C103-E114D

SHIMADZU
Excellence in Science

Fourier Transform Infrared Spectrophotometer

IRSpirit

reddot award 2018
winner

IRSpirit™, Ready to Run

Space-Efficient with High Expandability

- Compact FTIR that travels where it's needed.
- For sites with only a narrow space available, samples can be measured with the unit positioned horizontally or vertically.
- With the widest sample compartment in its class, it easily accommodates Shimadzu and third-party accessories.

Dedicated IR Pilot™ Program Ensures Immediate and Easy System Operation

- IR Pilot includes 23 application programs as standard.
- Includes an identification test program convenient for routine inspections as standard.
- Includes a pass/fail judgment program specialized for contaminant analysis as standard.

High Reliability Ensures the System Can Be Introduced with Confidence

- Stable interferometer performance based on technology inherited from high-end models.
- Designed to endure high-humidity environments (selectable KRS-5 window + optional electric dehumidifier).
- Instrument status monitoring function enables users to understand the instrument status easily.
- Anti-theft and anti-drop keylock can be installed.

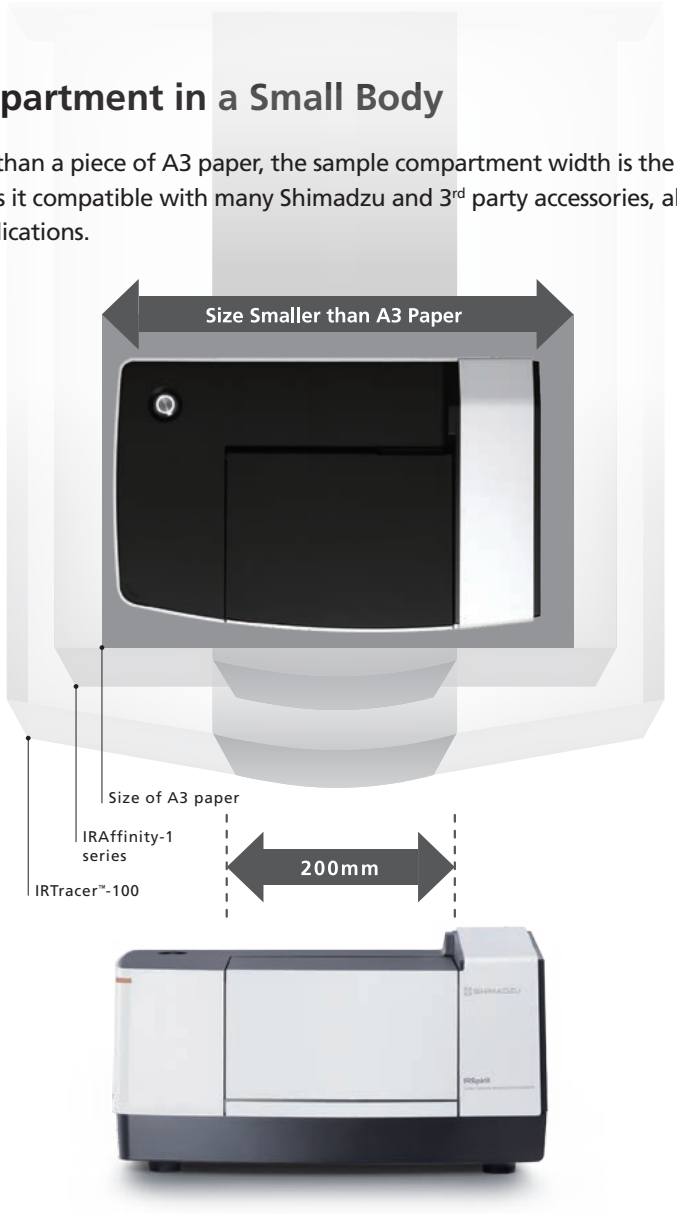
Space-Efficient with High Expandability

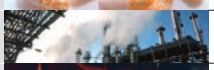
Even Fits in Small Spaces

There is a growing need for systems that can fit in tight spaces, such as for lining up a row of units used for student experiments or to enable measurements in an environment with many different samples and experimental tools laid out for use in chemical synthesis. For sites with only a narrow space available, samples can also be measured with the unit positioned vertically (see diagram below). The start switch is accessible and the humidity indicator is visible from both directions.
The prism and FTIR main unit are the same in height. Therefore, samples can be placed directly on the ATR attachment, which is integrated with the sample compartment. That can eliminate the trouble of having to cut large samples.

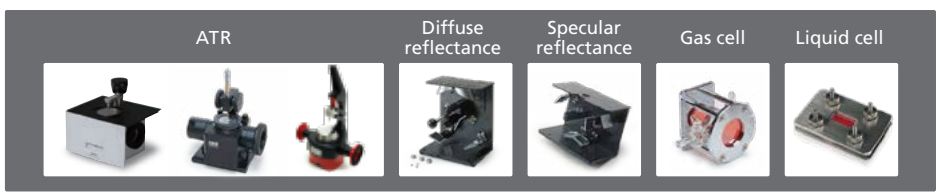
Large Sample Compartment in a Small Body

In spite of a body size smaller than a piece of A3 paper, the sample compartment width is the same as on higher-end models. This makes it compatible with many Shimadzu and 3rd party accessories, allowing it to be used for a wide variety of applications.



Fields \ Applications		Contaminant analysis	Raw materials acceptance inspection	Identification tests	Quantitative analysis	Spectral analysis
Pharmaceuticals and life sciences		○	○	○	○	
Chemicals and petroleum		○	○	○		
Academia				○	○	○
Environmental		○			○	○

○ : Applicable

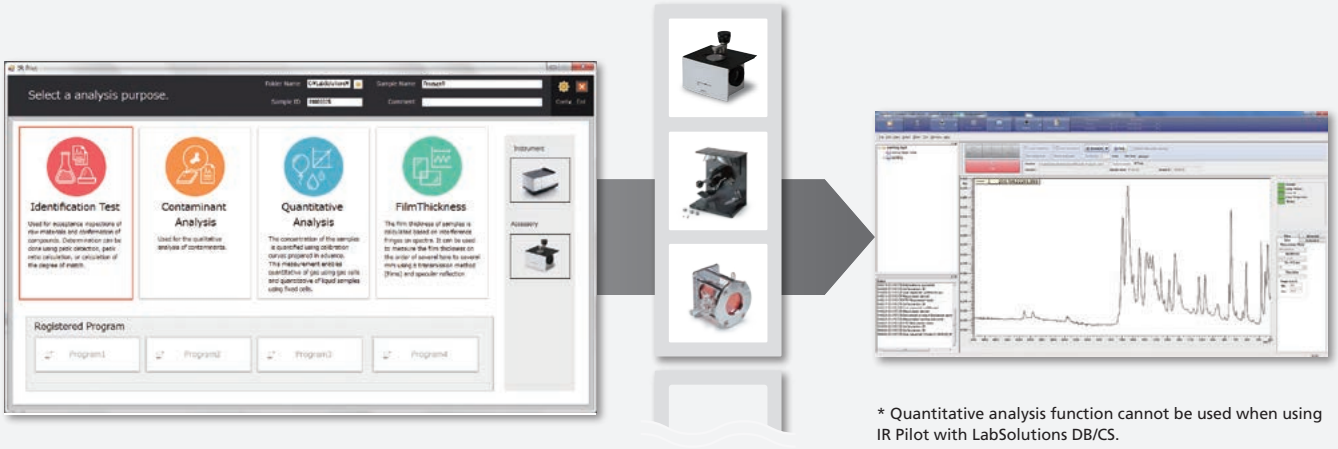


Dedicated IR Pilot Program Ensures Immediate and Easy System Operation

ANALYTICAL INTELLIGENCE

IR Pilot

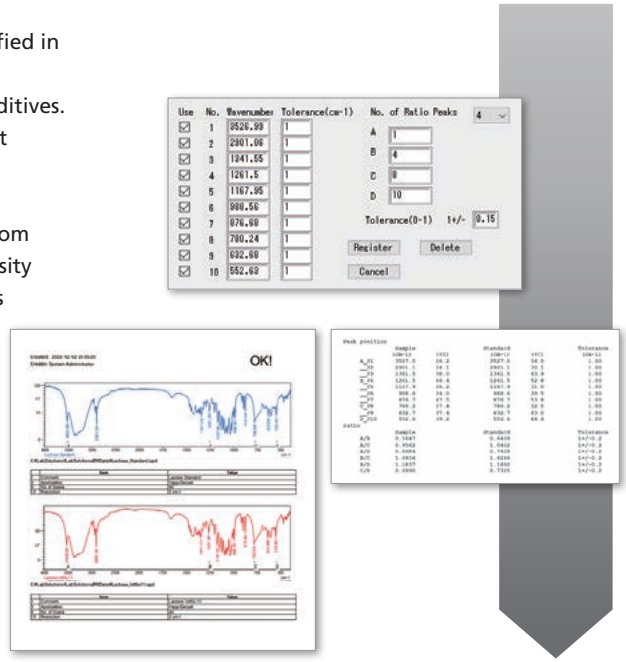
IR Pilot offers a total of 23 application programs as standard, making it easy for operators with minimal FTIR experience to analyze samples by simply selecting the analysis purpose and accessory. There is no need to set parameters. It enables the measurement of multiple samples with only one click.



* Quantitative analysis function cannot be used when using IR Pilot with LabSolutions DB/CS.

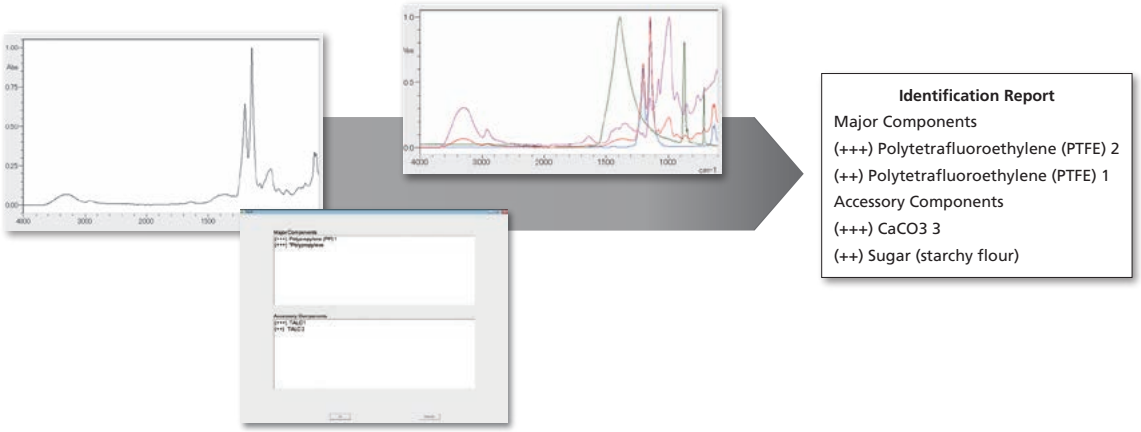
Identification Test Program

This program makes pass/fail judgments for test samples based on verification methods described in Pharmacopoeia and standards specified in each country, such as "Infrared Spectrophotometry" in the Japanese Pharmacopoeia and Japan's Specifications and Standards for Food Additives. In addition to identification tests for pharmaceutical and food product identification tests, the program can also be used for acceptance and pre-shipment inspections.
The program calculates the difference between peak wavenumbers from standard and test samples and the difference between the peak intensity ratios and then prints a report of pass/fail judgment results. It includes spectra for the 57 substances specified in Japan's Specifications and Standards for Food Additives.



Contaminant Analysis Program

The contaminant analysis program identifies measured contaminants using Shimadzu's proprietary identification algorithm (Japanese Patent No. 5205918) in combination with a spectral library containing more than 550 spectra for substances commonly detected as contaminants. After data analysis, it automatically makes a pass/fail judgment and creates a report. Even if the contaminant is a mixture, it searches for major and minor components and displays their ranks. Since the number of components in the mixture does not need to be specified, even operators with minimal infrared analysis experience can easily analyze samples.

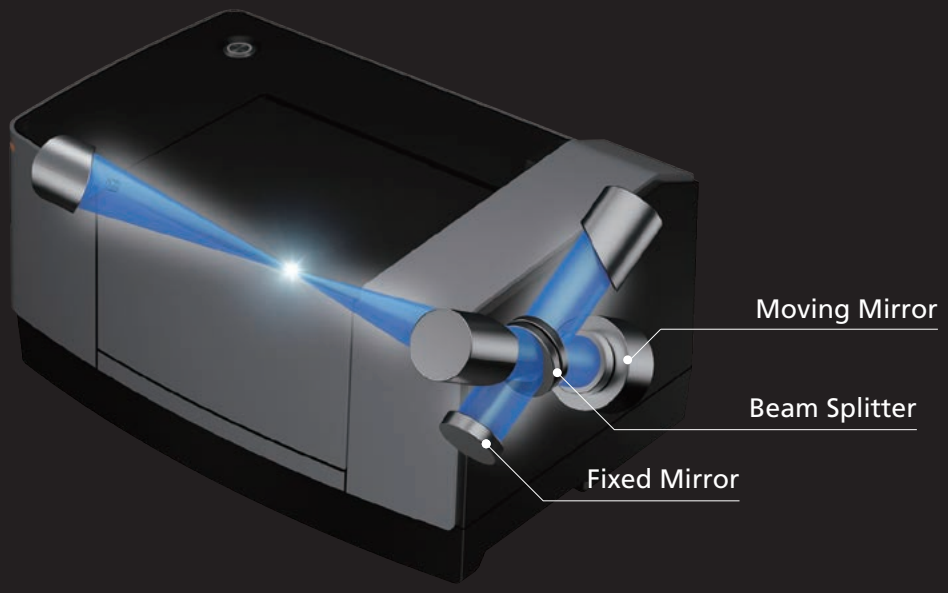


Identification Report
Major Components
(+++) Polytetrafluoroethylene (PTFE) 2
(++) Polytetrafluoroethylene (PTFE) 1
Accessory Components
(+++) CaCO3 3
(++) Sugar (starchy flour)

Shown here is an analysis of a contaminant attached to a tablet surface using the Contaminant Analysis Program. The results showed Polytetrafluoroethylene (PTFE) was the major component, and sugar and calcium carbonate were the accessory components. Since the two accessory components are often used as tablet components, it is estimated that the components were scraped up at the same time when scraping the contaminant.

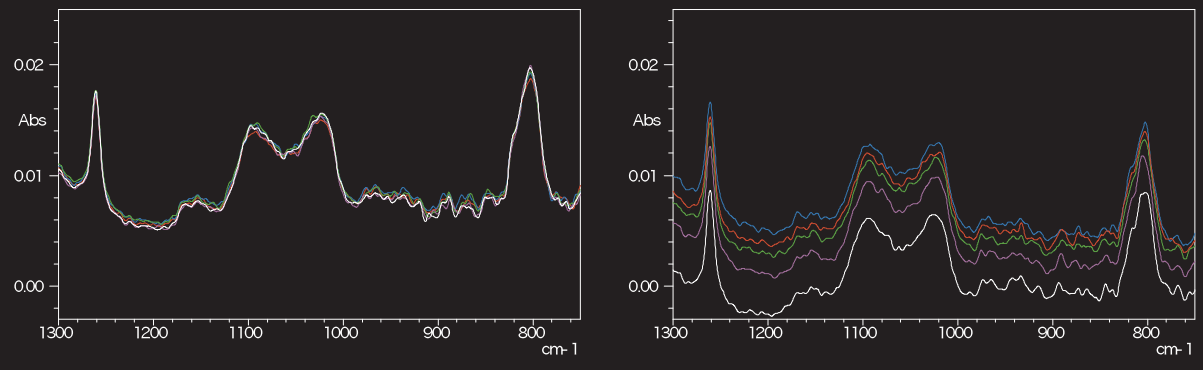
High Reliability Ensures the System Can Be Introduced with Confidence

Technology Inherited from Higher-End Models



- High stability and throughput
  (Features dynamic alignment at 5000 times per second and a high-brightness ceramic light source)
- High sensitivity comparable to general-purpose models (IRSpirit-T)
  (DLATGS detector with temperature control function)

The silicone oil content in the paraffin oil (1.0%) was obtained by repeating the single-reflection ATR method for five times. Data obtained using the DLATGS detector with temperature control is shown on the left and data obtained using the DLATGS detector without temperature control is shown on the right. The internal heat in the instrument and the environment temperature caused large baseline data fluctuations without temperature control. In contrast, using the detector with temperature control resulted in highly repeatable data.



ATR Spectrum of Silicone Oil Content in Paraffin Oil (measurement repeated five times)
Left: DLATGS detector with temperature control
Right: DLATGS detector without temperature control

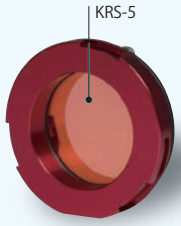
High Reliability Due to Humidity-Resistant Design

The robust optics are designed to ensure the system can be used reliably even under harsh temperature and humidity conditions.

- Optics sealed in an aluminum die cast body
- Status monitor function features electrical and paper-based indicators.
- Beam splitter includes a humidity-resistant coating.
- Select from a KBr window (to 70% RH) or a KBS-5 window (to 90% RH) which both include a humidity-resistant coating.*
- Optional electric dehumidifier can be installed.

*No condensation

KBr Window (Selectable)



KRS-5 Window (Selectable)

Aluminum die cast interferometer

Instrument Status Monitoring

Instrument status is automatically verified during start-up and results are saved in a report. This feature is especially convenient for instrument management. Pharmacopoeia-compliant programs* convenient for routine inspections are also included.

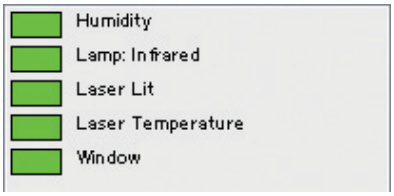
* See description of identification test program on page 7.

■ Self-diagnostic function

An automatic self-diagnostic function inspects the signal system and optics during instrument initialization. It obtains a variety of information and automatically outputs the results in one file, making instrument management easy.
The instrument status history can also be confirmed.

■ Status monitor function

This function continuously monitors and manages information about the light source, semiconductor laser, humidity inside the instrument, the window plate connection (interlock), and accessories.

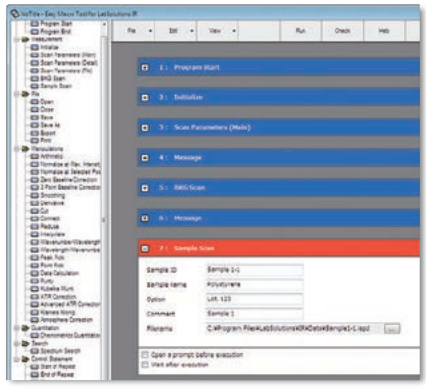


Macro Functions Provide Automation and Labor-Savings

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

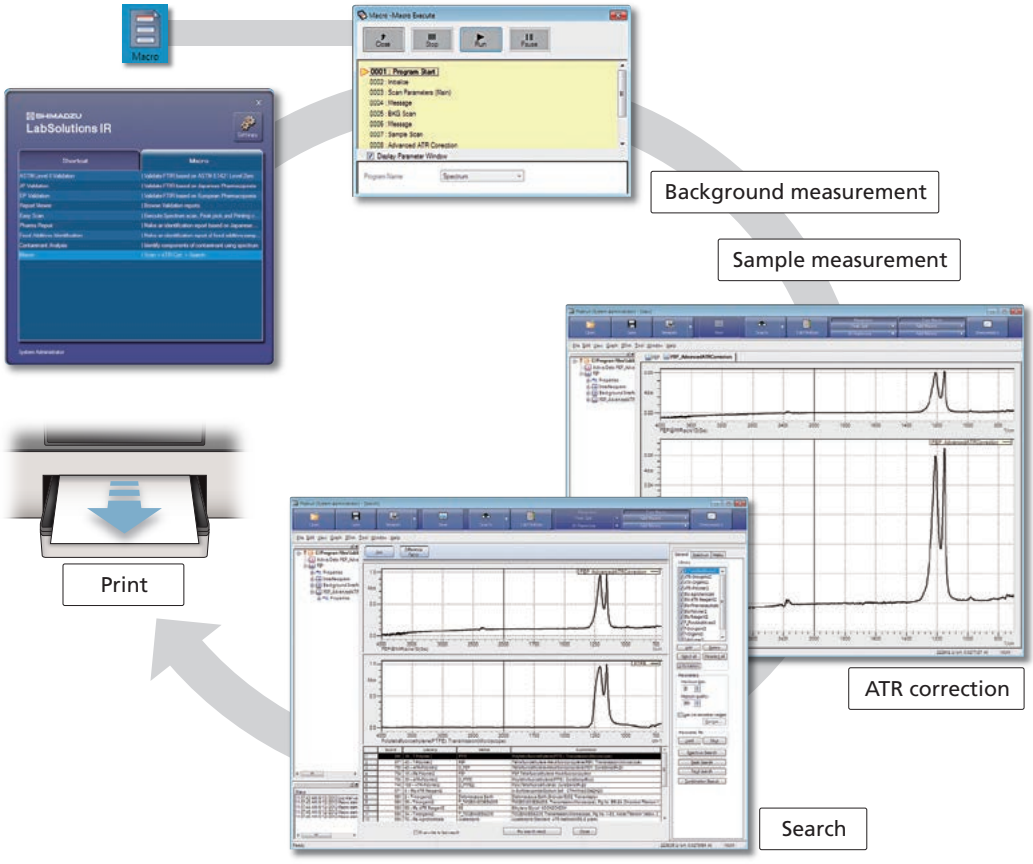
Easy Macro – Just a Single Click Launches Routine Work

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



Hardware Options

QATR™-S

The QATR-S is a single-reflection ATR measurement attachment. The prism is made of diamond, so the measurement wavenumber range is up to 400 cm^{-1} (wide-band). With a liquid sample, simply place a drop on the prism to measure spectra. For other samples, clamp the sample closely against the prism surface before measurement on the sample surface. Large samples (with a large area) can be measured without cutting. The incident angle is 45 degrees. Three prism materials are available: diamond (high-throughput), germanium (Ge) or zinc selenide (ZnSe). The Ge prism is best suited for samples with a high refractive index.
Functionality is included for automatically recognizing attached accessories.

(Samples Can Be Measured: Powders, Moldings, Thin Films, Films, Liquids, Rubber)

DRS-8000A (P/N 206-62301-58)

SiC sampler

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 200-66750-01) 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 LabSolutions IR software.
Functionality is included for automatically recognizing attached accessories.

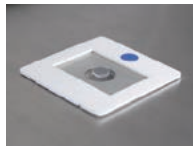
(Samples Can Be Measured: Powders, Moldings)

MHP-1 (P/N 200-66747-91)

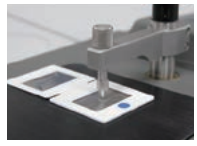
This is a compact, inexpensive hand-driven press used to produce 4 mm dia KBr pellets. A pellet produced in the frame is directly measured using the dedicated holder, which ensures exceptional simplicity of operation. No dies or vacuum pump are required.

(Samples Can Be Measured: Powders)

EDXIR-Holder™ (P/N 221-25890-41)



Measurement with EDX



Measurement with FTIR

This foldable holder consists of an adhesive layer with samples attached and polypropylene film designed for X-ray fluorescence analysis. It provides measurement by keeping the samples in the holder with EDX and FTIR. 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.
Close the holder after the measurement and it can be used as a sample stocker.

(Samples Can Be Measured: Powders, Moldings, Thin Films, Films, Liquids, Rubber)

Dehumidifier Unit (P/N 206-31050-46)

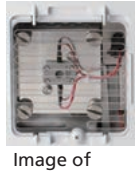


Image of Dehumidifier

Back Side of IRSpirit

This is the same electric dehumidifier unit used in the higher-end models (IRAffinity-1 series and IRTracer-100). The dehumidifier is driven by a stand-by power, so it is possible to maintain a low level of humidity inside the interferometer even when the FTIR is not used (AC power supply). It can reduce the labor and maintenance costs associated with replacing the silica gel.

Software Options

Contaminant Library for LabSolutions IR

(P/N 206-33179-91)

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 water supply maintenance parts commercially available in Japan, the library also includes X-ray fluorescence profiles (PDF files) to significantly improve the accuracy of contaminant searches. Unlike existing libraries, this contains data on mixed compounds and incorporates all the depth of knowledge and 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.

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 and number of scans. Maximum measurement time is 48 hours but it depends on scan parameters. The time course software includes a 3D Processing program.

EDXIR-Analysis™ Software

(P/N 206-33175-91)

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.

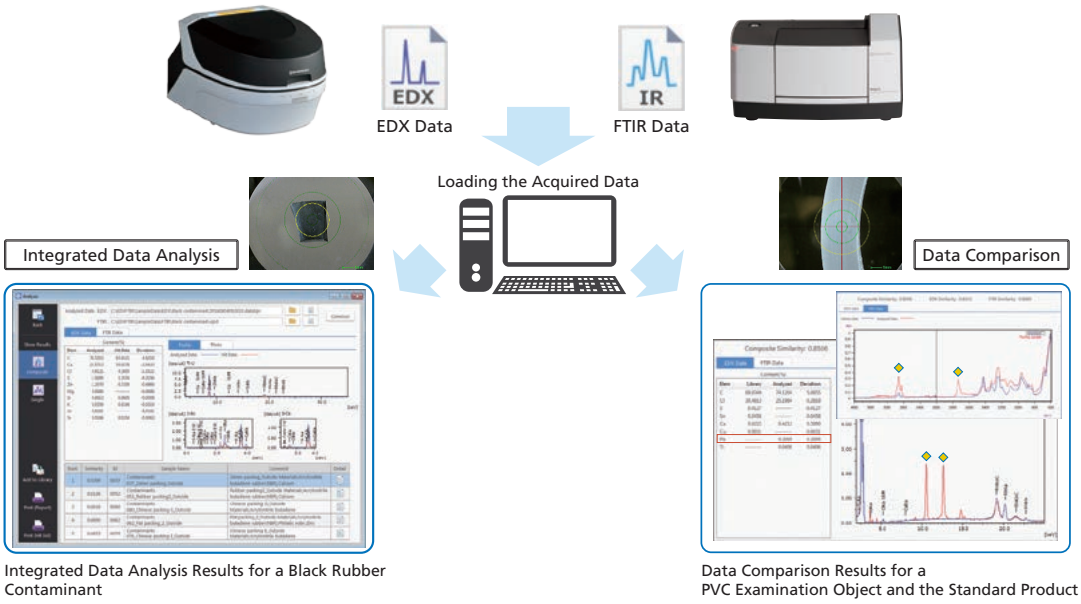
To perform qualitative analysis automatically, simply click "Analyze Both Data" and select the EDX/FTIR data*1. This heightens the efficiency of data analysis and provides strong support for contaminant analysis. In addition to a list of hits, the integrated data analysis results show EDX profiles and 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.

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.

*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 Analysis of Contaminant Data and Data Comparisons for Confirmation Tests

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.

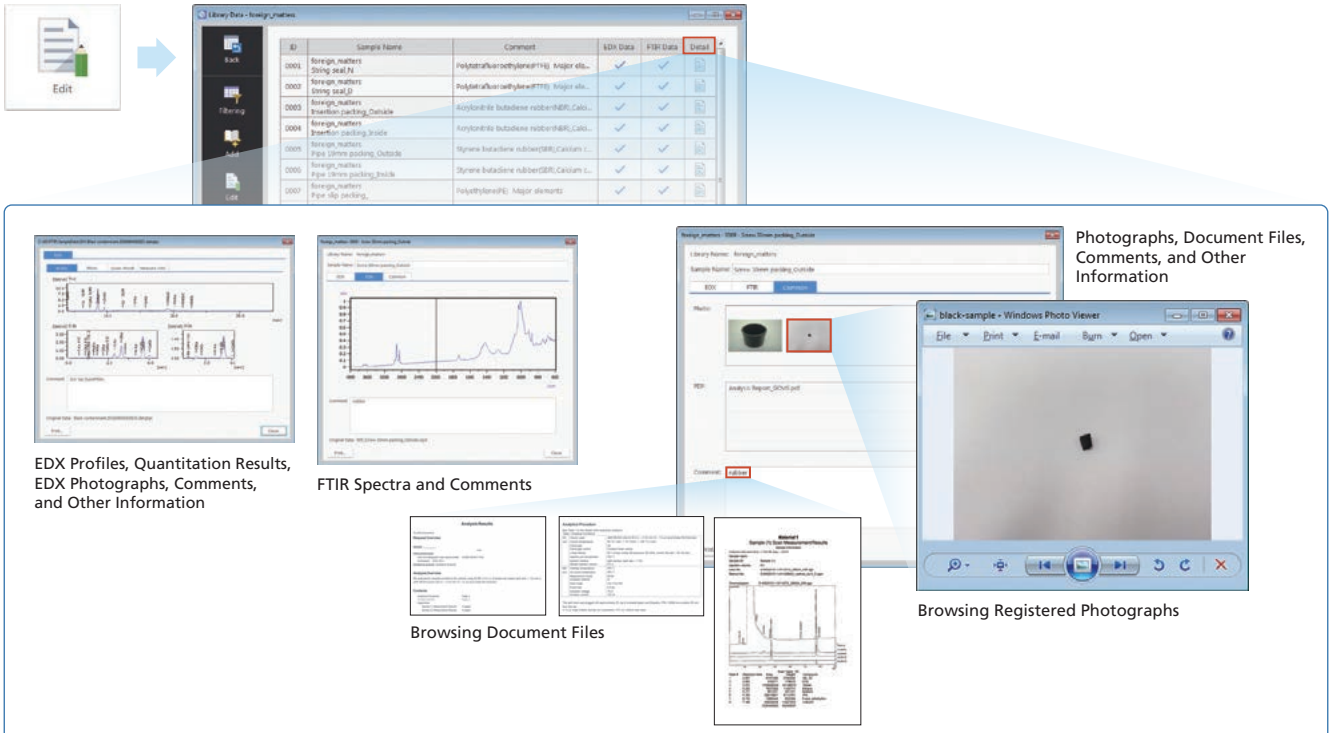


Integrated Data Analysis Results for a Black Rubber Contaminant

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

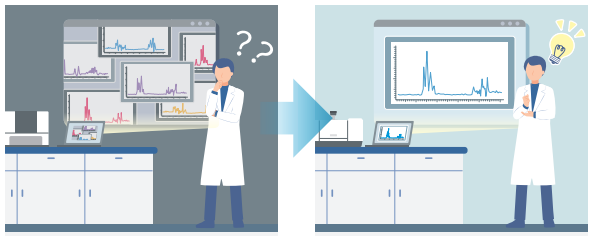
Data Browsing and the Registration, Editing, Deletion of Data, Images, Document Files

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.



Supporting Contaminant Analysis and Deteriorated Microplastics Analysis

When analyzing plastics, libraries are used to qualify their material properties. However, infrared spectra of plastics that have been denatured (have deteriorated) due to heat or UV rays differ in shape from standard spectra, and qualifying them can sometimes be difficult. To address this, the Plastic Analyzer includes a deterioration library, so highly accurate qualification can be performed reflecting the state of deterioration.

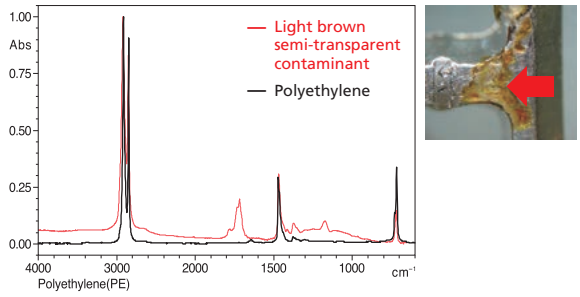


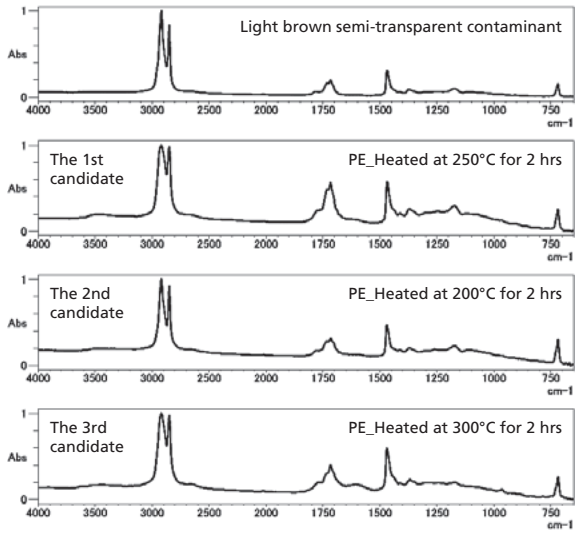
Unable to determine if a sample is deteriorated plastic or another substance

Capable of qualification reflecting the state of deterioration

Contaminant Analysis (Contaminants in Processed Items)

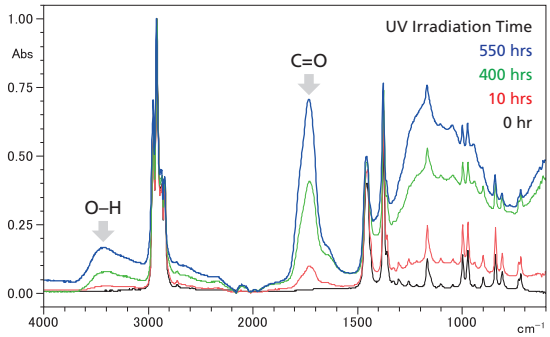
The measurement of a light brown semi-transparent contaminant on a plated item was performed. The figure below shows that the spectral pattern of the acquired infrared spectrum differs from the standard polyethylene (PE).
Plastic Analyzer shows the best match is heated PE. The Thermal-Damaged Library makes it useful for surmising the thermal history of the plastic.

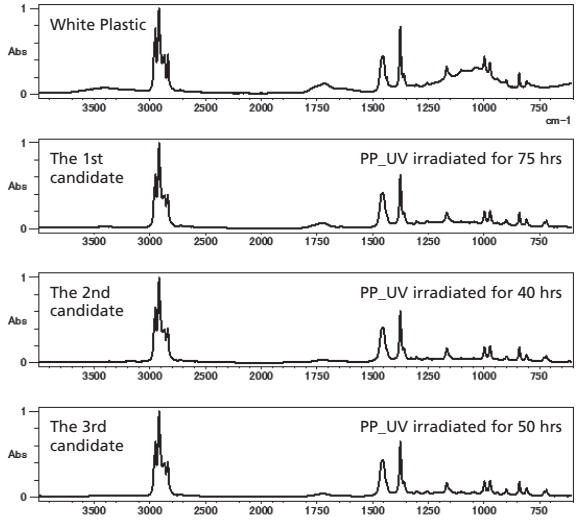




Evaluation of Deteriorated Samples

Plastics degrade as they experience molecular cleavage and cross-linking due to heat and light. As a result, in fault analysis and failure analysis, the qualities of deteriorated samples must be analyzed.
The figure at bottom left shows the infrared spectrum of a polypropylene (PP) sample that has been irradiated with UV rays. The UV irradiation has caused the plastic to deteriorate, and it is evident that the shape of the infrared spectrum has changed.
The figures at bottom right show the search results from measurements by Plastic Analyzer of a white plastic (PP material) that was left outdoors for an extended period and exposed to UV rays.
The infrared spectrum of the sample exposed to UV rays differs from the standard spectrum. Accordingly, in general library searches, different plastics such as polybutene are at the top of the results. In contrast, with Plastic Analyzer, PP denatured by UV rays is the top result.





Plastic Analyzer consists of the following.

- Fourier transform infrared spectrophotometer
- Single-reflection ATR attachment
- Plastic Analyzer method package
  1. UV-Damaged Plastics Library*1 **2** . Thermal-Damaged Plastics Library*1
  3. Macro Program for IR Pilot™/Parameter File*2

IRSpirit + QATR-S System

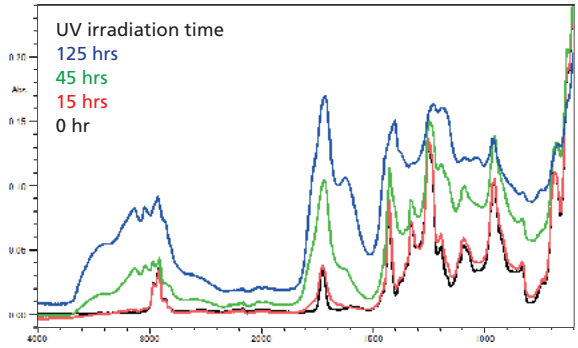
Plastic Analyzer Method Package

- Navigates from measurement to analysis without complicated parameter settings.*2
- UV-damaged plastics library and thermal-damaged plastics library are compatible with any FTIR models controlled by LabSolutions IR.

*1: Purchasing/Using a library is available.
*2: Only available with IRSpirit Fourier transform infrared spectrophotometer.

1 UV-Damaged Plastics Library

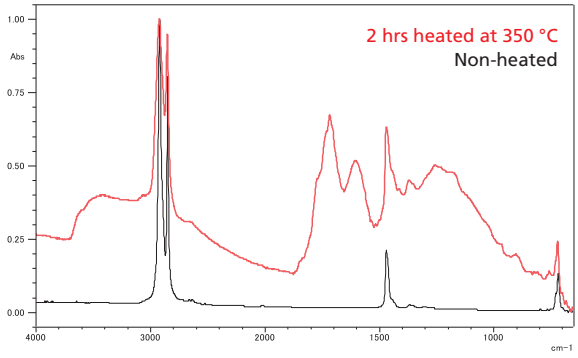
This library includes more than 300 spectra from the UV degradation of 14 types of plastic. This proprietary Shimadzu library includes the IR spectra for plastics degraded by UV rays for the equivalent of approximately 10 years using a super accelerated weathering chamber from Iwasaki Electric Co., Ltd.



Hard PVC Spectra Listed in the UV-Damaged Plastics Library

2 Thermal-Damaged Plastics Library

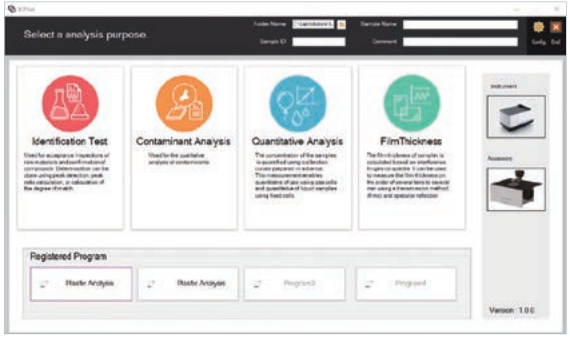
This library includes more than 100 spectra from the degradation of 13 types of plastic heated to between 200 and 400 °C.
This proprietary Shimadzu library contains IR spectra for plastics degraded by heating, acquired through measurements at the Hamamatsu Technical Support Center at the Industrial Research Institute of Shizuoka Prefecture.



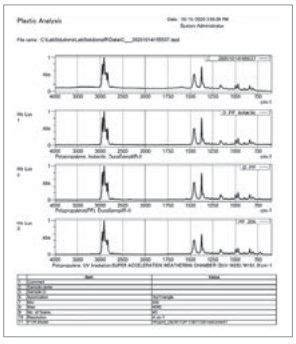
Polyethylene Spectra Listed in the Thermal-damaged Plastics Library

3 Macro Program and Parameters

The system includes plastic measurement parameters and IR Pilot, a special program for IRSpirit that simplifies spectral measurements and the creation of reports, enabling analysts to perform everything from the measurement of target samples to data analysis easily. Even users unfamiliar with FTIR analysis can start work immediately.



IR Pilot, a Special Program for IRSpirit



Report Output

Sample Positioning

Solutions Achieved with LabSolutions IR

Reliable LabSolutions Software

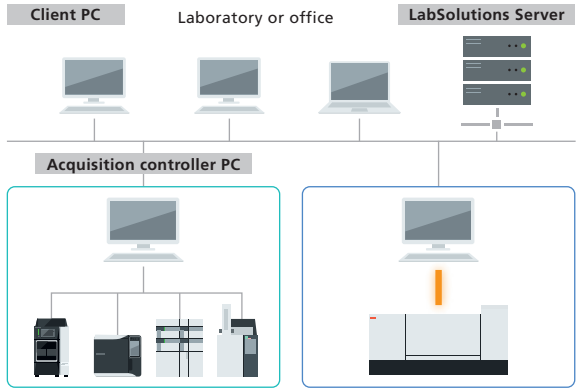
In addition to LabSolutions IR, which provides basic functionality, Shimadzu also offers LabSolutions DB IR and LabSolutions CS IR to meet the requirements of ER/ES regulations.

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

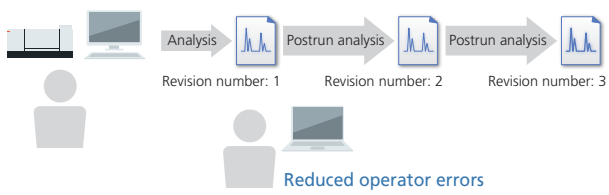
LabSolutions CS, which is freely accessible to the analysis network, can be connected to IR, eliminating the need for connecting a PC to the instrument. Since all the data are managed on a server, LabSolutions CS IR can be read from any personal computer on a network. With terminal service, LabSolutions 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.	

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.



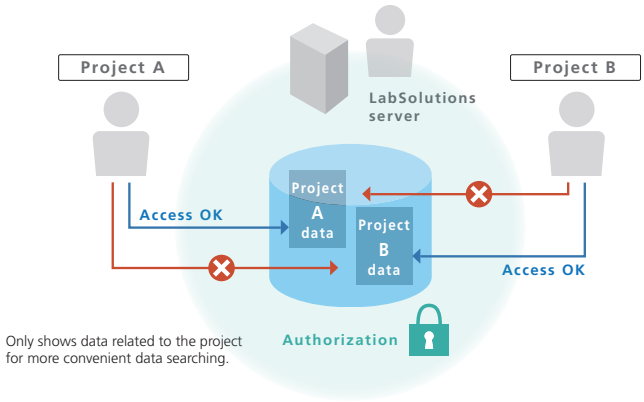
Solid Security

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.

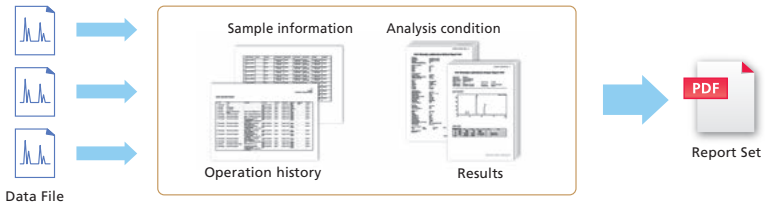
Management can be suited to tasks!



Visualization of a Series 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.

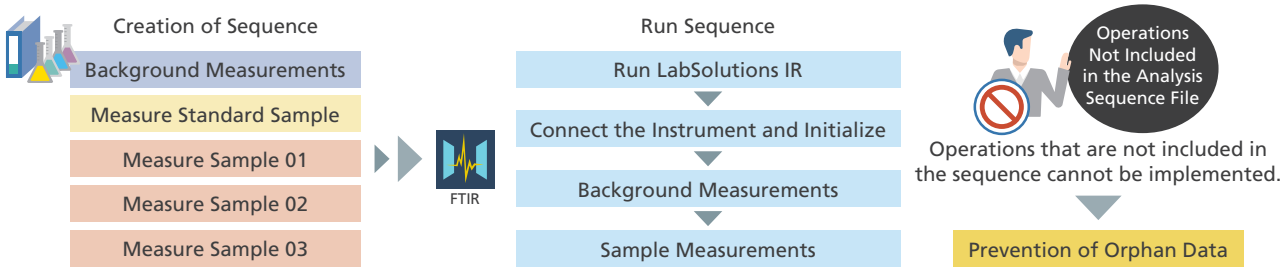


Prevention of Orphan Data by Using Analysis Sequence (Optional)

Ensuring data integrity requires a system that shows no data manipulation has occurred. Shimadzu has achieved this through the introduction of its Analysis Sequence for spectrometers. Using the Analysis Sequence, it is possible to verify that the full chain of analysis has been carried out according to experimental protocol (or SOP).
The LabSolutions Analysis Sequence (optional) provides a three-step workflow:

1. **A sequence is put together according to a given experimental protocol (or SOP). See the flow below for reference.**
2. **The operator conducts analysis in the order shown by the sequence file.**
3. **After analysis, a report set is created from the sequence file used in the analysis. The experiment leader uses the report set to review the data chain generated by the sequence.**

Until now, a problematic issue with data integrity in spectrometers has been the existence of orphan data (data which is isolated and not reviewed, despite being used in the analysis). However, the LabSolutions Analysis Sequence option not only meets the requirements for data integrity by preventing the creation of orphan data, but also allows for highly efficient spectrometer operation.




HUMOTY

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.

eco

This product is certified as Shimadzu's Eco-products Plus.
Energy savings: 62% reduction as compared to the previous model*
Space savings: 76% reduction of weight as compared to the previous model*
70% reduction of installation area as compared to the previous model*
*: IRAffinity-1S

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