**SHIMADZU**

Excellence in Science

Fourier Transform Infrared Spectrophotometer

# IRXross

# IR, Xross over

## Performance × Operability

The IRXross™ creates a new concept for infrared spectroscopy.

It offers the optimal solution for a new era with diverse application requirements.

## High-End Sensitivity for Countless Applications

## Built-in Analytical Intelligence

## Complies Fully with Regulations

**ANALYTICAL INTELLIGENCE**

- Automated support functions utilizing digital technologies, such as M2M, IoT, and Artificial Intelligence (AI), that enable higher productivity and maximum reliability.
- Allows a system to monitor and diagnose itself, handle any issues during data acquisition without user input, and automatically behave as if it were operated by an expert.
- Supports the acquisition of high quality, reproducible data regardless of an operator's skill level for both routine and demanding applications.

# High-End Sensitivity for Countless Applications

The IRXross is a mid-level FTIR model that achieves high-end level S/N. It enables best-in-class low noise with P-P values of 55,000:1 for one minute of integration.

**Moving mirror**

**Beam splitter**

**Fixed mirror**
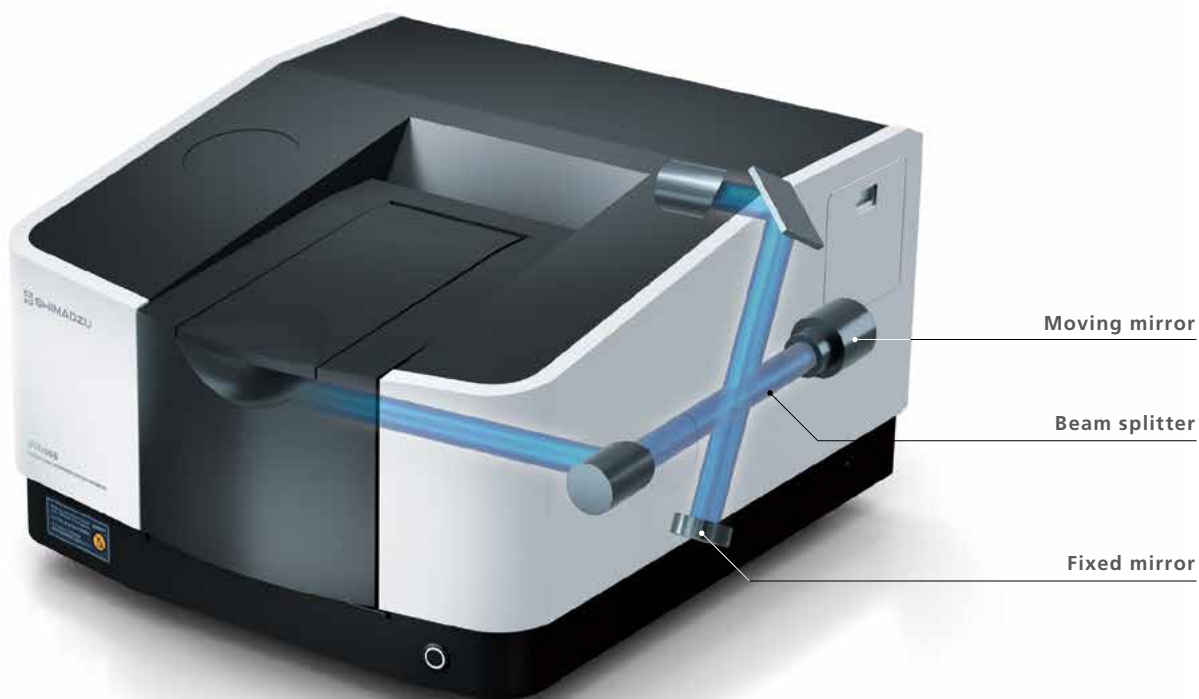
## Astoundingly Low Noise

The 100 %T line was obtained by successively measuring the background and sample values without placing a sample in the sample compartment. Excluding the peaks for water vapor and carbon dioxide, the noise level (P-P value) was within ±0.005 %T, which shows that it can acquire data with low noise.

± 0.005%T

IRXross 100 %T Line
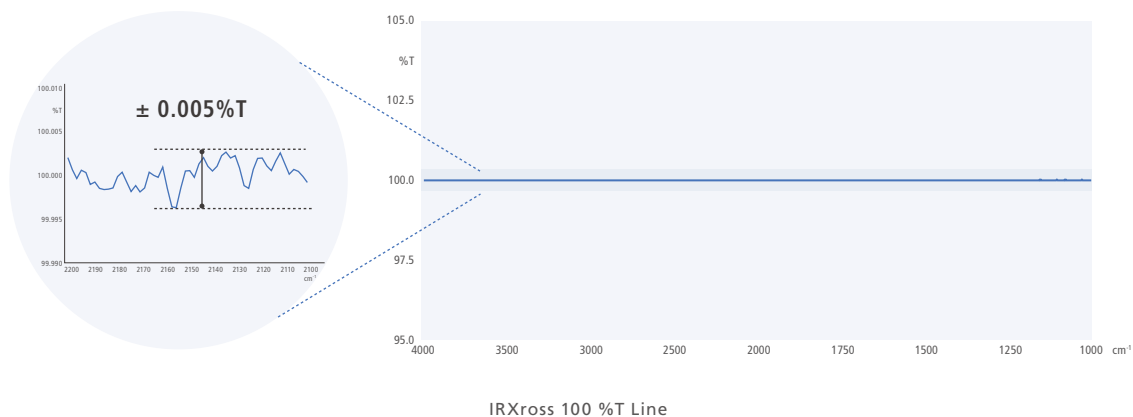
## 55,000:1 S/N Enables Ultra-High-Sensitivity Measurements

Using the IRXross with a single-reflection ATR attachment, an oil stain on paper was analyzed. Analyzing the sample directly without pretreatment would not result in good peaks, so n-hexane was applied to the stain area to extract the stain substances. Then a drop of the extract solution was placed on the ATR prism for analysis. The system is able to detect even the extremely weak 0.00023 absorbance signal with good sensitivity.
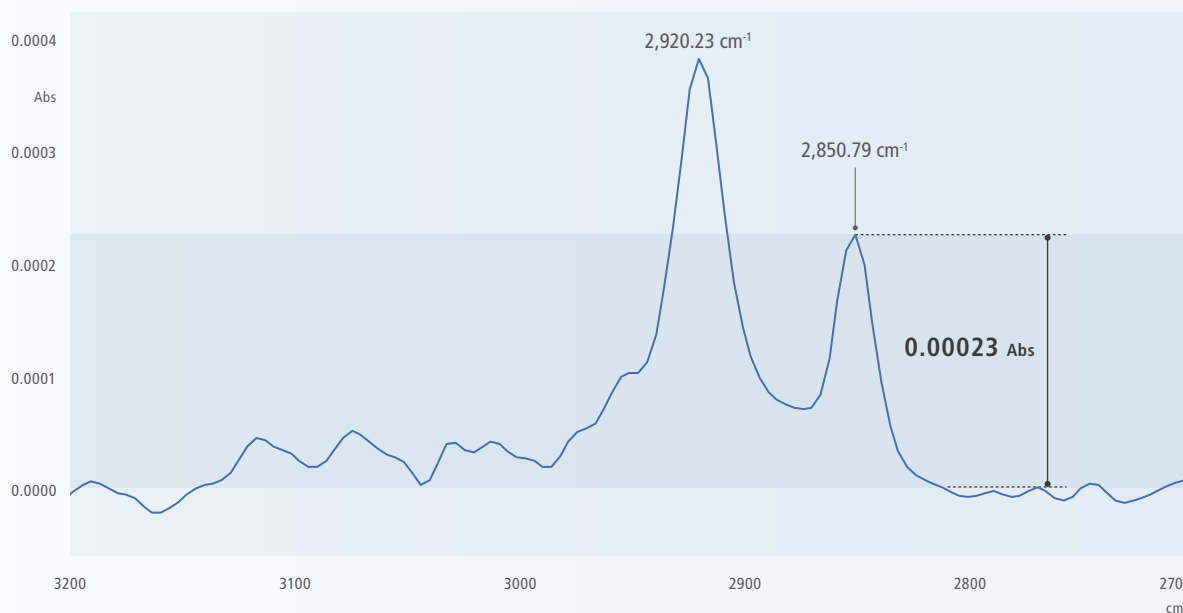


## 0.25 cm$^{-1}$ Resolution Enables High-Resolution Measurements

N$_2$O gas (500 ppm), considered an environmental problem as a greenhouse gas, was analyzed. Measuring the gas at high resolution shows the peaks near 2,230 cm$^{-1}$ properly separated, whereas a resolution of 1.0 cm$^{-1}$ only shows the peaks as two levels.
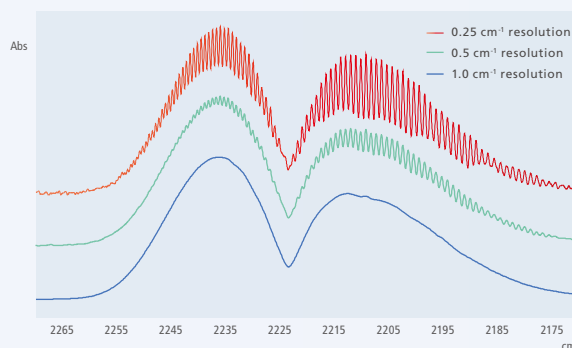


## High-Speed Measurement Enables Faster Reaction Tracking

When tracking the curing reaction in UV curable resin, the data shows that the intensity of the peak at 1,635 cm$^{-1}$ began decreasing 5.0 seconds after UV irradiation and the reaction was finished by 5.5 seconds.
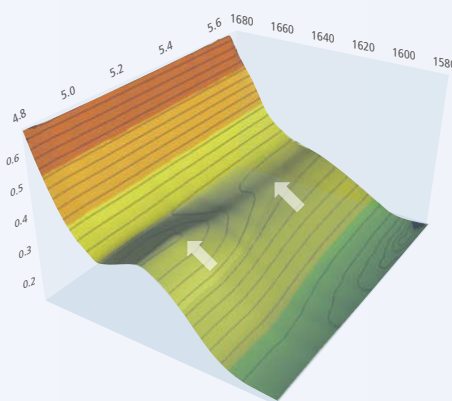
# Built-in Analytical Intelligence

## Easy Navigation with IR Pilot™ Ensures Anyone Can Get Started Easily


ANALYTICAL INTELLIGENCE

A total of 23 macro application programs are included. Even operators unfamiliar with FTIR analysis can analyze samples easily by simply selecting the purpose of analysis and attachment used. There is no need to set parameters. Multiple samples can be analyzed with a single click.

**1 Click**

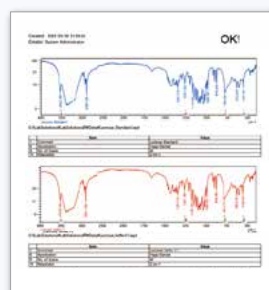**Selecting the purpose of analysis**
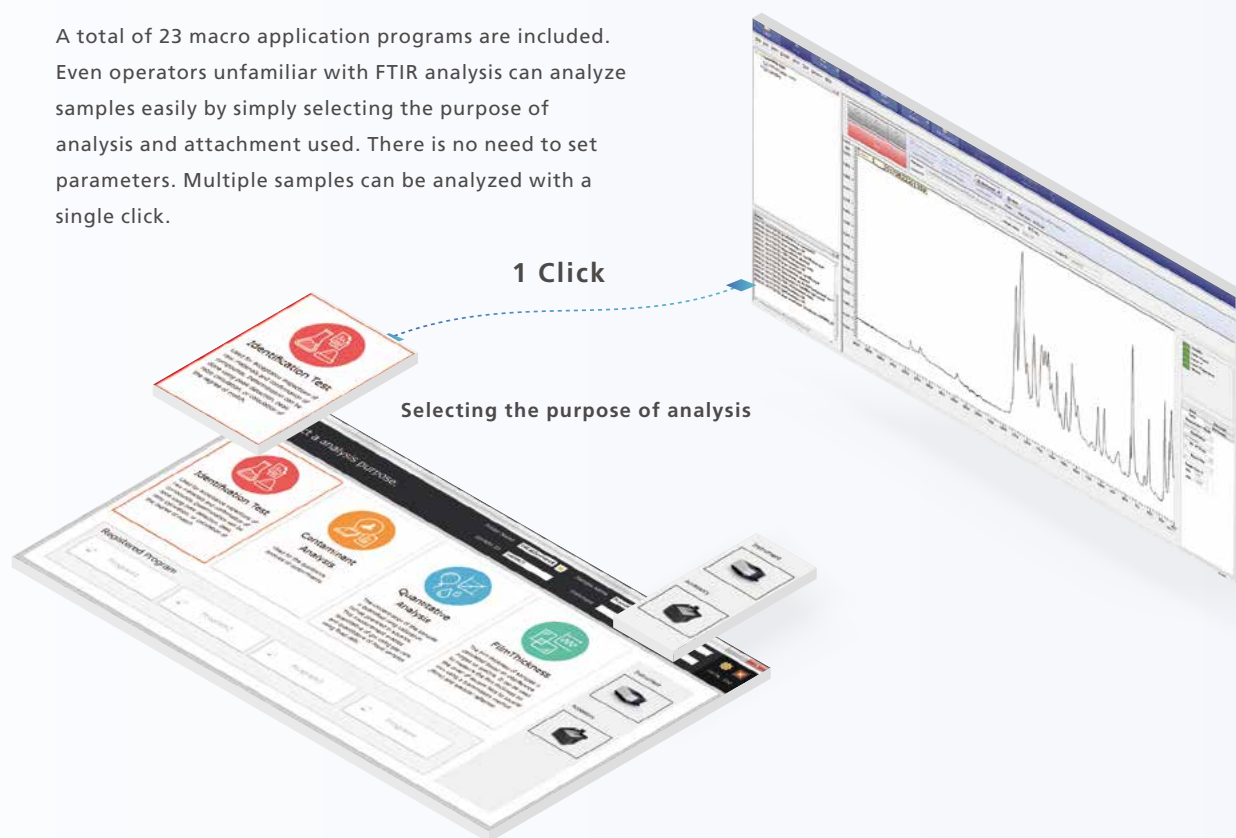
## Program Specifically for Supporting Identification Testing

This program makes pass/fail judgments for test samples based on verification methods specified in pharmacopoeia and official methods specified in respective countries. In addition to identification tests for pharmaceuticals and food products, the program can be used for acceptance and pre-shipment inspections. It calculates how much peak wavenumbers and the intensity ratio between peaks in test samples differ from the corresponding values in standard samples and then makes pass/fail judgments. The results are printed as a report.

## Program Specifically for Supporting Contaminant Analysis

This program can accurately identify measured contaminants using Shimadzu's proprietary algorithm (patent No. 5205918) in combination with a spectral library containing more than 550 spectra for substances commonly detected as contaminants. After analyzing the data, it automatically determines a pass/fail judgment and creates a report. Even for contaminants that are mixtures, the program searches possible principal and secondary components and indicates the certainty level of each substance identified. Because the number of components in the mixture does not need to be specified, even operators with minimal infrared analysis experience can easily analyze contaminants. It displays analysis results within a few seconds after selecting the spectrum.



**Identification Report**
Major Components
(+++) Polytetrafluoroethylene (PTFE) 2
(++) Polytetrafluoroethylene (PTFE) 1
Accessory Components
(+++) CaCO3 3
(++) Sugar (starchy flour)
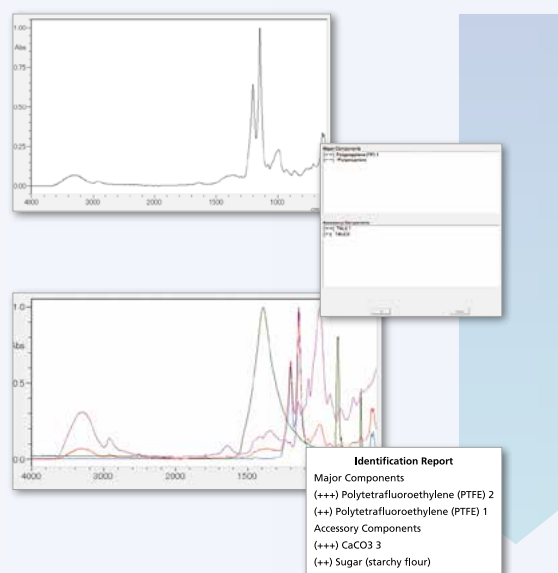
## Library Useful for Identification Testing and Contaminant Analysis

### 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.

| SHIMADZU Food additives library | Reagents | Pharmaceutical products, agrichemicals |
|---|---|---|
| SHIMADZU Contaminant library | Polymers | Inorganic compounds |

## Library Useful for Analyzing Contaminants and Microplastics (Optional)

### Plastic Analyzer method package

When analyzing a plastic, a library is used to qualify the type of material. However, unlike the infrared spectra shape for standard samples, the spectra from plastics that have been denatured (degraded) due to heat or ultraviolet rays can be difficult to qualify in some cases. With a plastic degradation library included, this product enables highly accurate qualitative analysis that takes into consideration the given degradation status.

# Complies Fully with Regulations

## Humidity-Resistant Window Material Compatible with the Wavenumber Measurement Range Specified in Pharmacopoeia

Either a KBr or KRS-5 window can be selected. The KRS-5 window maintains humidity resistance up to 90 %RH (for temperatures up to 30 °C) and is compliant with pharmacopoeia wavenumber range requirements (350 to 7,800 cm$^{-1}$).

| | KBr Window | KRS-5 Window |
|---|---|---|
| Window Material | KBr | KRS-5 |
| Humidity Resistance | With humidity-resistant coating Max. humidity at installation site: 70 %RH (with no condensation) | Max. humidity at installation site: 90 %RH (provided no condensation at temperatures up to 30 °C) |
| Wavenumber Range | 350 to 7,800 cm$^{-1}$ | |
| Transmittance | About 90 %T | About 70 %T |
| Characteristics | High transmittance and high sensitivity Could deliquesce in humid environments | Compared to KBr window: • Higher humidity-resistance • Lower S/N due to lower transmittance |
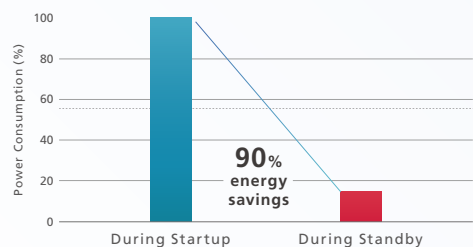


IRXross Power Consumption during Startup (with Start Switch ON) and during Standby (with Start Switch OFF and Dehumidifier ON)

## Internal Dehumidifier (Optional) Ensures High Durability

This dehumidifier removes moisture from inside the interferometer electrolytically using a solid polymer electrolytic membrane. It maintains low humidity levels inside the interferometer without leaving the light source ON. Using the dehumidifier can reduce power consumption by about 90 % compared to leaving the light source illuminated.

## 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.
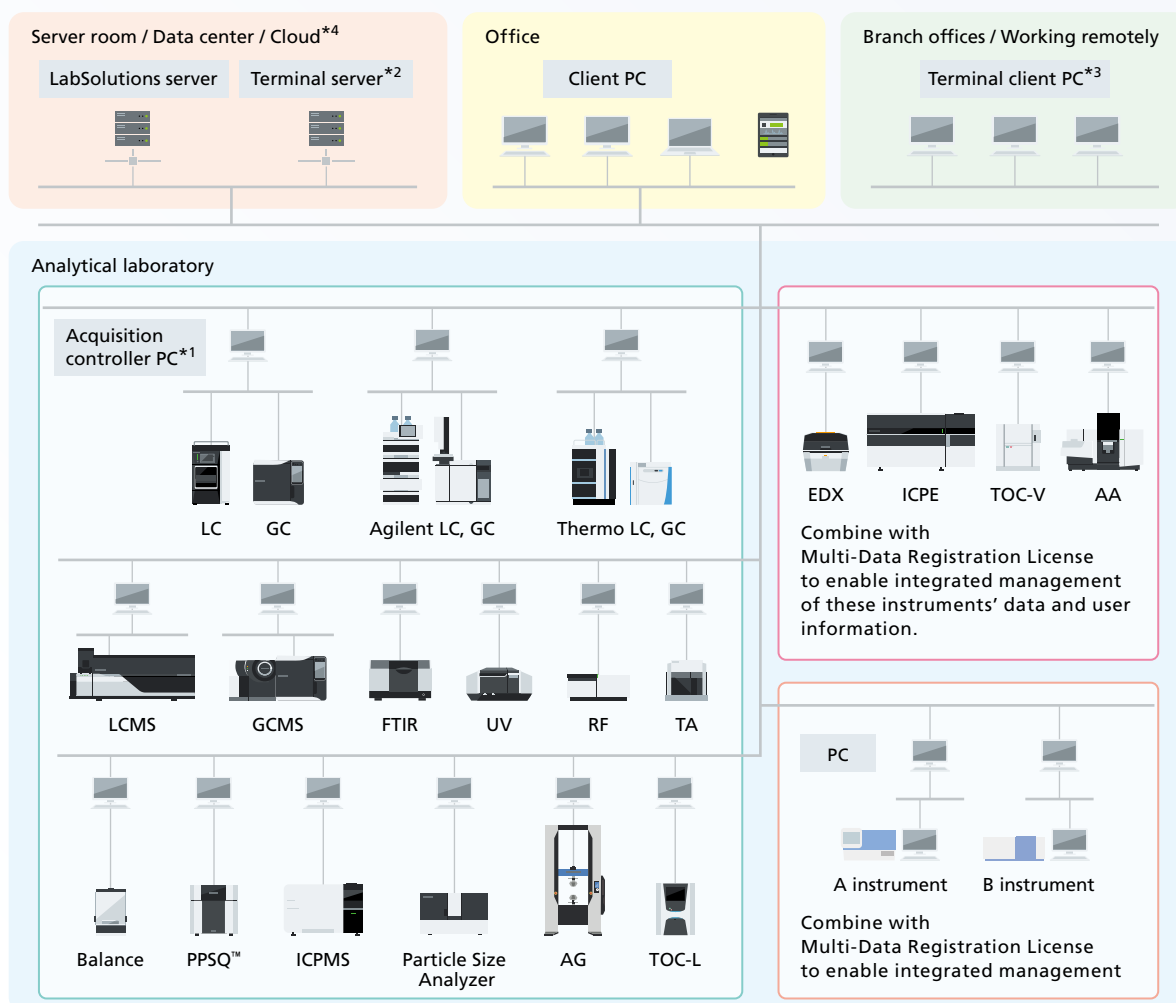
## LabSolutions DB IR

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 LabSolutions 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.



Server room / Data center / Cloud[*4]
LabSolutions server    Terminal server[*2]

Office
Client PC

Branch offices / Working remotely
Terminal client PC[*3]

Analytical laboratory

Acquisition controller PC[*1]

LC    GC    Agilent LC, GC    Thermo LC, GC

LCMS    GCMS    FTIR    UV    RF    TA

Balance    PPSQ™    ICPMS    Particle Size Analyzer    AG    TOC-L

EDX    ICPE    TOC-V    AA

Combine with Multi-Data Registration License to enable integrated management of these instruments' data and user information.

PC

A instrument    B instrument

Combine with Multi-Data Registration License to enable integrated management

*1  The acquisition controller PC controls analytical instruments.
*2  A terminal server is a server for using terminal services. Users can view data reports and perform electronic signature operations through terminal services. It is ideal for remote connections because of the low network load. Only LC, GC, LCMS, and GCMS support analysis and postrun operations through terminal services.
*3  If a terminal service is used, LabSolutions software does not need to be installed on client PCs or tablets.
*4  Servers can be built on various clouds (IaaS). AWS (Amazon Web Services), Microsoft® Azure®, GCP™ (Google Cloud Platform™)

## Data Integrity Compliance

**Project B**

**LabSolutions server**

**Project A**

## 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 status. In addition, a box can be selected to prevent overwriting a data file and outputting an item to a report can be performed.

## Essential 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

Report set includes test methods and test results for a series of samples analyzed as well as 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. It provides visibility of the individual analytical operations, and helps to check for operating errors and improve the efficiency and reliability of checking processes.

# Applications and Options

### Electrical/Electronic Applications

**(Defect Analysis and Contaminant Analysis)**

Microscopes are well suited to measuring micro-areas. Because they focus the light, there is greater light loss than with regular measurements, but they can accurately identify tiny peaks from a high-sensitivity interferometer.

### AIMsight™ Infrared Microscope

The automatic analysis systems can be used with ease even by users new to analysis work. It is equipped as standard with a variety of enhanced functions (Wide-field camera, Automatic contaminant recognition system, Length measurement function, Contaminant analysis program, Spectrum advisor function) that support analysis work.

### AIRsight™ Infrared/Raman Microscope

Infrared and Raman microscopy based on a combination of two analytical techniques to provide complementary molecular information. Both infrared and Raman spectra can be measured from the same position in the extremely small area without moving the sample. As it is equipped standard with 532 nm and 785 nm lasers, it is possible to analyze samples susceptible to fluorescence.

**For Infrared Measurement**
### ATR Objective

This objective lens is used when performing ATR measurements with the AIMsight infrared microscope. Using a cone-type prism, this single reflection objective features 15× 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.

**For Infrared/Raman Measurement**
### Mapping Program

The mapping program measures the absorption distribution on the surface of a sample and creates imaging data when used with the Shimadzu AIMsight infrared microscope and AIRsight infrared/raman microscope. It allows setting of mapping parameters, such as the mapping range, the scan intervals, and the background positions, on the composite visible images.
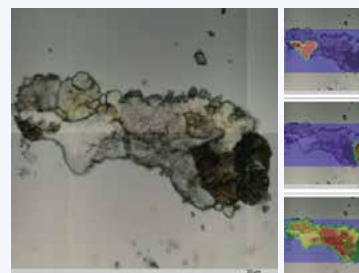
## Chemicals and Polymer Applications

**(Tracking Reactions in Materials)**

Rapid scan measurements are useful for tracking reaction changes in UV curable resins. Optional Rapid Scan software can visually display time-course changes in target peaks during each scan. As scan speeds increase, the sensitivity of the standard DLATGS detector can decrease due to the detector's frequency characteristics. However, an optional MCT kit can be installed to enable high-sensitivity measurements even at high scan speeds.

### QATR™ 10

This single-reflection ATR attachment features a prism made of only diamond to enable measurements up to 400 cm$^{-1}$ (wide range model). Spectra are measured from liquid samples by simply placing a droplet on the prism. Other samples are measured by placing them on the prism and clamping them against the prism surface. The angle of incidence is 45 degrees. Four types of prisms are available, including a Ge, ZnSe, and two diamond prisms (wide range and high-throughput models). The Ge prism is best suited for samples with a high refractive index.

### MIRacle™ 10

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.

### Rapid Scan

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.
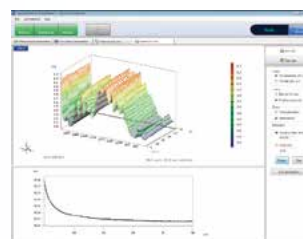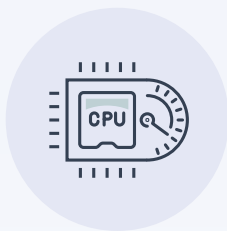
**Semiconductor Applications**

**(Monitoring Semiconductor-Related Gases)**



**Environmental Applications**

**(Exhaust Gas Analysis)**

Gas analysis requires selecting a cell length and window material appropriate for the type and concentration of gas being analyzed. Longer optical path lengths result in greater than normal light losses, but reliable data can be obtained using a high-sensitivity interferometer to suppress baseline noise. Additionally, an MCT kit can be installed to increase sensitivity.

## Time Course Software

The time course program is used to collect spectra in regular intervals. It 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. The scan interval is dependent on resolution, number of scans, and mirror speed. The fastest speed under a 16 cm$^{-1}$ resolution and a mirror speed of 9 mm/s is 7 seconds for 1 accumulated scan.



## 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.



5-cm Gas Cell

Long-Path Gas Cell

## MCT Kit

Use a high-sensitivity MCT detector for analyses where a large amount of light is not available, such as monomolecular film analysis on metal substrates, high-speed reaction tracking, and low-concentration gas analysis using a gas cell with a long path length. The kit installs an MCT detector on the IRXross. Switching between the standard DLATGS detector and the MCT detector is performed automatically from LabSolutions IR. In addition, the kit has a built-in liquid nitrogen sensor to terminate current flow when the detector element is not being cooled, thus protecting the MCT detector.

**SHIMADZU**

## Shimadzu Corporation

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