the ViewPrint function and Free-layout reports.

### Data Manipulation

- ▶ A wide variety of data manipulation functions, including Advanced ATR correction and Kubelka–Munk conversion, and quantitation functions, such as the multi-point calibration curve method and CLS method, are standard.

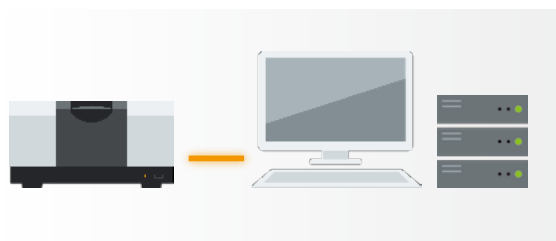
# Solutions Achieved with LabSolutions

## Reliable LabSolutions Software

In addition to LabSolutions IR, which provides basic functionality, Shimadzu also offers LabSolutions DB IR and LabSolutions CS IR to meet the requirements of ER/ES regulations.

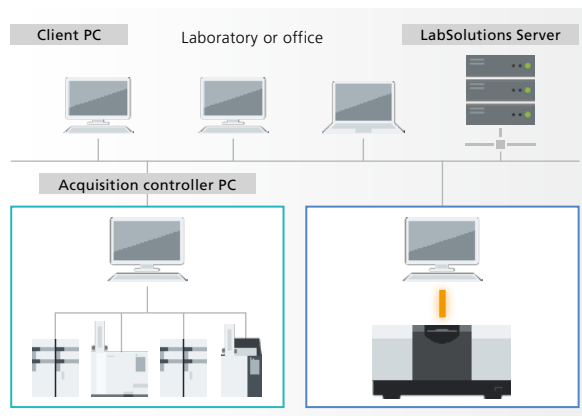
### LabSolutions DB IR

LabSolutions DB IR allows for secure data management by integrating a data management function with LabSolutions IR. Compliant with ER/ES regulations, the software is optimally configured for customers using a PC. It is recommended for facilities that do not require network connections and want to be ER/ES compliant.



### LabSolutions CS IR

LabSolutions CS, which is freely accessible to the analysis network, can be connected to IR, eliminating the need for connecting a PC to the instrument. Since all the data are managed on a server, LabSolutions CS IR can be read from any personal computer on a network. With terminal service, LabSolutions IR can be controlled from a client PC without installing LabSolutions IR on it. It is recommended for facilities that have a large number of users, manage data in a database, and want to be ER/ES compliant.



Name	LabSolutions IR	LabSolutions DB IR	LabSolutions CS IR
Data management method	Measured data files are saved and managed in folders on the PC.	Measured data files are saved and managed in the LabSolutions database.	
Data references	The software references files on drives or in folders on the PC.	The software references files in the database.	
LabSolutions database	Unavailable	Available (The database resides on a local PC)	Available (The database resides on a server)
User administration		Available	
Rights group administration		Available	
Project administration	Unavailable	Available	
Standalone/network	Either can be used.	Only the standalone configuration can be used.	Only databases on the network can be used. (LabSolutions IR data can be viewed using the database manager on a PC set up for viewing purposes. Note that LabSolutions IR must be installed on the PC used for viewing.)
Data backup	Performed on a file-by-file basis using Windows Explorer.	Performed for each database.	

Operate with LabSolutions, Shimadzu's reliable and popular workstation used in chromatography and spectroscopic analysis.



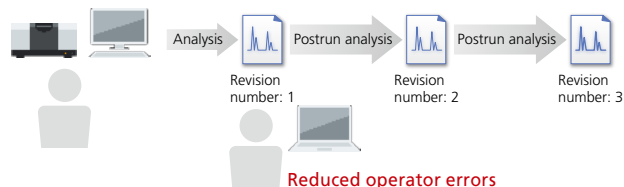
Spectral Measurement Screen



## Database Management Prevents Mistakes

With LabSolutions DB IR and CS IR, the analysis data are managed securely by the database. Overwriting, deletion and other mistakes typical of data file management do not occur.

In addition, when postrun analysis is performed using the acquired data, postrun analysis data revision numbers are automatically assigned, preventing the accidental overwriting of raw data.



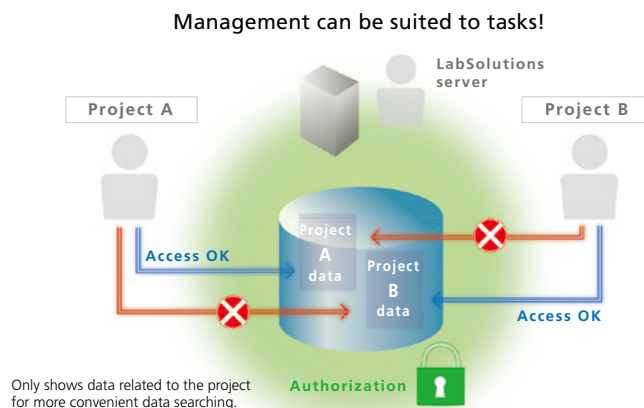
## Solid Security

An audit trail to ensure the reliability of data and document e-mail transmission functions when any event occurs in the system can be set up. User accounts are managed using passwords, where password length, complexity and term of validity must satisfy specified requirements. It is

also possible to set lockout functions to prevent illegal access, and set a registered user's deletion and change. In addition, a box can be selected to prevent overwriting a data file, and outputting an item to a report can also be performed.

## Pertinent Information is Managed for Every Project

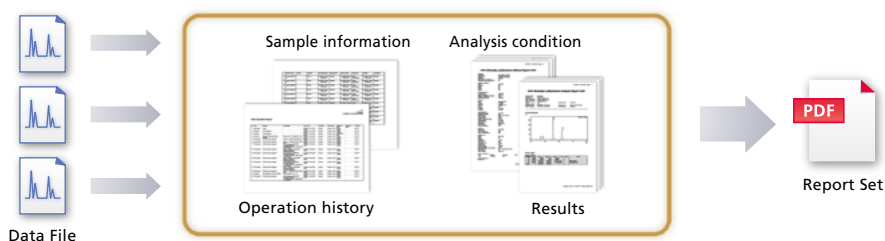
LabSolutions DB IR and CS IR provide a project management function enabling management suited to tasks and system operations. This function enables equipment and user management, security policy, and data processing to be set on a project by project basis, thereby improving the efficiency of data searches and management tasks.



## Visualization of the Sequence of Analysis Operations

Creating a report set\* provides visibility of the individual analytical operations involved in the overall analytical process. When analytical operations are visible, it is easier to check for operating errors, which helps improve the efficiency and reliability of checking processes.

\* Report sets include test methods and test results for a series of samples analyzed, and also a corresponding operation log (a record of all operating events from login to logout), which is automatically extracted from the data and summarized in a single report.

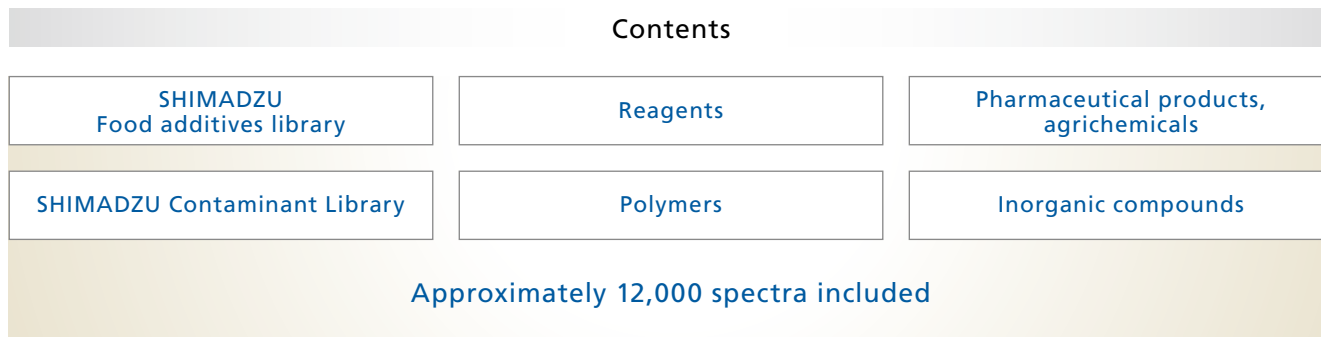


# Extensive Spectra Library and a High-Performance Search Function

Features a library containing approximately 12,000 spectra. Enables high-quality searching with standard libraries.

## Approx. 12,000-Spectra Library

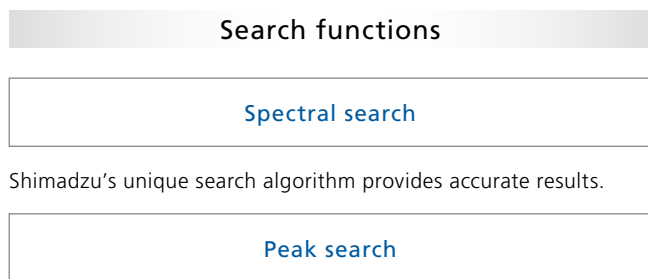
A wide variety of libraries, including Shimadzu's unique libraries, reagents, polymers and more, is included standard. Searching with standard libraries provides high-quality search results without purchasing extra libraries.



## High-Performance Search Functions

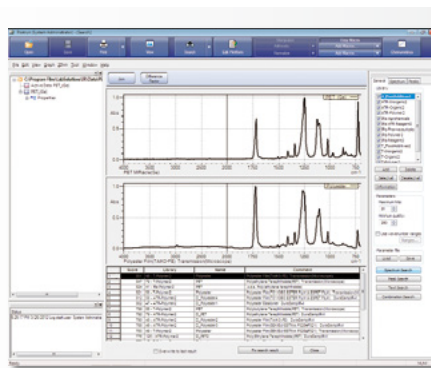
Obtain high-quality search results with four high-performance search methods (spectral search, peak search, text search and combination search) and a library containing 12,000 spectra. Libraries created on IRsolution and HYPER-IR and commercial

libraries such as Sadtler and S.T. Japan can also be used. Simply dragging spectra into a library creates a user library. In addition, editing spectral information or deleting a spectrum is very easy.



Shimadzu's unique search algorithm provides accurate results.

If you only have an old spectrum chart, searching can be performed with peak wavenumbers without a spectrum file.



## Other Optional Libraries

### ▶ Contaminant Library for LabSolutions IR

This is Shimadzu's latest original library. It is an effective tool for analyzing contaminants in tap water and food. In addition to containing information on actually sampled contaminants and information about commercially available water supply maintenance parts, the library also includes X-ray fluorescence profiles (PDF files) and significantly improves the accuracy of contaminant searches. Unlike existing libraries, this contains data on mixed compounds and incorporates all the depth of knowledge and wide experience needed to make qualitative assessments.

### ▶ Thermal-Damaged Plastics Library\*

Unlike existing libraries, this library contains data of degraded plastics that have been oxidized by heating. The library demonstrates its effectiveness when the contaminants include degraded substances, as is often the case.

\* The library was compiled by Shimadzu Corporation from spectra measured and acquired by the Hamamatsu Technical Support Center, Industrial Research Institute of Shizuoka Prefecture.

# Contaminant Analysis Program

By combining Shimadzu's own algorithms (patent pending) with that of library spectra for common contaminants, this program identifies contaminants with a high degree of accuracy. Reports are automatically created after analysis, thereby reducing post-processing time to a few seconds.

With automated reporting, this easy-to-use program allows operators with little FTIR knowledge to perform analysis easily.

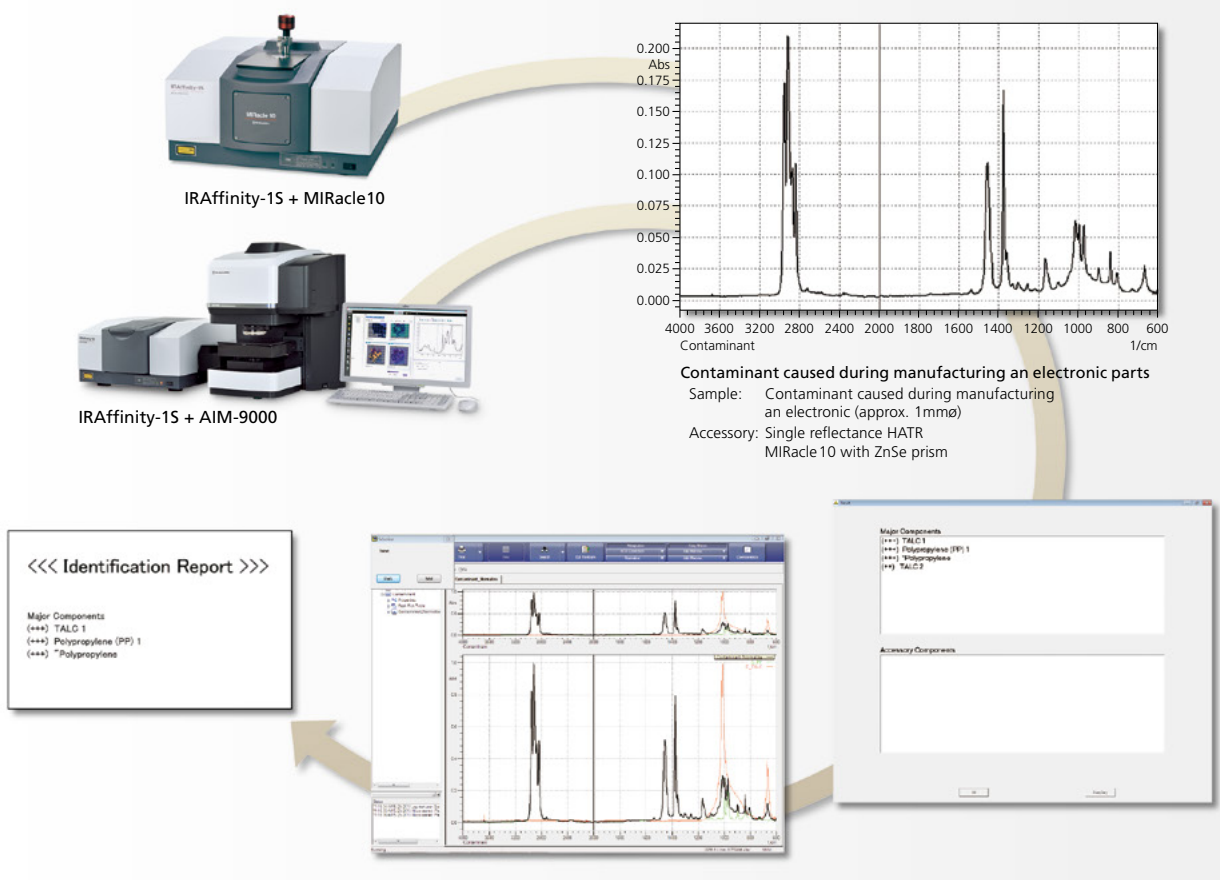
## 4 features of the Contaminant analysis program

Contains spectra for over 500 highly-selected inorganic substances, organic substances, and polymers that are often detected as contaminants in Shimadzu's Analytical Applications Department.

Allows automation of the process, including searching, judgment evaluation, and report creation.

Incorporates algorithms that focus on spectral characteristics, rather than performing simple spectrum searches.

Major and Minor components are found and their ranks are displayed.



# Automation and Labor-Savings with Macro Program Functions

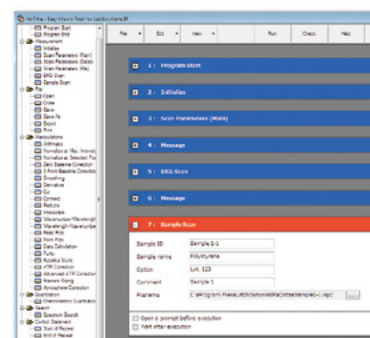
LabSolutions IR automates routine work, such as scanning, data manipulation, reporting, identification tests, and contaminants analysis. Launch programs from the Launcher or your PC desktop.

With LabSolutions IR, the following analysis operations can be automated for more labor-saving by using macro programs.

- ▶ **Routine tasks: Measurement, peak detection, and printing**
  - Common routine tasks for IR analysis performed with just one click
  - Identification tests for Pharmacopoeia and Food Additives standards
- ▶ **Japanese Pharmacopoeia and food additive identification tests**
  - Automate pass/fail judgment of test samples
- ▶ **Contaminant analysis**
  - Easy and quick contaminant analysis. Just a few seconds until the results are output
- ▶ **Validation program that complies with the Japanese, European, Chinese, and United States Pharmacopoeias, and with ASTM standards**
  - Easy undertaking of instrument inspections in accordance with official regulations

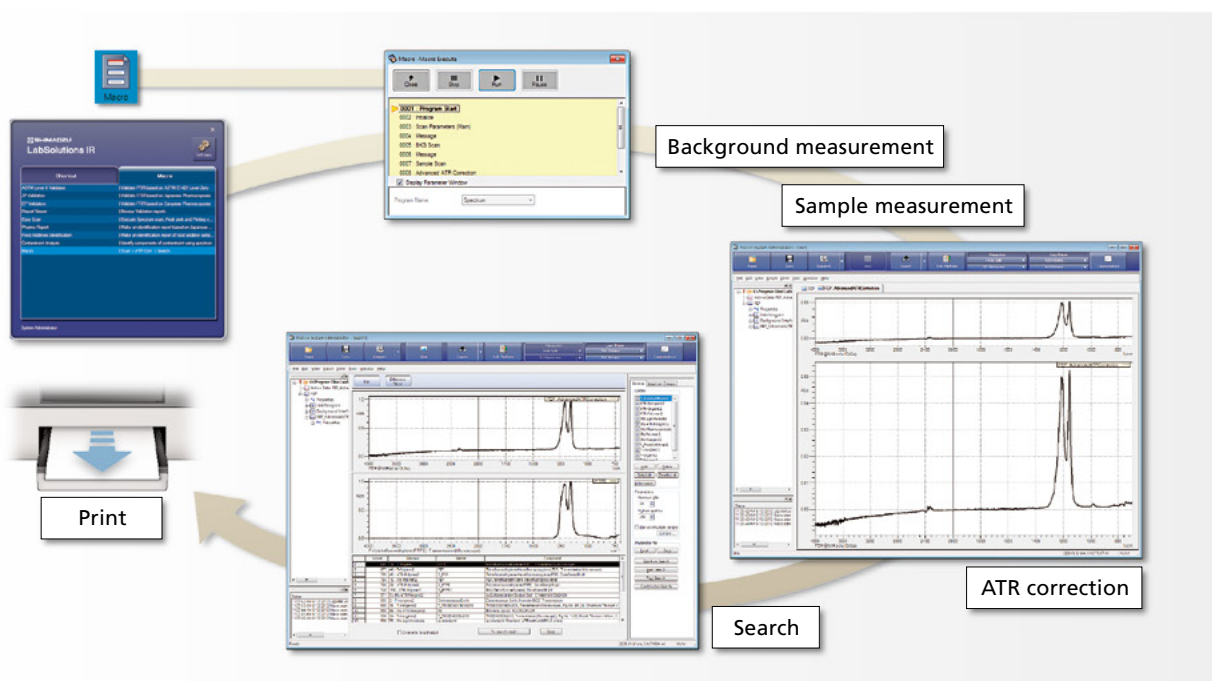
## Easy Macro — Just a Single Click Launches Routine Work

The "Easy Macro" function will create macros that are suitable for routine work, particularly when repetitive operations are used. The macro builder allows macros to be constructed by simply selecting and aligning operations from a list. Once constructed, the macros can be registered with the Launcher and desktop for quick execution. Operators who are not familiar with FTIR can easily operate the instrument.



### Easy Macro Operations

- ▶ Initialization of FTIR, configuration of scan parameters, spectrum measurement
- ▶ Data manipulations, search, quantitation, printing
- ▶ Repeat measurements, displaying messages, alarm sounds, external program execution



# Identification Tests

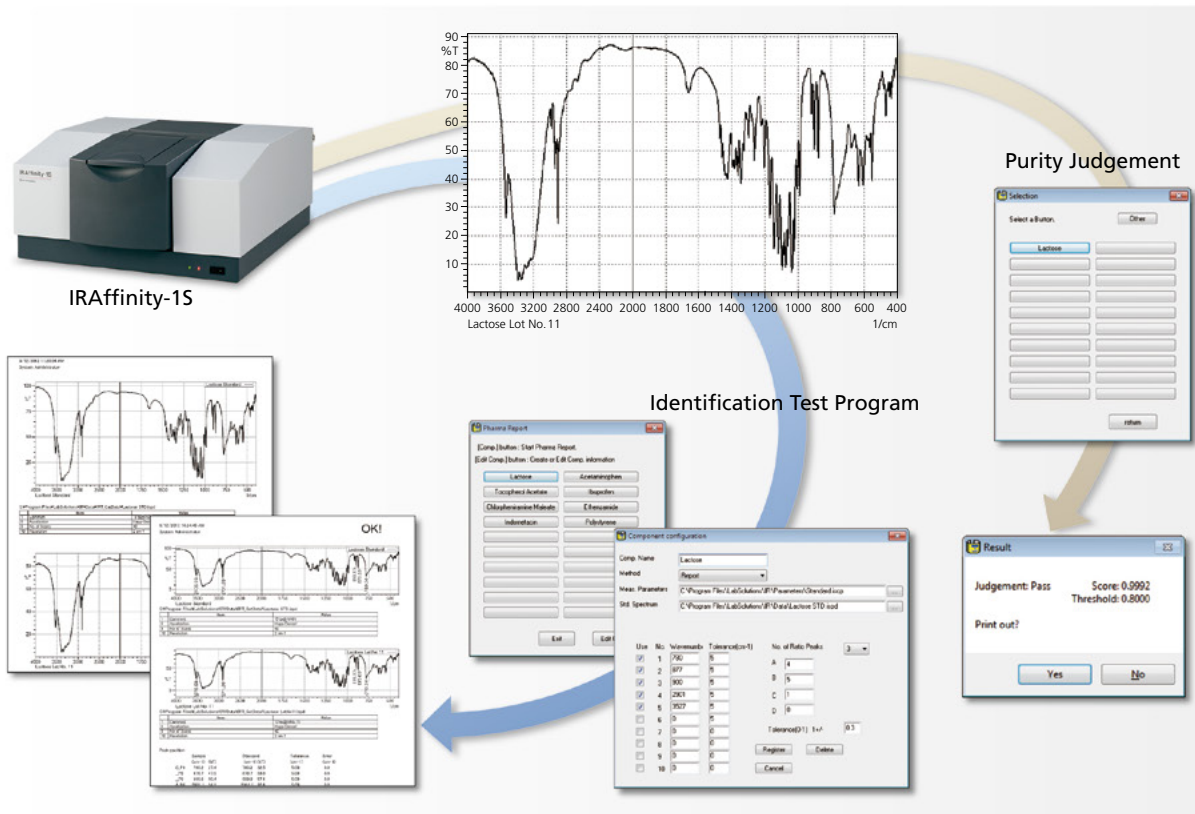
Two methods are used for Identification tests; a method performed in accordance with tests specified in the Pharmacopoeia and other standards, and a method using spectrum matching for judgments.

## Identification Testing Program

This program makes pass/fail judgments for test samples based on verification methods as described in the Pharmacopoeia and standards in each country such as "Infrared Spectrophotometry" in the Japanese Pharmacopoeia and Food Additive Standard. In addition to identification tests for pharmaceutical and food products identification tests, the program can also be used for incoming inspections and pre-shipment inspections.

### 4 features of the Identification test program

<p>Prints out the spectra for standards and samples in order to facilitate easy comparison.</p>	<p>Calculation of the differences between the peak wavenumbers for standards and samples, differences in intensity ratios between peaks, pass/fail judgments, and print out of reports.</p>
<p>Detection and printing just the peaks that are specified for pass/fail judgment.</p>	<p>Spectra of 57 samples on Japanese Standards of Food Additives are stored in LabSolutions IR.</p>



## Purity Judgement

The Purity Judgement calculates the similarity (Purity) between a reference spectrum and a test spectrum, and judges Pass or Fail. It judges similarity of spectra in a quantitative way.



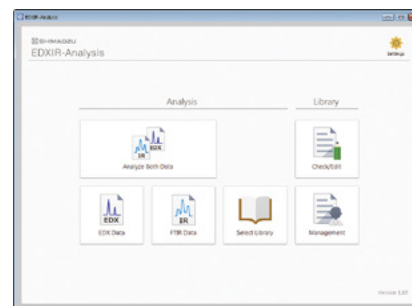
# EDXIR-Analysis Software (Option)

EDXIR-Analysis software is specially designed to perform qualitative analysis using data acquired by an energy dispersive X-ray (EDX) fluorescence spectrometer and a Fourier transform infrared spectrophotometer (FTIR).

This software is used to perform an integrated analysis of data from FTIR, which is excellent at the identification and qualification of organic compounds, and from EDX, which is excellent at the elementary analysis of metals, inorganic compounds and other content. It then pursues identification results and the degree of matching. It can also be used to perform EDX or FTIR data analysis on its own.

The library used for data analysis (containing 485 data files) is original to Shimadzu, and was created through cooperation with water supply agencies and food manufacturers.

Additional data can be registered to the library, as can image files and document files in PDF format. It is also effective for the linked storage of various types of data as electronic files.



## Integrated Analysis of Contaminant Data and Data Comparisons for Confirmation Tests

To perform qualitative analysis automatically, simply click "Analyze Both Data" and select the EDX/FTIR data\*1. This heightens the efficiency of data analysis and provides strong support for contaminant analysis.

In addition to a list of hits, the integrated data analysis results show EDX profiles and FTIR spectra found as hits from the library. If the user wishes to browse the respective data analysis results, they can be checked by clicking "Single".

In addition, with the data comparison function, which calculates the degree of matching between the actual measured data and the data registered in the library, the software can be used for countermeasures against "silent change"\*2 and for other confirmation tests.

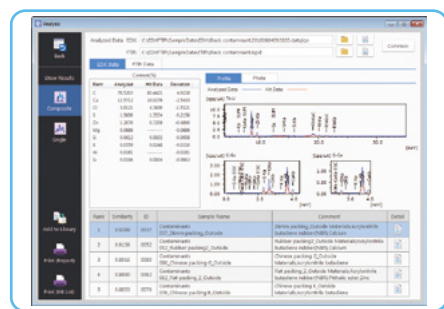
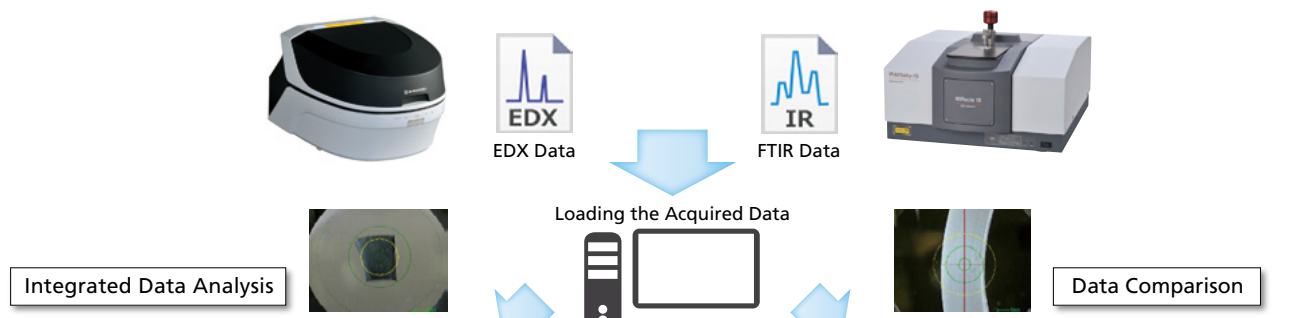
Clicking the "Print" button prints the results in a fixed format and also saves them in Word format\*3.

The examples here show an integrated analysis of black rubber contaminant data and a data comparison for a polyvinyl chloride (PVC) examination object and the standard product. From the integrated data analysis results, it is evident that the black rubber contaminant is acrylonitrile-butadiene rubber (NBR), which contains calcium carbonate and zinc stearate. In addition, from the data comparison, the degree of matching between the PVC examination object and the standard product is 0.8506. Lead (Pb) and acrylic were detected from the EDX and FTIR data, but not detected in the standard product. Accordingly, it is surmised that the examination object contains components different to those in the standard product.

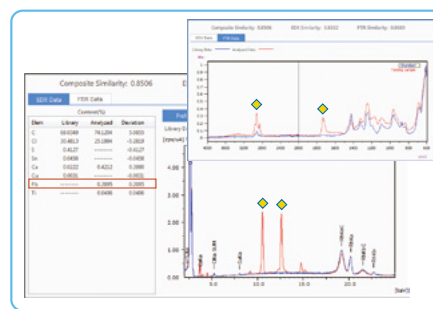
\*1: Using the EDX profile, data are classified as inorganic, organic, and mixture. Integrated data analysis is performed by applying priority levels to each classification. (Patent pending)

\*2: A term used in Japan to indicate changes to materials by suppliers without the knowledge of the manufacturers.

\*3: Microsoft Word must first be installed.



Integrated Data Analysis Results for a Black Rubber Contaminant

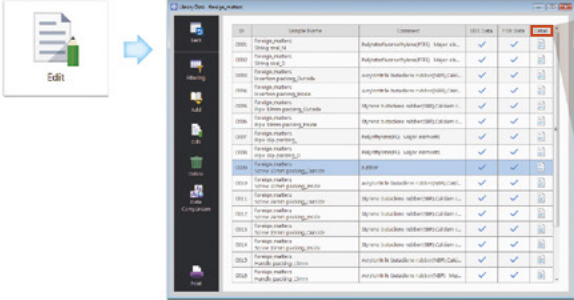


Data Comparison Results for a PVC Examination Object and the Standard Product



## Data Browsing and the Registration, Editing, Deletion of Data, Images, Document Files

By clicking "Edit" and selecting an existing library, the data, images and documents registered in the selected library can be browsed. Data can be newly registered, edited and deleted. A new library can also be created. In addition, if data for a sample were acquired by instruments other than EDX and FTIR instruments (such as a chromatograph, mass spectrometer, or surface observation system), it can be converted into PDF format and then registered, enabling linked storage to the EDX/FTIR data.



**Edit**

ID	Sample Name	Comment	EDX Link	FTIR Link
0000	For sample analysis			
0001	Sample analysis			
0002	Sample analysis			
0003	Sample analysis			
0004	Sample analysis			
0005	Sample analysis			
0006	Sample analysis			
0007	Sample analysis			
0008	Sample analysis			
0009	Sample analysis			
0010	Sample analysis			
0011	Sample analysis			
0012	Sample analysis			
0013	Sample analysis			
0014	Sample analysis			
0015	Sample analysis			
0016	Sample analysis			
0017	Sample analysis			
0018	Sample analysis			
0019	Sample analysis			
0020	Sample analysis			

**Photographs, Document Files, Comments, and Other Information**

**EDX Profiles, Quantitation Results, EDX Photographs, Comments, and Other Information**

**Browsing Registered Photographs**

**Browsing Document Files**

**FTIR Spectra and Comments**

**All Data Are Linked and Stored**

## Sample Holder/Stocker for Contaminant Measurement EDXIR-Holder (Option)

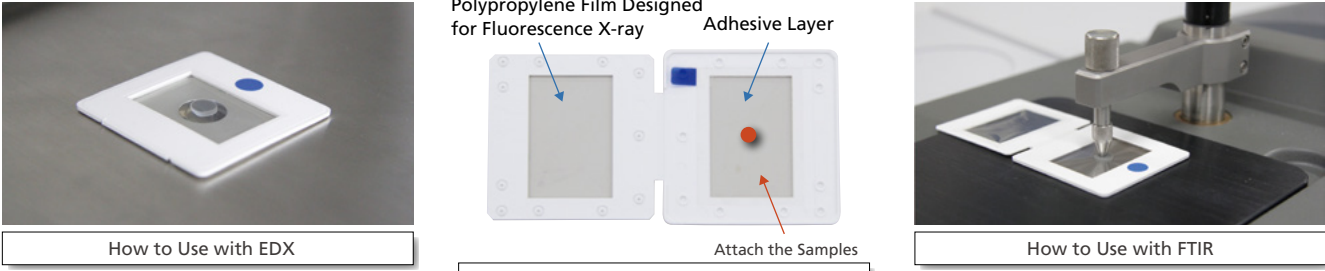
Measure the Samples Kept in the Holder with EDX and FTIR  
The Holder Can Be Used as the Sample Stocker after the Measurement

### Enables More Efficient Analyses

This foldable holder consists of adhesive layer with samples attached and polypropylene film designed for fluorescence X-ray. When using EDX for measurement, close the holder and place the polypropylene film directly to the irradiation side (downside). When using FTIR for measurement, open the holder and press the samples attached to the adhesive layer against the ATR prism. This enables the replacement of samples, at a minimum, saving on labor and making analysis more efficient.

### Prevents Loss of Samples

Close the holder after the measurement and it can be used as a sample stocker. It is not necessary to transfer the samples to other containers, so there is no danger of losing samples.



**Polypropylene Film Designed for Fluorescence X-ray**

**Adhesive Layer**

**Attach the Samples**

**How to Use with EDX**

**How to Use with FTIR**

**When the Holder is Open (Inside of the Holder)**

**Close the holder and place the polypropylene film to the irradiation side (downside).**

**Open the holder and press the samples attached to the adhesive layer against the prism.**

# Software Options

LabSolutions IR incorporates data processing functions such as Advanced ATR correction and Kubelka–Munk conversion, quantitation functions such as the multi-point calibration curve method and the CLS method, as well as the spectral searching function as standard features. However, adding the following optional software products makes it possible to further increase the application range.

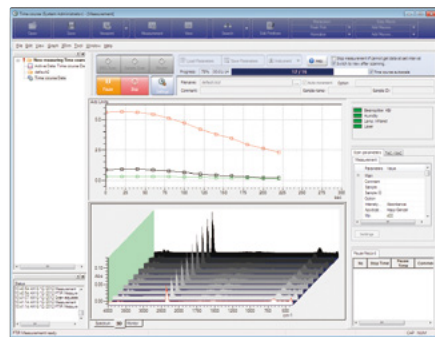
LabSolutions IR

## Time course software

(P/N 206-74558-91)

The time course program is used to collect spectra in regular intervals and creates a time course dataset used to follow reactions as a function of time. Changes in peak height and peak area can be used to calculate values related to reaction kinetics. Time course information is saved and displayed in 3D (bird's eye view) or in a contour plot. It can be recalculated by modifying parameters.

The scan interval is dependent on resolution, number of scans and mirror speed. The fastest speed under a  $16\text{cm}^{-1}$  resolution and a mirror speed of  $9\text{mm/s}$  is 7 seconds for 1 accumulated scan. Maximum measurement time is 48 hours but it depends on scan parameters. The time course software includes a 3D Processing program.



LabSolutions IR

## Mapping program

(P/N 206-74559-91)

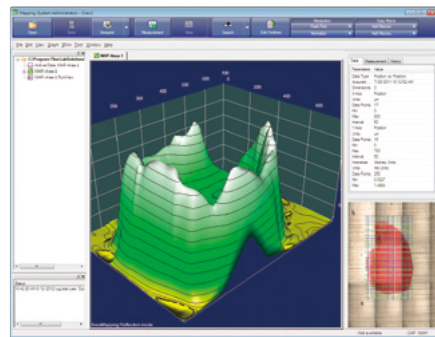
The Mapping software allows one to map absorption information on a sample surface as a function of position when using the Shimadzu AIM-8800 Infrared Microscope.

Mapping parameters, such as the mapping range, the scan intervals, and the background positions, can be set on the composite images. Area mapping, line mapping and random mapping modes are supported.

In addition to mapping in the conventional transmittance and reflectance modes, micro-ATR mapping with an optional ATR objective is also available. From the acquired mapping data, it is possible to extract spectra and to perform calculations for functional-group mappings for specific peaks. The data can be displayed as 3D images or contour plots, or in spectral overlay mode.

Mapping program includes a 3D Processing program.

AIMsolution Mapping Program (P/N 206-32936-41) is necessary when mapping in combination with Shimadzu AIM-9000 Infrared Microscope.



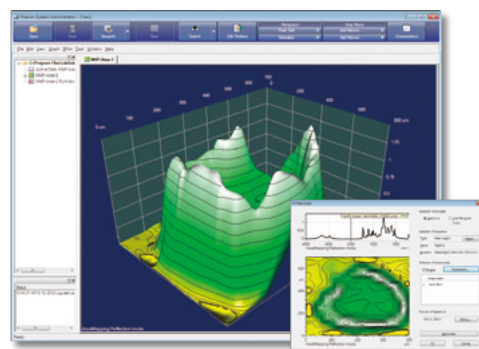
LabSolutions IR

## 3D processing program

(P/N 206-74563-91)

The 3D processing program offers the following functionality

- ▶ **Changes the method of displaying data**
  - Data can be displayed in bird's eye view (3D), as an intensity distribution or using contour lines, as a spectral overlay, or rotated.
- ▶ **3D data processing**
  - Changes at specific wavenumbers can be isolated.
  - Functions include data extraction, data points thinning, smoothing, zero-baseline, background correction, normalization, log conversion, first- or second-order derivative, and ATR correction.
- ▶ **Creation of 3D data from spectra**
  - Spectra measured at fixed intervals, such as by repeated measurements, can be arranged consecutively to create 3D data.



Note: The 3D processing program cannot control mapping measurements or AIM-8800 series infrared microscopes.

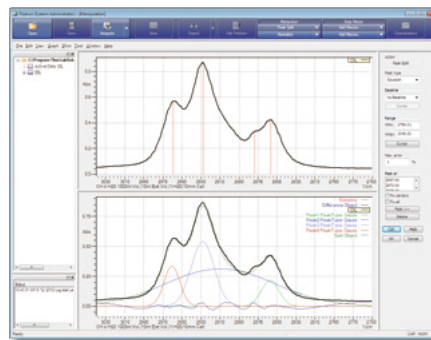
LabSolutions IR

## Curve-fitting (Peak-splitting) program

(P/N 206-74561-91)

Usually, absorption bands in infrared spectra consist of overlapping peaks. The curve-fitting (peak-splitting) program can be used to separate absorption bands into individual peaks, separate peaks that have been influenced by hydrogen bonding, and identify the peaks of functional groups that are hidden by absorption bands. Six types of curves, such as Gaussian, Lorentzian, and Gaussian+Lorentzian, are available for separation analysis.

The curve can be selected in accordance with the form of the peaks in the absorption band. The separated component peaks are displayed together with the resultant spectra, making it possible to accurately evaluate the separation.



LabSolutions IR

## PLS quantitation program

(P/N 206-74560-91)

PLS (partial least squares) quantitation is a chemometrics method that, like multiple linear regression analysis, is widely used for the simultaneous quantitation of multiple components. The PLS quantitation program incorporates PLS I and PLS II methods. It is possible to display calculation values based on input values. PLS factors are based on "PRESS" values, loading vectors, and score values. Analysis can be performed on the regression equations obtained with the PLS method.

LabSolutions IR

## Macro platform

(P/N 206-74562-91)

The Macro Platform is required to run the customized macro programs created by Shimadzu (for a fee). If, for example, you wish to perform routine work in which certain functions are used in a pre-determined order, or you wish to run an automatic measurement system in combination with an auto sample changer, please contact your SHIMADZU representative for details.

## Contaminant Library for LabSolutions IR

(P/N 206-30390-91)

This is Shimadzu's latest original library. It is an effective tool for analyzing contaminants in tap water and food. In addition to containing information on actually sampled contaminants and information about commercially available water supply maintenance parts, the library also includes X-ray fluorescence profiles (PDF files) and significantly improves the accuracy of contaminant searches. Unlike existing libraries, this contains data on mixed compounds and incorporates all the depth of knowledge and wide experience needed to make qualitative assessments.

## Thermal-Damaged Plastics Library\*

(P/N 206-33039-91)

Unlike existing libraries, this library contains data of degraded plastics that have been oxidized by heating. The library demonstrates its effectiveness when the contaminants include degraded substances, as is often the case.

\* The library was compiled by Shimadzu Corporation from spectra measured and acquired by the Hamamatsu Technical Support Center, Industrial Research Institute of Shizuoka Prefecture.

## A Wide Range of Accessories

If an accessory is installed in the sample compartment, the name and identification (machine) number of the installed accessory is displayed in LabSolutions IR.

In addition to being displayed on the status monitor, it is also recorded in the log file.

The optimum measurement parameters for the installed accessory are automatically set.

This is a series of horizontal ATR accessories integrated with sample compartments. The ease of purging has been improved, and there is no concern with dust entering the IRAffinity-1S sample compartment.



### MIRacle 10

(P/N 206-74127-XX)

This is a single-reflection ATR accessory. To measure the spectrum of a liquid, simply drip it on the prism. To measure the spectrum of the surface of other samples, clamp them firmly on the surface of the prism. Large samples (with a large surface area) can be measured without cutting them. The incidence angle is 45°.

Select from three types of prism: ZnSe, Ge, and diamond/ZnSe. Also, select whether the respective prism is equipped with a pressure sensor. The Ge prism is ideal for samples with a high refractive index.



(P/N 206-74128-91)

### GladiATR 10

(With pressure sensor P/N 206-74128-93)

This is a single-reflection ATR accessory. Since the prism is made solely of diamond, it is capable of measuring spectra up to 400  $\text{cm}^{-1}$ . To measure the spectrum of a liquid, simply drip it on the prism. To measure the spectrum of the surface of other samples, clamp them firmly on the surface of the prism. The incidence angle is 45°. Select whether the prism is equipped with a pressure sensor. The Ge prism is ideal for samples with a high refractive index.



(P/N 206-74126-91)

### HATR 10

This is a horizontal ATR accessory. There are prisms for liquids and solids. To measure the spectrum of a liquid sample, simply drip it on the prism. To measure the spectrum of the surface of film and rubber samples, clamp them firmly on the surface of the prism. The incidence angle is 45°, and the number of reflections is 10. The ZnSe prism is included as standard, but the Ge prism is ideal for samples with a high refractive index.



## DRS-8000A

(P/N 206-62301-58)

Although powder samples are mixed with KBr, as with the KBr pellet method, they are analyzed in their original state. It is not necessary to create pellets. For plastic moldings, part of the surface is scraped off with the emery paper attached to the SiC sampler (P/N 200-66750), and the powdered sample formed on the paper is analyzed. Diffuse reflectance spectra that are similar to transmittance spectra are produced by Kubelka–Munk conversion.



Powders



Moldings



SiC Sampler  
(Option)

## SRM-8000A

(P/N 206-62304-91)

A specular reflectance accessory with a 10° incidence angle is used for the analysis of thin films on a metal plate with a mm order of thickness. In the case of mirror-like plastic samples, the light specularly reflected from the sample surface is measured. Specular reflectance spectra that are similar to transmittance spectra are produced by Kramers–Kronig analysis.



Thin Films



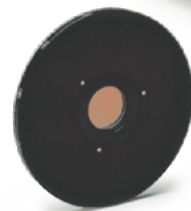
## RAS-8000A

(P/N 206-62302-91)

A high-sensitivity reflection measurement accessory with incidence angles of 70° and 75° is used for the analysis of thin films on a metal plate with an nm order of thickness. Using it in combination with the GPR-8000 infrared polarizer (P/N 206-61550) enables measurement with an even higher level of sensitivity.



Thin Films



GPR-8000  
(Option)

## ATR-8000A

(P/N 206-62303-91)

This accessory obtains spectra for the surfaces of film-like samples that are clamped firmly on the surface of a prism. Incidence angles of 30°, 45°, and 60° can be selected. The KRS-5 prism is standard.

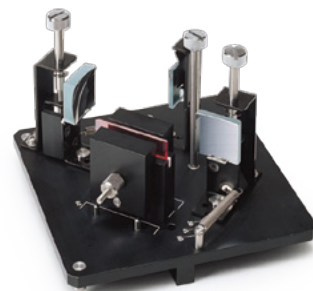
A Ge prism is also available for samples with a high refractive index.



Films



Rubber



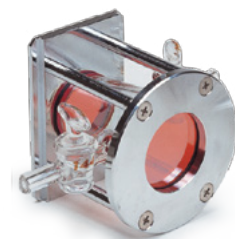
\* ATR spectra similar to transmittance spectra are produced by ATR correction.

**5-cm Gas Cell**  
**10-cm Gas Cell**  
**Long-Path Gas Cell**

(P/N 202-32006-XX)

(P/N 202-32007-XX)

Gas cells are used for the analysis of gas samples, and the path length is selected according to the concentration. There are gas cells with short path lengths of 5 or 10 cm, and long path lengths of 10 m or more. Please contact your Shimadzu representative for details on long-path gas cells.



5-cm gas cell



Long-path gas cell



Gases

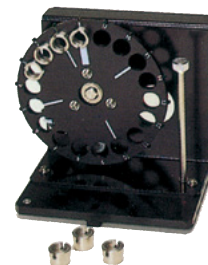
**Accessories for Automated Analysis**

An automatic measurement system can also be configured using an autosampler. The autosampler is controlled by LabSolutions IR.

**ASC-8000T**

(P/N 206-63900)

An auto sample changer that can perform automatic transmission measurement for up to 18 KBr pellets with a diameter of 13 mm. Film holders and cell plates for Nujol mulls are available as options.



Powders

Films

Liquids

**DRS-8010ASC**

(P/N 206-62308)

An automatic diffuse reflectance accessory that can automatically analyze up to 24 powder samples.



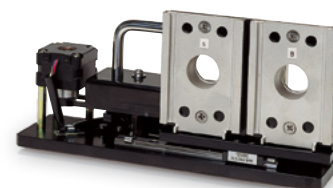
Powders

**Sample Switcher 21**

(P/N 206-63663-92)

Transmission-type sample switcher that switches between the sample and the background.

Note: This accessories is not applicable CE marking. Please check with your Shimadzu representative for detail.



Powders

Films

Liquids

\* An optional ASC cable is required.



Minute Samples

## Accessories for Minute Samples

A single-reflection ATR accessory is useful for the analysis of sample sizes of the order of a few mm. The sample is taken out, placed on a prism, and firmly secured with the clamp provided.

An infrared microscope is useful for the analysis of sample sizes from a few mm down to approximately 10  $\mu\text{m}$ .

In addition to transmission and reflection modes, the ATR mode is also available, enabling the analysis of various forms of minute samples.

### Infrared Microscope AIM-9000

(P/N 206-32000-58 (Narrow band MCT))

The AIM-9000 incorporates a bright, optimized optical system and a high-sensitivity MCT detector. Not only enabling high-sensitivity measurement of micro samples, but the system has also been automated to ensure all steps involved in micro analysis can be performed quickly and easily.

#### Features of the AIM-9000

- Incorporates a bright, optimized optical system and a high-sensitivity MCT detector to enable high-sensitivity measurement.
- Enables reflection/ATR measurements on samples up to 40 mm thick.
- Comes with a digital zoom function of up to 330 $\times$  magnification using the wide-view camera (optional) and the microscope camera. Enables the measurement position to be quickly determined.
- Includes an automatic contaminant recognition system that automatically determines the measurement position as a standard feature.
- Up to 60 measurement position can be recorded.
- Includes a contaminant analysis program to identify the cause of failures as a standard feature.



Note: In order to use this attachment, an external beam extraction kit (P/N 206-32570-42), an AIM connection kit (P/N 206-32607-42), and accessories for the AIM-9000 (P/N 206-32799-41) are required.

### ATR Objective

(Ge prism: P/N 206-32600-41)

This objective lens is used when performing ATR measurements with the AIM-9000 infrared microscope. Using a cone-type prism, this single reflection objective features 15 $\times$  magnification and a 45-degree mean incident angle. The slide-on type prism makes it easy to switch back and forth between visible observation and infrared measurement.



### Mapping Program (AIMsolution)

(P/N 206-32936-41)

The mapping program measures the absorption distribution on the surface of a sample and creates imaging data when used with the AIM-9000 infrared microscope.

It allows setting of mapping parameters, such as the mapping range, the scan intervals, and the background positions, on the composite visible images. It also supports area mapping and random mapping modes. In addition to mapping in the conventional transmittance and reflectance modes, micro-ATR mapping is also available. (An optional ATR objective is required. It also requires a separate pressure sensor.) From the acquired mapping data, it is possible to extract spectra and to perform calculations for specific peaks and functional group mapping by multivariate analysis.

## Other Accessories

In addition to Shimadzu genuine accessories, unique FTIR accessories from all over the world can be used with the IRAffinity-1S. Please contact your Shimadzu representative about accessories that are not listed in this brochure. We will provide details on accessories that are appropriate for specific samples and applications. Also, note that it may not be possible to use the previous FTIR-8000 series accessories. If necessary, please check with your Shimadzu representative.

## Specifications

### Hardware

<b>Interferometer</b>	Michelson interferometer (30° incident angle) Equipped with dynamic alignment system Sealed interferometer with auto dryer
<b>Beam splitter</b>	Germanium-coated KBr
<b>Light source</b>	High-energy ceramic light source with 3 years guaranteed
<b>Detector</b>	DLATGS detector equipped with temperature control mechanism
<b>Wavenumber range</b>	7,800 to 350 cm <sup>-1</sup>

<b>Resolution</b>	0.5, 1, 2, 4, 8, or 16 cm <sup>-1</sup>
<b>Mirror speed</b>	4-step selection of 2.0, 2.8, 5, or 9 mm/sec
<b>Data sampling</b>	He-Ne laser (guaranteed for 1 year)
<b>Sample compartment</b>	Equipped with automatic accessory recognition mechanism W200 × D230 × H170 mm Center focus
<b>Power requirements</b>	AC 100–240 V, 50–60 Hz
<b>Power consumption</b>	150 VA (when used), 4 VA (standby)

### LabSolutions IR Software

<b>OS</b>	Windows 10 Pro 64 bit edition Windows 7 Professional 32/64 bit edition
<b>Interface</b>	USB 2.0, USB 3.0
<b>Programs</b>	Postrun, Spectrum, Quantitation, Photometric, Time course (option), Mapping (option)
<b>Manipulation functions</b>	Four Arithmetic Operations, Normalize, Zero Baseline Correction, 3 Point Baseline Correction, Multipoint Baseline Correction, Smoothing, Derivative, Cut, Connect, Reduce, Interpolate, Frequency Convert, X Adjust, Time-Temperature Conversion, Peak Pick, Film Thickness, Data Calculation, Purity, Deconvolution, FFT, Kubelka-Munk, ATR Correction, Kramers-Kronig, Atmosphere Correction, 3D Reprocess, 3D Extract, Purity Judgement
<b>Search functions</b>	Spectrum search (based on similarity), peak search, text search, combination search, setting of search conditions, search of user library and commercial library, creation of user library Library of approx. 12,000 spectra of organic compounds, polymers, pharmaceutical products, inorganic compounds, food additives, contaminants, etc. included

<b>Quantitative functions</b>	Multi-point calibration curve method, CLS quantitative method, PLS quantitative method (option), Photometrics, Recalculation function for quantitative and photometric results
<b>Printing functions</b>	Report template creation, Printing using report templates, Easy printing using the ViewPrint function (patent pending)
<b>Validation program</b>	Complies with Chinese, European, US, and Japanese Pharmacopoeias and ASTM
<b>GLP/GMP support</b>	Tree-structured audit trail function, Recording of operation logs and data logs (history), Saving by overwriting the same filename is prohibited
<b>Security functions</b>	Coordination with LabSolutions security functions, User-group based privilege settings
<b>File formats</b>	Files of JCAMP-DX, ASCII, CSV, IRsolution, HYPER-IR can be loaded and saved.



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