

Fourier Transform Infrared Spectrophotometer

# IRTracer-100



# New Levels of Performance and Quality Created by Excellent Sensitivity, Speed and Resolution



## Excellent Sensitivity, Speed and Resolution

- ▶ Quickly and easily obtain high-quality data for any kind of sample.
- ▶ Quickly analyze data with user-friendly LabSolutions IR software.
- ▶ High-speed generation of analysis reports.

Shimadzu's technologies provide the high performance needed for your IR Analysis.

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# IRTracer-100

Fourier Transform Infrared Spectrophotometer

## Excellence in Sensitivity and Reliability

High Sensitivity, Resolution, and Speed:  
Techniques to stabilize and optimize the interferometer provide high sensitivity.

## New Generation of Workstation

LabSolutions IR software 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.

## Meeting the Needs of a Wide Range of Analyses

Two main application programs support all analyses.  
A wide variety of options to meet every application is available.



This product conforms to Shimadzu's Eco-labeled designation.

\*Energy savings: 34% reduction as compared to the previous model

# New Levels of Performance and Quality Created by Excellent Sensitivity, Speed and Resolution

Quickly and easily obtain high-quality data for any kind of sample.

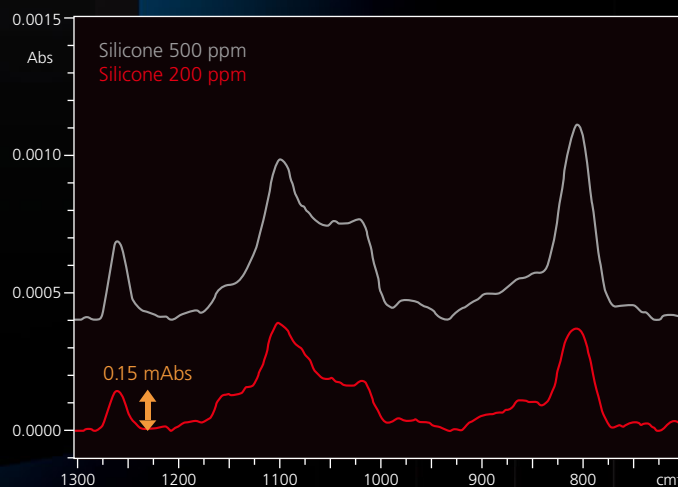


## High-Sensitivity Measurements, with an SN Ratio of 60,000:1\*1

Trace quantities of silicone oil contained in paraffin oil were measured using the IRTracer-100 and a single-reflection ATR accessory. Even the very faint peak (1260  $\text{cm}^{-1}$ ) from the silicone, with a mere 0.00015 Abs, was measured with a high SN ratio.

### Remarks:

- Difference spectrum obtained by subtracting the paraffin spectrum
- Measured with a resolution of 4  $\text{cm}^{-1}$ , using the DLATGS detector





## High Sensitivity, High Resolution and High Speed

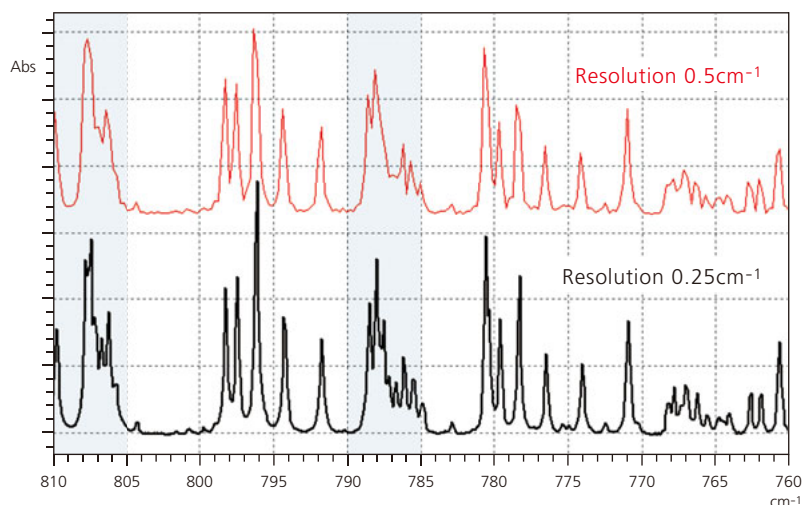
The IRTracer-100 features the highest SN ratio in its class at 60,000:1, 0.25cm<sup>-1</sup> resolution, and high-speed scanning capable of 20 spectra/second.

### Acquire High-Resolution Spectra with a 0.25cm<sup>-1</sup> Resolution Setting

Highly accurate quantitation and identification can be achieved with 0.25cm<sup>-1</sup> resolution.

For example, this resolution is suitable for the detailed analysis of each peak in a gas sample.

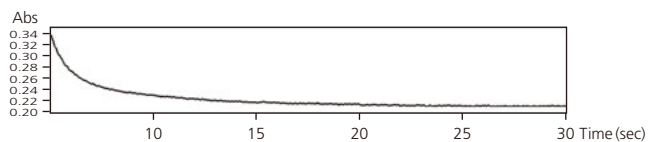
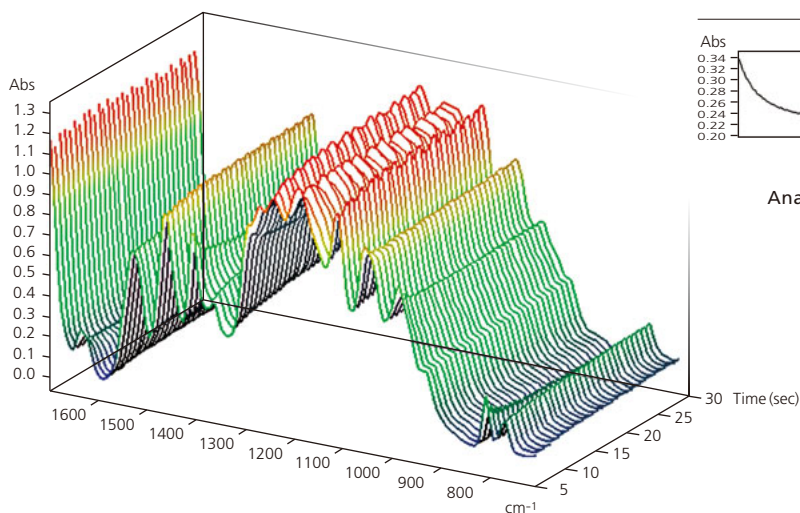
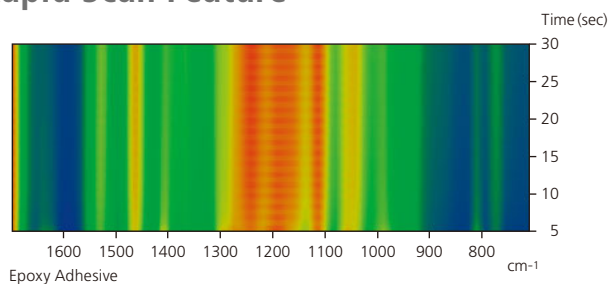
When ammonia gas was run at 0.25cm<sup>-1</sup> resolution, peaks in the 805 – 810 and 785 – 790cm<sup>-1</sup> ranges were clearly resolved.



### Achieve High-Speed Analysis with a 20 Hz Rapid Scan Feature<sup>\*2</sup>

The rapid scan function allows a maximum of 20 spectra per second to be obtained. This makes the IRTracer-100 suitable for fast reactions that occur within a few seconds and for kinetic studies occurring in less than one second.

Rapid, high-sensitivity analysis with a 2,000: SN is available.



#### Analysis of curing reaction of UV light curable resin

Sample: UV light curing adhesive  
Resolution: 16cm<sup>-1</sup>  
Scan accumulation: 1 scan  
Total scans: 600  
Interval: 50msec  
Monitor: Peak at around 1,400cm<sup>-1</sup>  
Detector: MCT

\*1 peak-to-peak, 4cm<sup>-1</sup> resolution, in a neighborhood of 2,200cm<sup>-1</sup>, 1-minute accumulation \*2 16cm<sup>-1</sup> resolution. Rapid scan program is optional.

## Reliable High Performance

An automatic dehumidifier and advanced dynamic alignment enable easy maintenance of the interferometer.

### Built-in Automatic Dehumidifier Allows for Easy Maintenance

Beam splitters used in FTIR interferometers are susceptible to humidity. In order to maintain the long-term stability of the interferometer, the beam splitter must be protected from moisture. To address this issue, the IRTracer-100 has been engineered with an airtight interferometer that incorporates a unique internal Automatic Dehumidifier.

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

The interferometer is sealed in an airtight housing.

An electronic Automatic Dehumidifier continuously removes any moisture, ensuring a dry interferometer chamber.

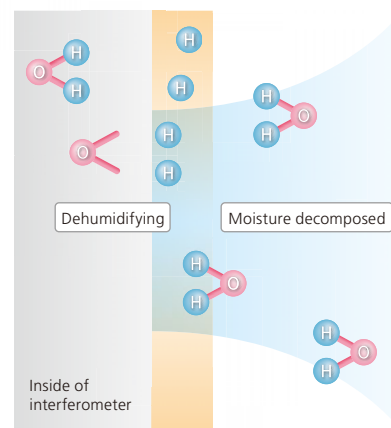
The beam splitter is covered with a moisture-resistant protective coat.

#### Principle of the Automatic Dehumidifier

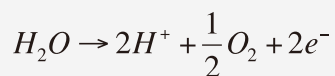
The IRTracer-100 incorporates an Automatic Dehumidifier that electrolytically removes the moisture inside the interferometer using a solid polymer electrolytic membrane.

Because the electric power required to operate the Automatic Dehumidifier is less than the continuous operation of the FTIR, it can reduce CO<sub>2</sub> emissions by approximately 400 kg/year.\*

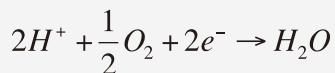
- 1 When porous electrodes are attached to a solid polymer electrolytic membrane and direct current is applied, moisture on the anode side (i.e., the desiccation side) dissociates into hydrogen ions and oxygen.
- 2 The hydrogen ions travel through the solid polymer electrolytic membrane and reach the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



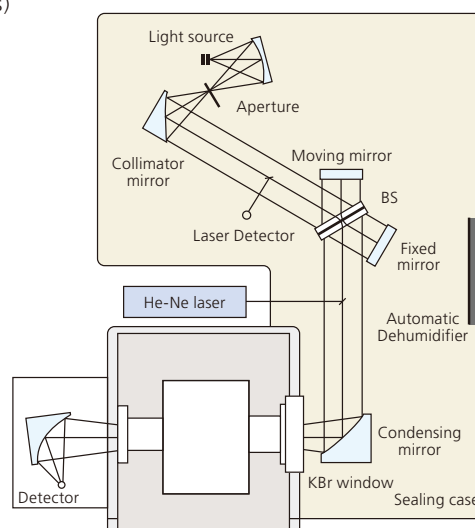
Anode  
(desiccation side)



Cathode  
(moisture discharge side)



Replacing the window (KBr) at the sample compartment with an optional KRS-5 window (P/N 206-74211-46) ensures safe operation with no concern for the window plate becoming cloudy under a high humidity environment.



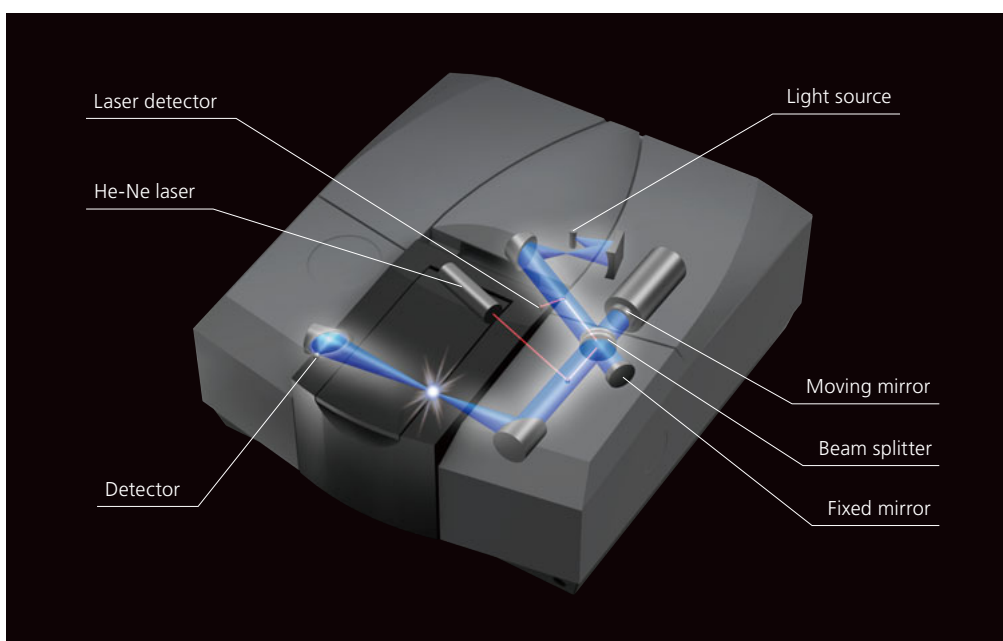
\* Model case by SHIMADZU

The IRTracer-100's interferometer is optimized and stabilized using a combination of a smooth moving mirror system and the Advanced Dynamic Alignment. To assure that the IRTracer-100 is always in the optimum operating condition, a self diagnoses routine monitors the operation of the system at initialization and constantly during operation. In addition, standard EP/CHP/JP/USP/ASTM validation programs are provided to evaluate the FTIR performance.

## Incorporation with Advanced Dynamic Alignment

Achieving reproducible optical interference in a spectrophotometer requires a robust interferometer design. The interferometer in the IRTracer-100 easily meets this requirement. The smooth moving mirror system monitored by the Advanced Dynamic Alignment system allows the IRTracer-100 to provide optimum and stable quality spectra

after only a short warm-up time. Sampling at over 5000 times/second the Advanced Dynamic Alignment keeps the IRTracer-100 in optimum operating condition. In addition, the Advanced Dynamic Alignment system automatically aligns the interferometer when the beam splitter is changed for NIR or FIR analysis.



### Four Benefits of Advanced Dynamic Alignment

Removes the influence of environmental variations

Allows the FTIR to be powered off when not in use\* (saving electricity and reducing the environmental impact)

Shorter warm-up times and enhanced stability

Provides for a maintenance-free system

### Scheme of Advanced Dynamic Alignment

- 1 The interference pattern of the He-Ne laser light is detected by the Laser Detector.
- 2 The quality of the produced interference is calculated.
- 3 The calculated interference is compared with stored patterns obtained under optimum operating conditions.
- 4 The difference between these interference patterns is calculated by an advanced digital signal processor.
- 5 The inclination of the fixed mirror is continuously adjusted to eliminate any difference and maintain optimum operating sampling conditions.

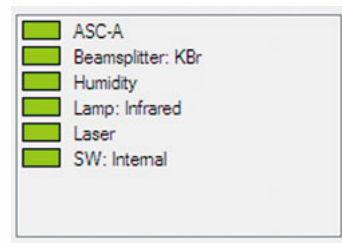
\* Automatic Dehumidifier is working.

# Reliable High Performance

Self-diagnostics and monitoring technology allow for quick, easy instrument management.

## Five Self-Diagnostic Functions

▶ The IRTracer-100 executes a self-diagnosis at instrument initialization, checking the electrical, signaling, and optical systems. If the interference conditions are not optimum, they are adjusted and optimized using the Advanced Dynamic Alignment mechanism.

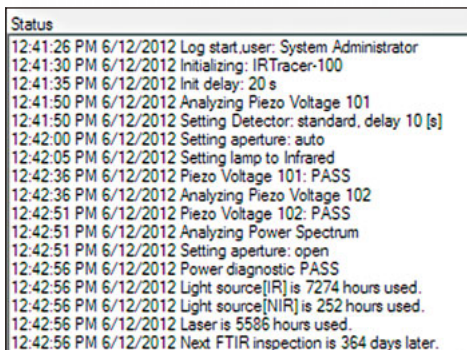
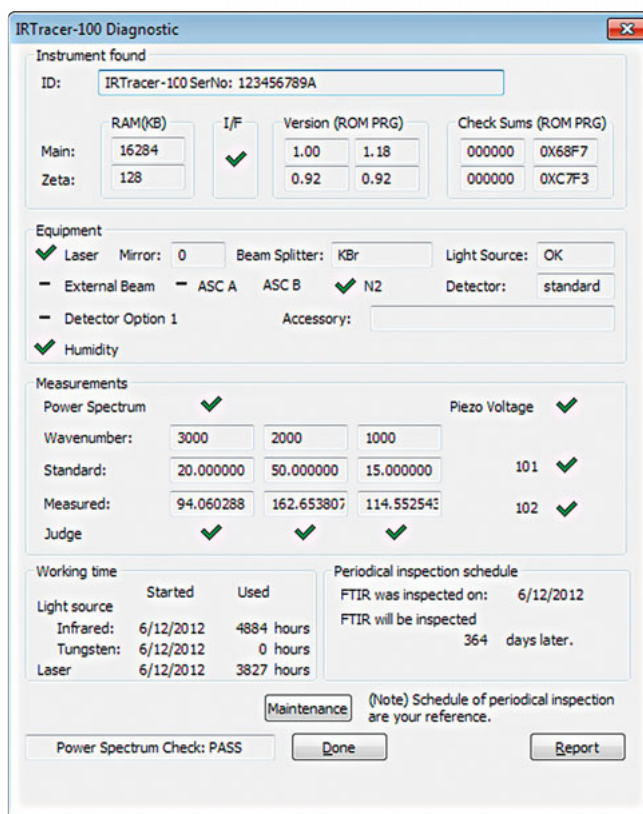


▶ The internal status monitor function offers continuous monitoring of the beam splitter type, the light source, the He-Ne laser, humidity condition, and information related to auto-start accessories.

▶ The hours\*1 used on the ceramic source and He-Ne laser as well as the time remaining before the next periodic inspection are monitored.

▶ When the beam splitter is exchanged for Near IR and Far IR analysis, the IRTracer-100 automatically detects the new beam splitter. In addition, when an accessory is installed, the accessory is automatically identified and optimum measuring conditions are automatically set\*2.

▶ Diagnostic and monitoring results are recorded in logs for reference.



\*1 3-year warranty for light source and 30-month warranty for He-Ne laser \*2 Only when QuickStart accessories are installed.



## Validation Program Verifies FTIR Performance

The IRTracer-100 is equipped with a validation program that complies with the European<sup>\*</sup>, Japanese, Chinese, and U.S.<sup>\*\*</sup>) Pharmacopoeias and with ASTM (American Society for Testing and Materials) specifications. The validation program checks

the basic performance of the instrument using a polystyrene film, and creates reports of the results. If any failure is detected, simply use the Advanced Dynamic Alignment mechanism to adjust and optimize the IRTracer-100.

### Test Specifications Complying with the European, Japanese, Chinese, and U.S. Pharmacopoeias

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

### Test Specifications for ASTM (ASTM E1421 Level Zero)

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

SHIMADZU IRPrestige/IRAffinity/IRTracer/FTIR-8000 Series ASTM Level 0 Report						
Instrument	: IRTracer-100	Overall Judgement	: PASS			
Serial No.	: IR 1	Temperature	: 25			
Sample name	: PS1	Relative Humidity	: 35			
Inspected by	: Admin	Date/Time	: 2012-06-12/10:01:02			
Approved by	:	Date	:			
<b>1. ASTM Level 0 Test - Energy Spectrum Test</b>						
Item	Today	Prev.	Error	Standard	Judge	
E(4000)/E(2000)	0.29	0.28	0.00	0.30	PASS	
E(2000)/E(1000)	1.44	1.43	0.01	0.30	PASS	
E(150)/E(max)	0.00	0.00	0.00	0.30	PASS	
at	%T	Error	Standard	Judge		
cm-1	%T	%T	%T			
4000	101.41	1.41	30.00	PASS		
2000	100.07	0.07	30.00	PASS		
1000	99.60	0.40	30.00	PASS		
500	99.43	0.57	30.00	PASS		
Ignore following bands due to water vapor (Peaks at 2200-1300cm-1, 4000-3300cm-1) and CO2 (Peaks at 2400-2250cm-1).						
<b>2. ASTM Level 0 Test - 100%T Line Test</b>						
<b>P-P Noise Value</b>						
W.N.	P-P	Standard	Judge			
cm-1	%T	%T				
4000	0.03	1.00	PASS			
2000	0.03	0.10	PASS			
1000	0.01	1.00	PASS			
500	0.32	8.00	PASS			
<b>RMS Noise Value</b>						
W.N.	RMS	Standard	Judge			
cm-1	%T	%T				
4000	0.007	0.50	PASS			
2000	0.006	0.05	PASS			
1000	0.003	0.50	PASS			
500	0.071	4.00	PASS			
<b>Average of Transmittance</b>						
W.N.	Average	Standard	Judge			
cm-1	%T	%T				
4000	100.20					
2000	100.03					
1000	99.99					
500	99.98					
<b>3. ASTM Level 0 Test - Polystyrene Test</b>						
at	%T	Standard	Judge			
cm-1	%T	%T				
4000	-1.20	+/-10.00	PASS			
2000	-0.37	+/-10.00	PASS			
1000	-0.41	+/-10.00	PASS			
500	0.88	+/-10.00	PASS			
Ignore following bands due to Strong Polystyrene bands at 3050-2850cm-1, 1550-1400cm-1, 800-650cm-1, 600-500cm-1						

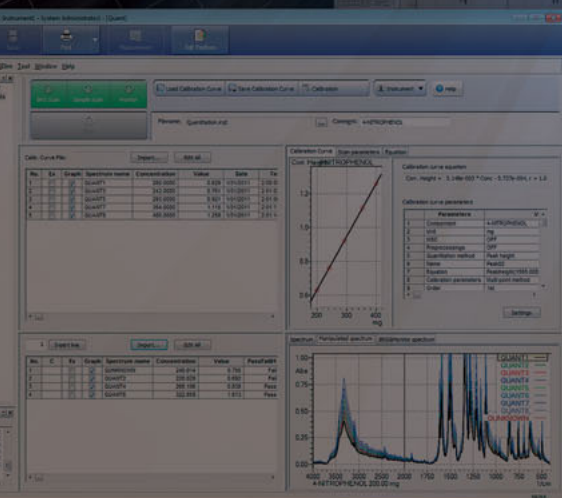
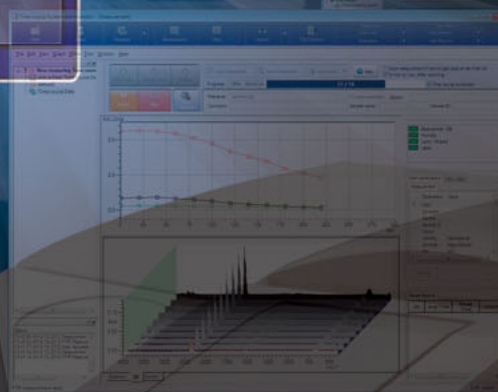
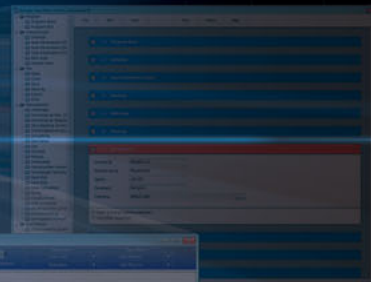
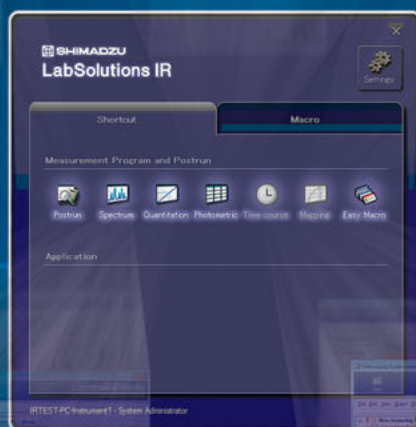
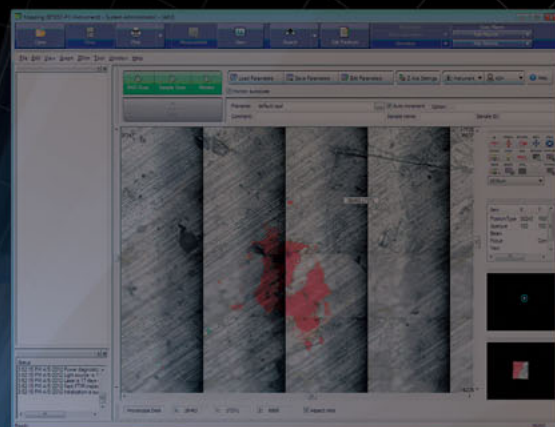
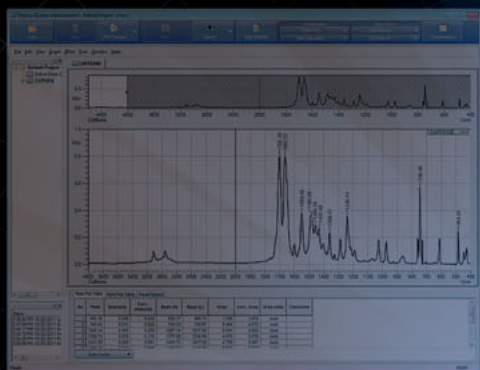
SHIMADZU IRPrestige/IRAffinity/IRTracer/FTIR-8000 Series Validation Report(EP7.0)						
Instrument	: IRTracer-100	Overall Judgement	: PASS			
Serial No.	: IR 1	Temperature	: 25			
Sample name	: PS1	Relative Humidity	: 35			
Inspected by	: Admin	Date/Time	: 2012-06-12/09:51:31			
Approved by	:	Date	:			
<b>1. Power spectrum</b>						
Wavenumber	Measured	Standard	Judge			
cm-1	E	E				
4600.0	16.26	8.41	PASS			
4000.0	29.75	21.02	PASS			
3000.0	50.42	42.04	PASS			
at Maximum	84.00	50.00	PASS			
700.0	28.74	8.41	PASS			
500.0	11.33	1.68	PASS			
403.0	2.70	0.42	PASS			
351.0	0.16	0.01	PASS			
<b>2. Resolution</b>						
Wavenumber	Measured	Standard	Judge			
cm-1	ABS	ABS				
2870.0	2870.2	0.448				
2849.5	2849.9	1.024	0.33	PASS		
Peak depth(ABS)	0.576					
1589.0	1588.4	0.278				
Peak depth(ABS)	0.201	0.08	PASS			
<b>3. Wavenumber accuracy</b>						
Wavenumber	Measured	Error	Tolerance			
cm-1	cm-1	cm-1	cm-1			
3060.0	3060.2	0.2	+/-1.0	PASS		
2849.5	2849.9	0.4	+/-1.0	PASS		
1942.9	1942.4	-0.5	+/-1.0	PASS		
1601.2	1601.0	-0.2	+/-1.0	PASS		
1583.0	1582.7	-0.3	+/-1.0	PASS		
1154.5	1154.4	-0.1	+/-1.0	PASS		
1028.3	1028.1	-0.2	+/-1.0	PASS		
<b>4. Reproducibility of Wavenumber</b>						
Wavenumber	No.1	No.2	Error	Tolerance		
cm-1	cm-1	cm-1	cm-1	cm-1		
2849.5	2849.9	2849.9	0.0	+/-5.0	PASS	
1601.2	1601.0	1601.0	0.0	+/-1.0	PASS	
1028.3	1028.1	1028.1	0.0	+/-1.0	PASS	
<b>5. Reproducibility of Absorbance</b>						
Wavenumber	No.1	No.2	Error	Tolerance		
cm-1	ABS	ABS	ABS	ABS		
2849.5	1.024	1.026	-0.002	+/-0.03	PASS	
1601.2	1.334	1.339	-0.005	+/-0.05	PASS	
1028.3	0.869	0.873	-0.004	+/-0.03	PASS	

\*): The Indian Pharmacopoeia has been unified with the European Pharmacopoeia.

\*\*): The United States Pharmacopoeia states that validation should be performed according to the method specified by the equipment manufacturer.

# 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

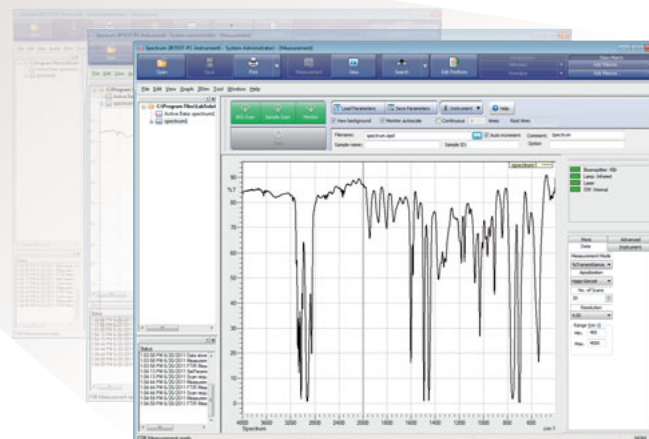
LabSolutions IR easily executes FTIR operations such as scanning, data manipulation, quantitation, reporting, saving, user administration, and more. High-level administrative functions and a variety of data manipulation functions provide for an easier, more user-friendly analysis environment. In addition, 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 ERES 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, LabSolution 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 IR Series

Designed to solve problems that can arise in laboratories!

## Provides a Comfortable Operating Environment

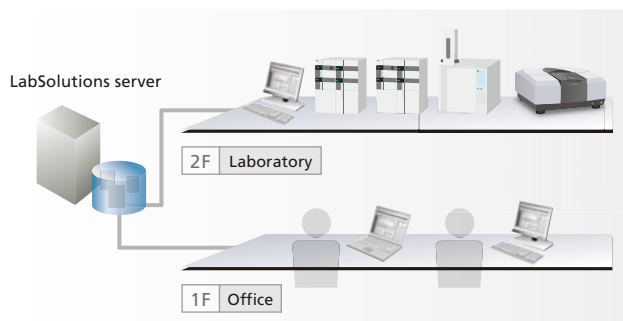
- ▶ The equipment operating status in a network is available at a glance.
- ▶ Analysis is possible from PCs other than the analysis PC.
- ▶ An enormous quantity of data can be quickly searched.

## Safe and Secure Data Management

- ▶ Database management prevents mistakes.
- ▶ Solid security

## Control and Analysis are Possible from PCs Other than the Analysis PC

With LabSolutions CS, equipment can be accessed freely, from any location, while maintaining security. For example, before starting an analysis, the equipment can be operated from a PC in the laboratory. After analysis starts, a PC in the office can be used to confirm operating status and analyze the data. This improves the efficiency of analysis status monitoring, report creation and other procedures.



## More Efficient Managerial Procedures

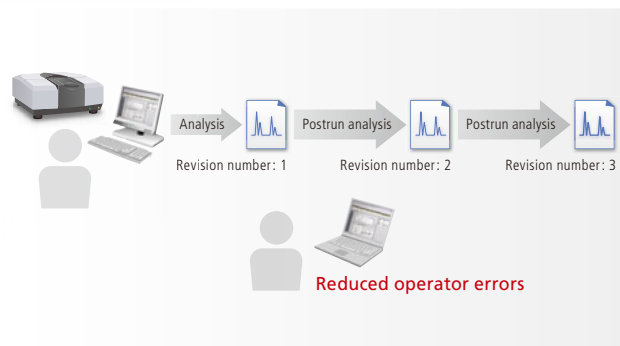
- ▶ System information, including data and users, is integrated with a server.
- ▶ Pertinent information is managed for every project.

## Total Support for Regulatory Compliance

- ▶ Support functionality for CSV (IQOQ validation) procedures.
- ▶ With terminal service, the configuration management of LabSolutions software in a client PC is unnecessary.

## Database Management Prevents Mistakes

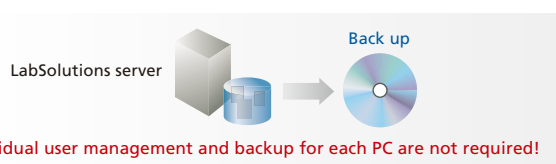
With LabSolutions DB and CS, the analysis data is managed securely by the database. Overwriting, deletion and other mistakes typical of data file management do not occur. In addition, when postrun analysis is performed using the acquired data, postrun analysis data revision numbers are automatically assigned, preventing the accidental overwriting of raw data.



## System Information, Including Data and Users, Is Integrated with a Server

Currently, since user information is managed for every PC, as the number of PCs increases, so too does the burden on the administrator. LabSolutions CS provides integrated server-based management of user information. As a result, user management is not required individually for each PC, reducing the administrator's time and effort.

Data backup is also important. Since the data can be managed with a server, data does not remain in each PC. It can be stored on the server or saved to media such as a DVD. The data can be referred to



directly, without returning to the original database. (Restoration unnecessary).

## 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.

## ||| LabSolutions IR Series |||

### LabSolutions IR

LabSolutions IR is a File Based FTIR Control and Analysis Software. This blended software package incorporates the improved software from IRsolution with LabSolutions' administration functions. The software is designed to improve operation and data processing for a more user-friendly environment. LabSolutions IR can also be connected with the conventional CLASS-Agent system.



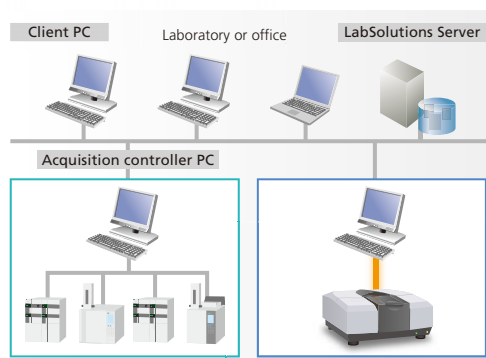
### LabSolutions DB IR

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

LabSolutions CS is Freely Accessible to the Analysis Network, eliminating the need for connecting a PC to the instrument. Since all the data is managed on a server, LabSolutions CS 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
<b>Data management method</b>	Measured data files are saved and managed in folders on the PC.	Measured data files are saved and managed in the LabSolutions database.	
<b>Data references</b>	The software references files on drives or in folders on the PC.	The software references files in the database.	
<b>LabSolutions database</b>	Unavailable	Available (The database resides on a local PC)	Available (The database resides on a server)
<b>CLASS-Agent database</b>	Available (Option)	Unavailable (The contents of the CLASS-Agent database can be transferred to the LabSolutions database.)	
<b>User administration</b>		Available	
<b>Rights group administration</b>		Available	
<b>Project administration</b>	Unavailable	Available	
<b>Standalone/network</b>	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.)
<b>Data backup</b>	Performed on a file-by-file basis using Windows Explorer.	Performed for each database.	



# 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.

### Contents

SHIMADZU  
Food additives library

Reagents

Pharmaceutical products,  
agricultural chemicals

SHIMADZU  
Contaminants library

Polymers

Inorganic compounds

Approximately 12,000 spectra included

## 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.

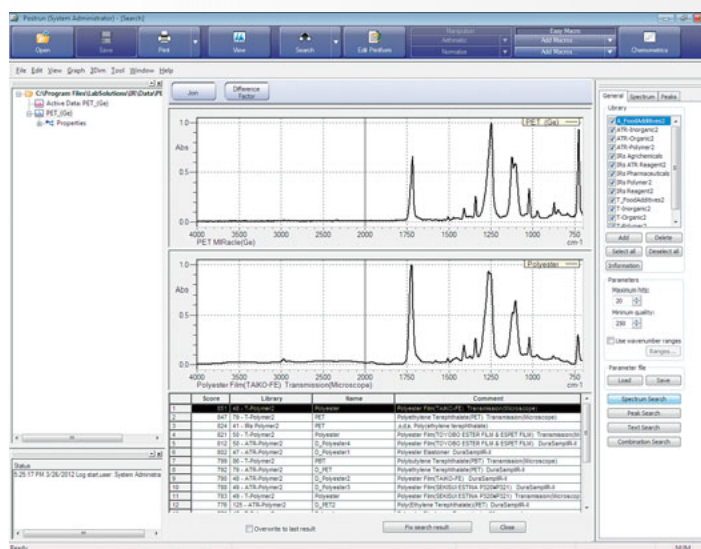
### Search functions

#### Spectral search

Shimadzu's unique search algorithm provides accurate results.

#### Peak search

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



# Automation and Labor-savings with Macro Program Functions

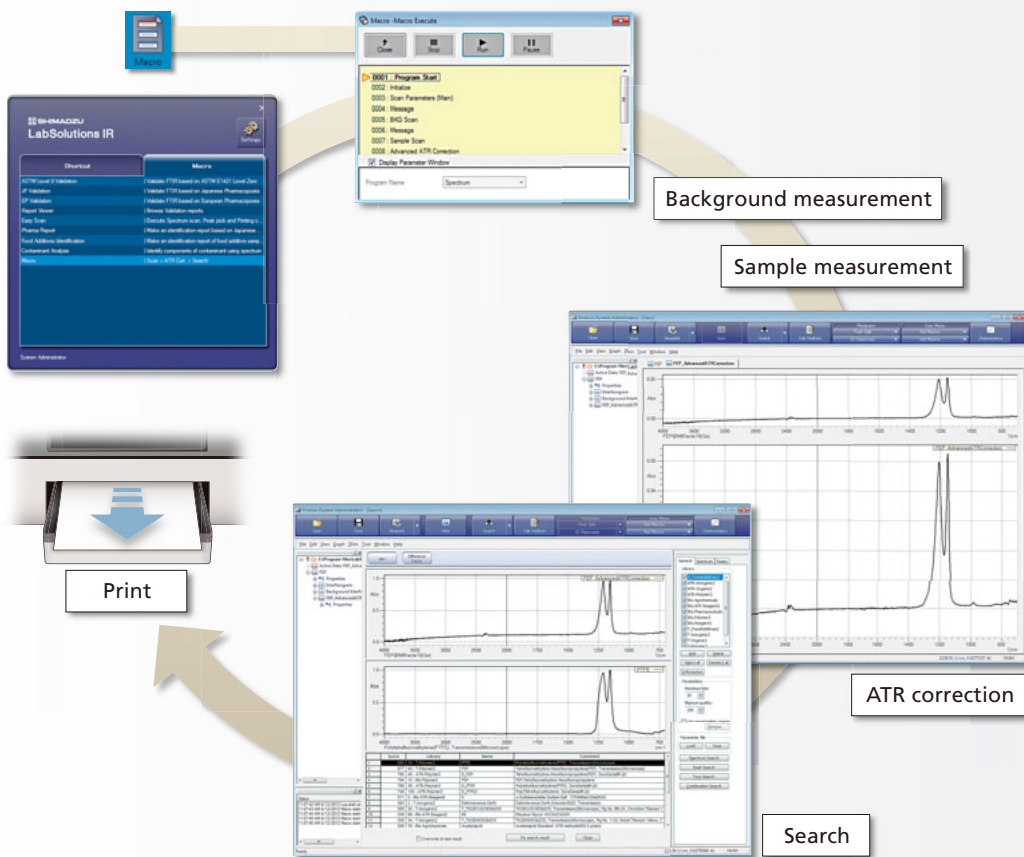
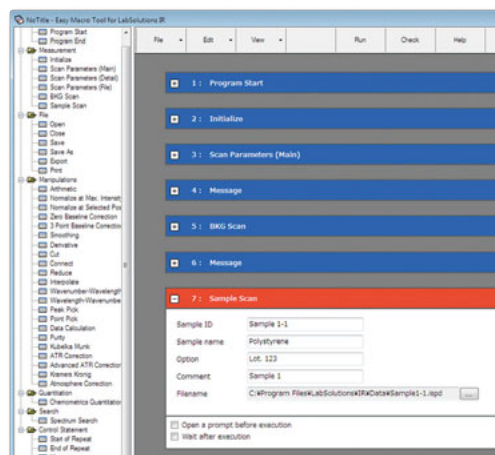
LabSolutions IR automates routine work, such as scanning, data manipulation, reporting, identification tests, and contaminants analysis. Launch programs from the Launcher or your PC desktop.

## 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

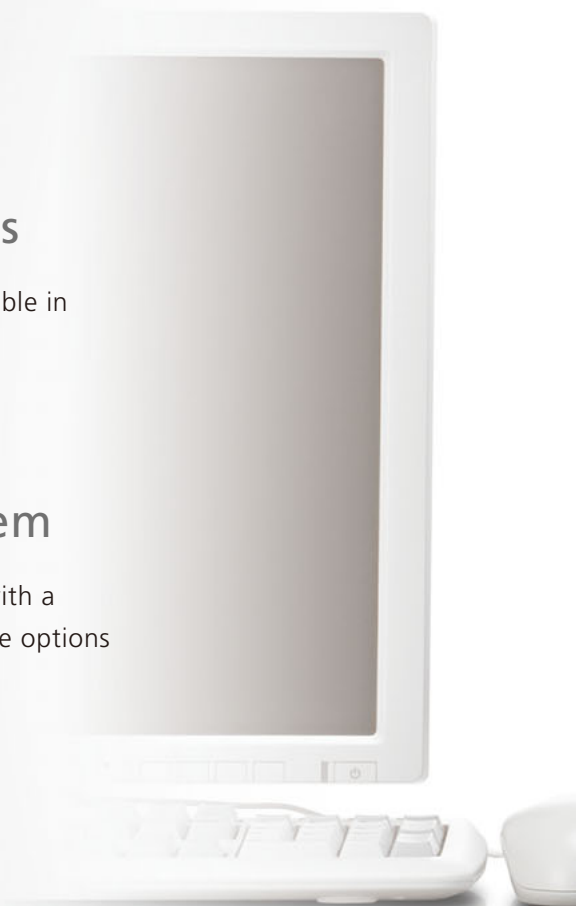


## Meeting the Needs of a Wide Range of Analyses

A wide variety of programs and accessories is available in order to meet the needs of various customers.

## Customize Your Own IRTracer-100 System

You can customize your own IRTracer-100 system with a wide variety of accessories and easy-to-use software options to meet the needs of your specific application.



## Meeting the Needs of a Wide Range of Analyses



### Pharmaceuticals

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

### Cosmetics

- Material identification tests
- Analysis of contaminants
- Failure analysis

### Food Products

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

### Environmental

- Water analysis
- Soil analysis
- Exhaust gas analysis
- Measurement of particles in water or air
- Analysis of asbestos
- Oil in water 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 contaminants
- Quantitative analysis
- Recycle



### Electrical, 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 (RoHS)
- Analysis of thin films
- Analysis of contaminants
- Failure analysis
- Analysis of semiconductor gases
- WEEE

### Automobiles

- Material identification tests
- Analysis of contaminants
- Failure analysis

### Metals

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

### Construction

- Material identification tests
- Degradation analysis of coatings

### Academia

- Research & Development
- Educational laboratories

## Two Main Application Programs Support All Analyses

LabSolutions IR includes two main application programs - for contaminant analysis and identification tests. Even operators unfamiliar with FTIR analysis can easily use these programs and create reports in just a few seconds.

### Contaminant Analysis Program

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. This easy-to-use program is conducive to all levels of operators. Reports are automatically created after analysis, allowing operators with little knowledge of infrared analysis to easily perform analysis.

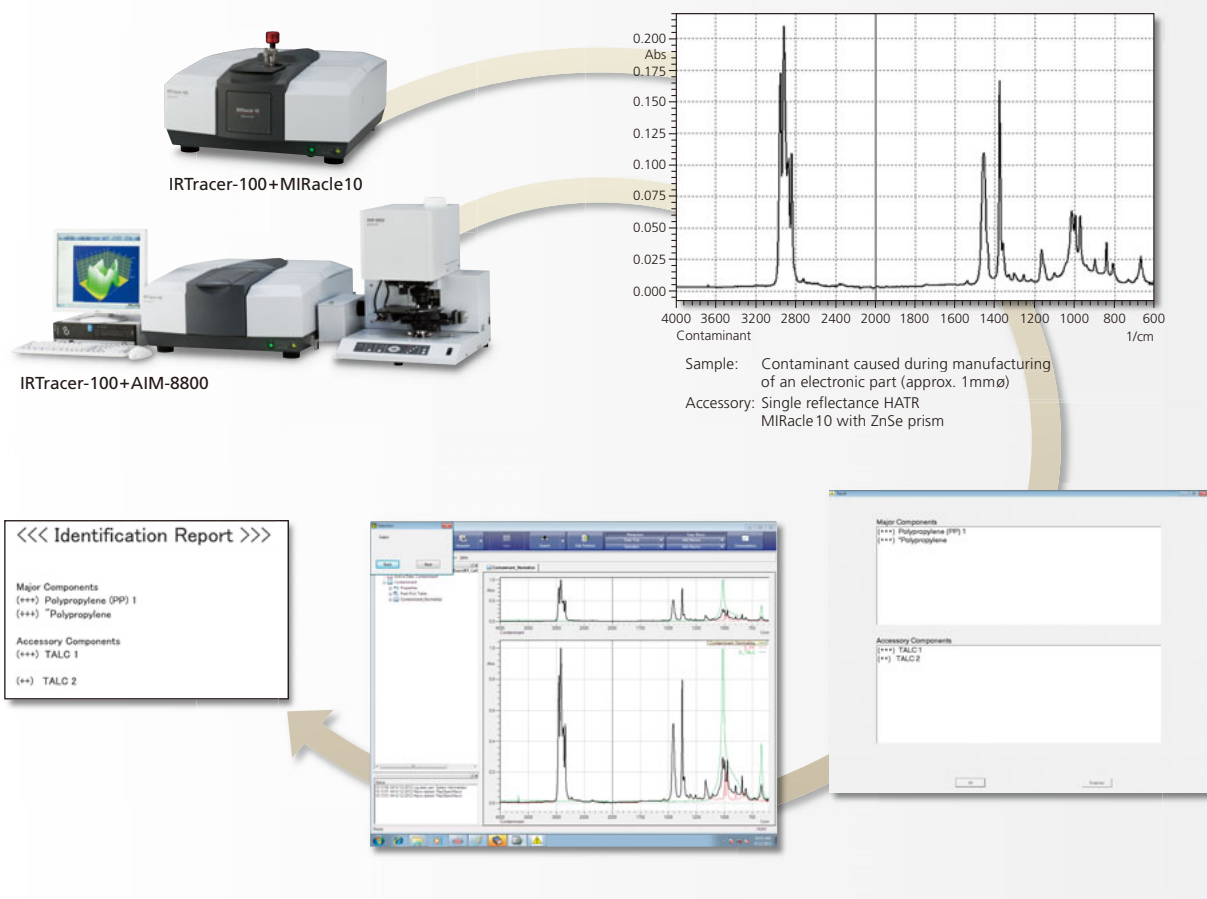
#### Four Features of the Contaminant Analysis Program

Contains spectra for over 550 inorganic substances, organic substances, and polymers that are often detected as contaminants in Shimadzu's Analytical Applications Department.

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

Automates the process, including searching, judgment evaluation, and report creation.

Finds major and minor components and displays their ranks.





## Identification Test Program

This program makes pass/fail judgments about samples in accordance with the tests specified in the Pharmacopoeia. In addition to identification tests for pharmaceutical products, this program can be used for incoming and pre-shipment inspections.

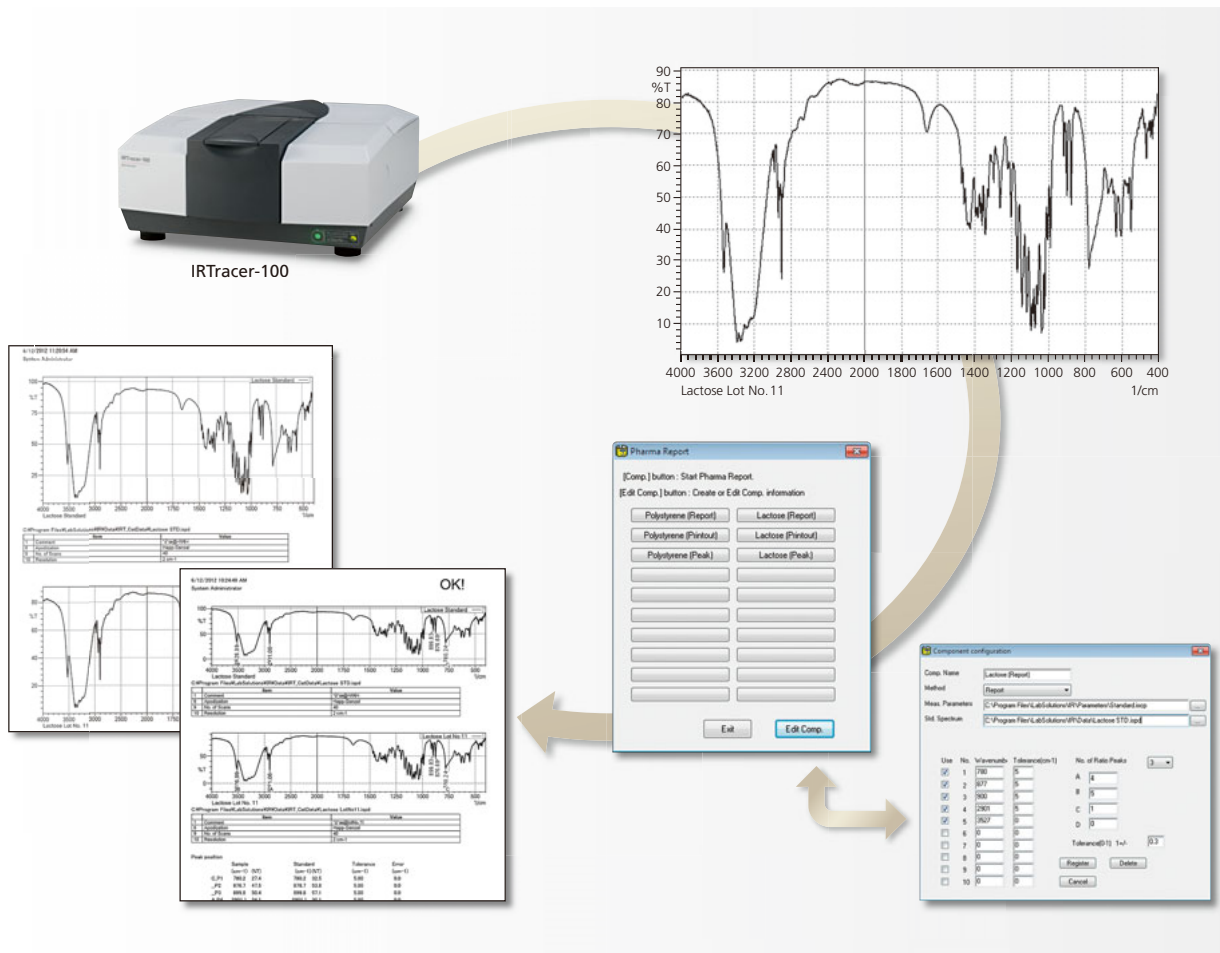
### Four Features of the Identification Test Program

Prints out the spectra for standards and samples to facilitate easy comparison.

Detects and prints just the peaks that are specified for pass/fail judgment.

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.

Contains spectra of 57 samples of Japanese Standards of Food Additives in LabSolutions IR.



## Hardware Options

Integrated with sample compartments, the series of horizontal ATR accessories offers improved purging performance, and eliminates the concern of dust entering the IRTracer-100's sample compartment. When an accessory is installed, the software displays its name and serial number and sets the optimum scan parameters.

### MIRacle 10

(P/N 206-74127-9x)

This is a single-reflection ATR accessory. To measure the spectrum of a liquid, simply place it on the surface of the prism drop-wise. Measure solid samples by simply clamping them onto the surface of the prism using the provided pressure clamp. In addition, the MIRacle-10 enables easy measurement of large samples (with a large surface area) without compromising sample integrity. The incidence angle is 45°. Select from three prism options: ZnSe, Ge, and diamond/ZnSe, and whether the prism is equipped with a pressure sensor. The Ge prism is ideal for samples with a high refractive index.



Powders



Moldings



Thin Films



Films



Liquids



Rubber



### GladiATR 10

(P/N 206-74128-9x)

This is a single-reflection ATR accessory. Because the prism is made solely of diamond, it is capable of measuring spectra down to 400  $\text{cm}^{-1}$ . To measure the spectrum of a liquid, simply place it on the prism drop-wise. To measure the spectrum of the surface of other samples, clamp them firmly on the surface of the prism. The incidence angle is 45° and you can select whether the prism is equipped with a pressure sensor.



Powders



Moldings



Thin Films



Films



Liquids



Rubber



### HATR 10

(P/N 206-74126-91)

This is a horizontal ATR accessory. There are flat prisms for solids and troughs for liquids. To measure the spectrum of a liquid sample, simply place it on the prism drop-wise. 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 ten. It includes a ZnSe prism as standard; use an optional Ge prism for samples with a high refractive index.



Films

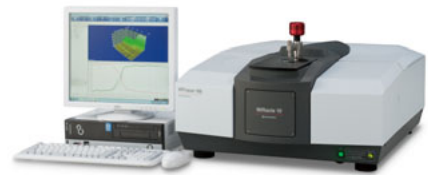


Liquids



Rubber





## DRS-8000A

(P/N 206-62301-91)

Although powder samples are mixed with KBr, as with the KBr pellet method, the DRS-8000A analyzes the samples in their original state; creating pellets is not necessary. For plastic moldings, emery paper attached to the SiC sampler (P/N 200-66750) scrapes off part of the surface, forming a powdered sample that can be analyzed. Easily obtain diffuse reflectance spectra similar to transmittance spectra using the built-in Kubelka-Munk conversion in the LabSolutions IR software.



Powders



Moldings



SiC sampler

## SRM-8000A

(P/N 206-62304-91)

Use this specular reflectance accessory, featuring a 10° incidence angle, for the analysis of thin films on a metal plate with a  $\mu\text{m}$  order of thickness. For mirror-like plastic samples, it measures the specular light reflected from the sample surface. Kramers-Kronig analysis, available with LabSolutions IR software, produces specular reflectance spectra similar to transmittance spectra.



Thin Films



## RAS-8000A

(P/N 206-62302-91)

Use this high-sensitivity reflection measurement accessory, featuring incidence angles of 70° and 75°, for the analysis of thin films on a metal plate with a 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

## IR Microscope AIM-8800

(P/N 206-73700-xx)

The AIM-8800 incorporates a bright, optimized optical system and a highly sensitive MCT detector, enabling the high-sensitivity analysis of minute samples. It offers many features that meet the needs of today's FTIR microscopist, such as the auto aperture and auto focus functions, which greatly simplify the

analysis of micro-sized samples. The design of the automated transfer mirror allows the user to easily switch between measurements in the IRTracer-100 sample compartment and those in the infrared microscope.

- ▶ The auto aperture, auto centering, and auto X-Y stage functions simplify determination of the analysis location.
- ▶ The auto focus function simplifies focusing.
- ▶ Up to 10 sample positions and 2 background measurement positions can be stored in memory.
- ▶ LabSolutions IR software enables automatic measurements.
- ▶ All microscope operations, such as stage movement, aperture setting and focusing, and switching between transmission/reflection and measurement/observation modes, can be controlled from the computer screen.
- ▶ Operation is also possible from the microscope's own keyboard.



Minute Samples

\* Beam switching kit (P/N 206-74250-41) and AIM connection kit (P/N 206-72019-93) must be purchased separately.

## ATR Objective (Slide-On Type) ATR-8800M

(P/N 206-70450-91)

A single-reflection ATR objective that uses a semicircular Ge prism with a diameter of 3 mm is used when performing ATR measurement with the AIM-8800 infrared microscope. The prism can be conveniently slid to one side when positioning the sample and then slid back into position for measurement.



Minute Samples

## 5-cm Gas Cell (P/N 202-32006-xx)

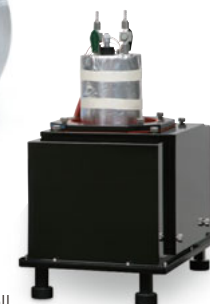
## 10-cm Gas Cell (P/N 202-32007-xx)

## Long-Path Gas Cell

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



5-cm Gas Cell



Long-Path Gas Cell



Gases

## MCT Kit

(P/N 206-74254-91)

Use a high-sensitivity MCT detector when analyzing minute or low transmittance samples, or when performing measurement using a long path-length gas cell. The kit installs an MCT detector on the IRTracer-100. Switching between the standard DLATGS detector and the MCT detector is performed automatically from

LabSolutions IR. In addition, the software has a built-in liquid nitrogen monitor to terminate current flow when the detector element is not being cooled, thus protecting the MCT detector. The liquid nitrogen dewar is made of glass and does not require periodic evacuation or yearly maintenance.

\* This kit cannot be mounted at the same time as the Near IR Kit (P/N 206-74253-91). Liquid nitrogen is required when using the MCT detector.

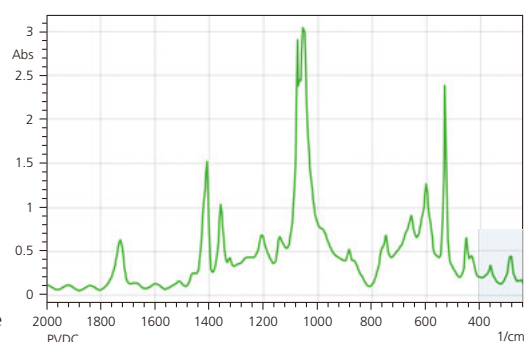
## Far IR Kit

(P/N 206-30616-41)

Bands related to inorganic compounds and organometallic complexes are typically observed in the far infrared region to  $240\text{ cm}^{-1}$ . The Far Infrared Kit contains a CsI beam splitter that can be mounted on the IRTracer-100 for measuring spectra in this region.

Since absorption due to water is greater in the  $400\text{ cm}^{-1}$  to  $240\text{ cm}^{-1}$ , the instrument should be purged with desiccated air before performing measurements. The CsI beam splitter should also be stored in a desiccator when not in use since it is highly sensitive to moisture.

Spectrum of Polyvinylidenechloride



## Near IR Kit

(P/N 206-74253-91)

Attached to the IRTracer-100, this kit enables near-infrared measurement. LabSolutions IR switches between the mid-infrared and the near-infrared.

- [ Specifications ]
- ▶ Measurement Range:  $12,500$  to  $3,800\text{ cm}^{-1}$
  - ▶ Beam Splitter: Si/CaF<sub>2</sub>
  - ▶ Light Source: Tungsten iodine lamp
  - ▶ Detector: InGaAs

\* This kit cannot be mounted at the same time as the MCT Kit (P/N 206-74254-91).

## NIR Integrating Sphere IntegratIR A

(P/N 208-97272-92)

- ▶ Powders, tablets, liquids, fibers, plastic pellets and molded samples can be placed on the sample stage for measurement (reflectance measurement).
- ▶ Pre-treatment such as KBr dilution is not required.
- ▶ Samples stored in a plastic bag or glass bottle can be measured.
- ▶ Applications include qualitative or identification tests in acceptance inspections and quantitative analysis of components in measured samples.
- ▶ Features a built-in highly sensitive InGaAs detector.

\* The IntegratIR installation kit (P/N 206-72715-93) must be purchased separately.



### For Other Accessories

Please contact your Shimadzu representative about accessories that do not appear in this catalog. Also note that it may not be possible to use FTIR-8000 Series accessories. Please consult your Shimadzu representative for assistance with using FTIR-8000 Series accessories.



## Software Options

Fast, easy-to-use LabSolutions IR can be equipped with a variety of optional software programs and applications. Adding these options makes it possible to further increase the application range.

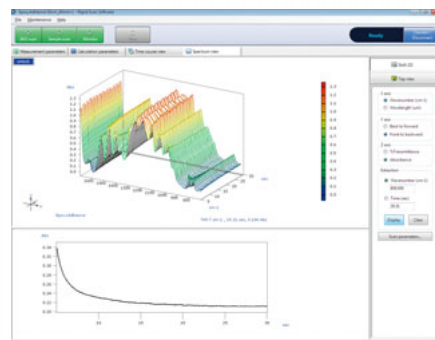
### Rapid Scan

(P/N 206-30200-91)

The Rapid Scan option provides the capability of collecting and recording a maximum of 20 spectra/second. This is especially suitable for fast reactions kinetics, where reactions are completed in a few seconds. Spectra obtained from Rapid Scan measurements can be used to calculate peak heights and areas, which are used to determine kinetic rates.

The Rapid Scan interval is dependent on the resolution, number of scans, and mirror speed. The fastest speed under a  $16\text{cm}^{-1}$  resolution and a mirror speed of  $40\text{mm/s}$  is 0.05 seconds for 1 accumulated scan. Maximum measurement time depends on scan parameters.

The 3D Processing Program (P/N 206-74563-91) is required for analysis of Rapid Scan spectra.



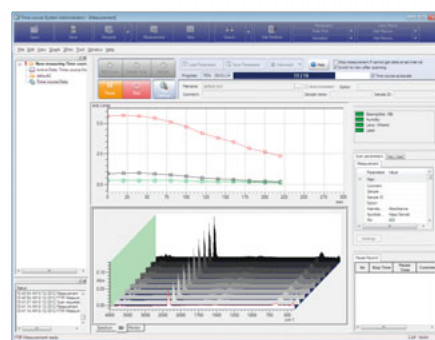
LabSolutions IR

### 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. Simply modify parameters to recalculate the information.

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

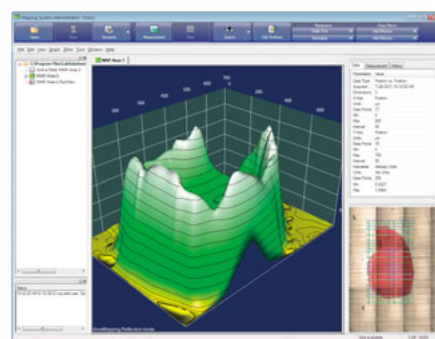
### Mapping Program

(P/N 206-74559-91)

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

The program allows setting of mapping parameters, such as the mapping range, the scan intervals, and the background positions, on the composite images. In addition, it supports area mapping, line mapping and random mapping modes. 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.

This program includes a 3D Processing Program.



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 more advanced applications in which certain functions

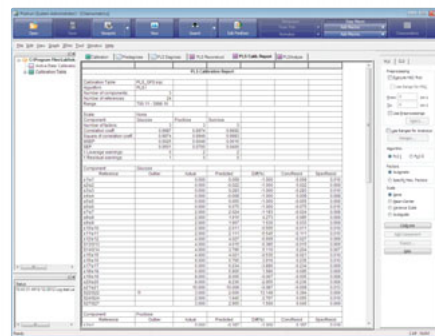
are used in a pre-determined order, or you wish to run an automatic measurement system in combination with an auto sample changer, please contact your Shimadzu representative for details.

LabSolutions IR

## PLS Quantitation Program

(P/N 206-74560-91)

Like multiple linear regression analysis, PLS (partial least squares) is a chemometrics method 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.

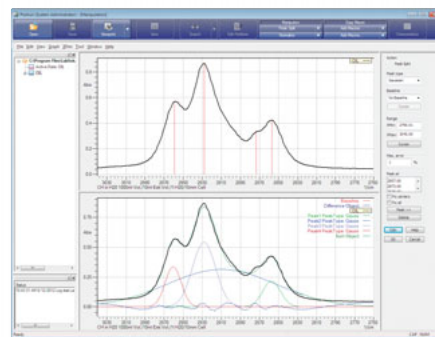


LabSolutions IR

## 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, including 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 evaluate the separation accurately.



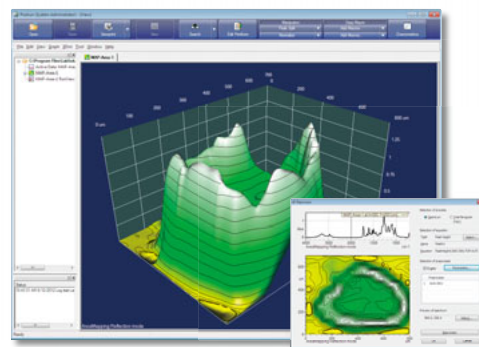
LabSolutions IR

## 3D Processing Program

(P/N 206-74563-91)

The 3D processing program offers the following functionality:

- ▶ **Changes the method of displaying data**
  - Display data in bird's eye view (3D), as an intensity distribution or using contour lines, as a spectral overlay, or rotated.
- ▶ **3D data processing**
  - Isolate changes at specific wavenumbers.
  - 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**
  - Create 3D data by consecutively arranging spectra measured at fixed intervals, such as by repeated measurements.



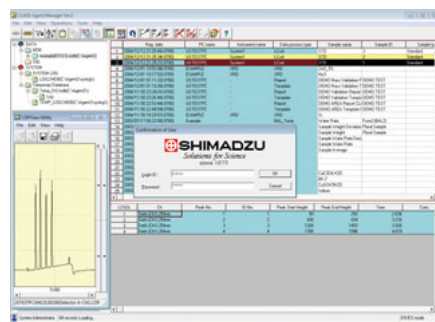
\* The 3D processing program cannot control mapping measurements or AIM-8800 series infrared microscopes.

## CLASS-Agent Connection Kit

(P/N 206-74557-91)

This program connects LabSolutions IR (File edition) to the CLASS-Agent system. Spectra collected using LabSolutions IR are managed in an existing CLASS-Agent database. This database enables data management for the entire recording life cycle, which consists of the creation (measurement), inspection, approval, storage, browsing, backup, and disposal of analysis data. Requires CLASS-Agent Manager and Public Agent.

\* Only spectra are saved in the CLASS-Agent database. Mapping data, Time course data, Calibration curve and Quantitation result tables cannot be stored.



# Specifications

## Hardware

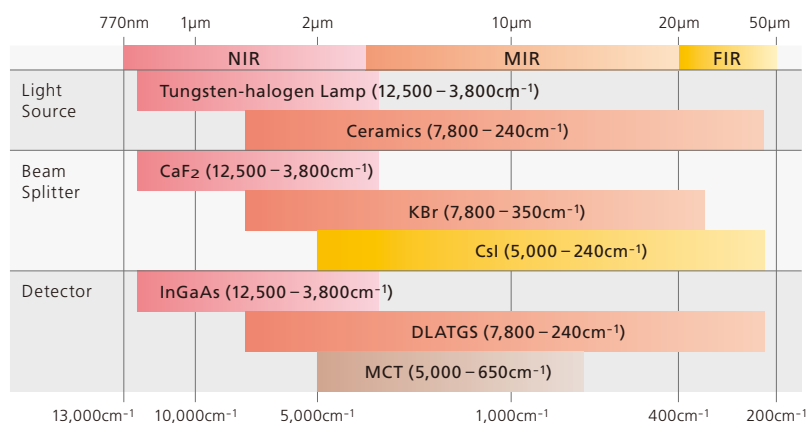
Interferometer	Michelson interferometer (30° incident angle) Equipped with Advanced Dynamic Alignment system Sealed interferometer with Automatic Dehumidifier
Optical system	Single-beam optics
Beam splitter	Germanium-coated KBr for Middle IR (Standard) Germanium-coated CsI for Middle/Far IR (Optional) Silicon-coated CaF <sub>2</sub> for Near IR (Optional)
Light source	High-energy ceramic for Middle/Far IR (Standard) with 3 years guaranteed Tungsten lump for Near IR (Optional)
Detector	DLATGS detector with temperature control for Middle/Far IR (Standard) MCT (Hg-Cd-Te) with liquid nitrogen cooling for Middle/Near IR (Optional) InGaAs for Near IR (Optional)
Wavenumber range	7,800 to 350cm <sup>-1</sup> (Standard) 12,500–240cm <sup>-1</sup> (Optional, See figure for details)
Resolution	0.25, 0.5, 1, 2, 4, 8, 16cm <sup>-1</sup> (Middle/Far IR) 2, 4, 8, 16cm <sup>-1</sup> (Near IR)
Wavenumber accuracy	0.01cm <sup>-1</sup>
SN ratio	60,000:1 or higher (Standard; 4cm <sup>-1</sup> resolution, 1 min. scan, around 2,200cm <sup>-1</sup> , peak-to-peak) 6,000:1 or higher (Microscope; Transmittance mode, aperture 50×50μm, 8cm <sup>-1</sup> resolution, 120 scans) 8,000:1 or higher (MCT measurement; 4cm <sup>-1</sup> resolution, mirror speed 9mm/s, 120 scans, MCT detector) 2,000:1 or higher (Rapid scan; 16cm <sup>-1</sup> resolution, mirror speed 40mm/s, 1 scan, MCT detector) 10,000:1 or higher (NIR measurement; 4cm <sup>-1</sup> resolution, mirror speed 2.8mm/s, 34 scan, InGaAs detector) * SN ratio with a DLATGS detector is 48,000:1 or higher when a MCT kit or an NIR kit is mounted. * When a sample compartment window is changed to a KRS-5, the SN ratio is 75% of that attained with a KBr window.
Mirror speed	4-step selection of 2.0, 2.8, 5, or 9mm/sec 10, 20, 30, or 40mm/sec for Rapid Scan (option)
Data sampling	He-Ne laser with 30 months guaranteed
Sample compartment	Equipped with automatic accessory recognition mechanism 200(W) × 230(D) × 170(H) mm Center focus
Dimensions	600(W) × 665(D) × 295(H) mm
Weight	47kg

## Scan range

Light Source	Beam Splitter	Detector	Scan Range (cm <sup>-1</sup> )	Necessary parts
Tungsten	CaF <sub>2</sub>	InGaAs	12,500–3,800	Near IR Kit (P/N 206-74253-91)
Ceramic	KBr	DLATGS	7,800–350	Standard
		MCT	5,000–720	MCT Kit (P/N 206-74254-91)
	CsI	DLATGS	5,000–240	Far IR Kit (P/N 206-30069-91)

## Scan wavenumber with options

The orange bar expresses the wavenumber range that can be measured with the standard configurations. The red, yellow and brown bars express the wavenumber range that can be measured when utilizing various options.



## Software (LabSolutions IR)

OS	Microsoft Windows 7 Professional 32bit edition
Interface	USB 2.0
Programs	Postrun, Spectrum, Quantitation, Photometric, Time course (option), Mapping (option)
Measurement	Spectrum measurement, continuous measurement, atmospheric correction measurement, continuous measurement using ASC, simple measurement mode
Hardware monitor	Self-diagnosis function, status monitor
Manipulation functions	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
Manipulation functions (option)	Peak split, 3D recalculation, spectrum extraction from 3D data
Analysis support programs	Contaminant (patent pending), Pharma Report, Food Additives Identification
Search functions	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
Quantitative functions	Multi-point calibration curve method CLS quantitative method PLS quantitative method (option) Photometrics Recalculation function for quantitative and photometric results
Printing functions	Report template creation Printing using report templates Easy printing using the ViewPrint function (patent pending)
Validation program	Complies with Chinese, European, US, and Japanese Pharmacopoeias and ASTM
GLP/GMP support	Tree-structured audit trail function Recording of operation logs and data logs (history) Saving by overwriting the same filename is prohibited
Security functions	Coordination with LabSolutions security functions User-group based privilege settings
Macro functions	Easy macro function <ul style="list-style-type: none"> <li>• Collective execution of multiple operations by simply arranging operations in the order of the procedure</li> <li>• Execution possible from the desktop</li> </ul> Macro platform (option)
Optional software	Rapid Scan, Time course, Mapping, PLS Quantitation, Peak split, 3D processing, Macro platform, CLASS-Agent connection kit
File formats	Files of JCAMP-DX, ASCII, CSV, IRsolution, HYPER-IR can be loaded and saved.

## Computer / Printer

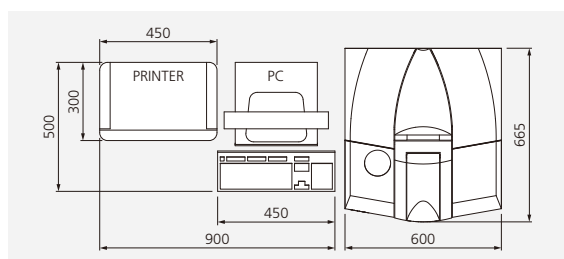
Type	Desktop
Specifications	Provide a computer and printer of a type recommended by SHIMADZU. Enquire separately for detailed specifications.

## Other Specifications

Installation site	Temperature: 15°C to 30°C; humidity regulated by air-conditioning equipment Humidity: 70% max.; with no condensation Provide local ventilation systems as required by applicable laws and regulations when analyzing or using organic solvents.
Power requirements*	100–240 VAC, 50/60 Hz, 150 VA for operation, 8 VA for standby

\* An additional power supply is required for the computer.

## Dimensions (PC and printer dimensions are examples.)





Shimadzu Corporation

[www.shimadzu.com/an/](http://www.shimadzu.com/an/)

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