SHIMADZU
Excellence in Science

Solutions offered by Shimadzu Corporation
Data Integrity Compliance in the Analytical Laboratory

Improving the Data Integrity of Spectrometers

LabSolutions UV-Vis
UVProbe

Data Integrity

LabSolutions IR
AIMsolution

LabSolutions RF

Improving the Data Integrity of Spectrometers
Shimadzu's Total Support for Data Integrity

Why Data Integrity Is Important?

The following warning letters have been issued by the FDA, demanding swift response regarding analytical instruments that do not support data integrity.

FDA Warning Letter Example A

Warning Letter: 320-18-55   Issue Date: May 23, 2018

You did not have procedures for reviewing audit trails or electronic data for the **Fourier-transform infrared spectroscopy or ultraviolet systems**.

FDA Warning Letter Example B

Warning Letter: 320-17-25   Issue Date: February 24, 2017

Our investigator observed that your laboratory systems lacked controls to prevent your staff from altering or deleting electronic data. Analysts manipulated and deleted audit trails. You lacked adequate controls for all HPLC, gas chromatography, and **ultra-violet systems**.

FDA Warning Letter Example C

Warning Letter: 320-17-01   Issue Date: October 13, 2016

In response, to this letter, provide details of your retrospective review of HPLC and other laboratory data, such as **Fourier transform infrared spectroscopy**, gas chromatography, **UV spectrophotometry**, and (b)(4) analyzer data.

FDA Warning Letter Example D

Warning Letter: 320-15-09   Issue Date: April 6, 2015

You lacked controls to prevent the unauthorized manipulation of your laboratory's electronic raw data. Specifically, your **infrared (IR) spectrometer** did not have access controls to prevent deletion or alteration of raw data.

Data Integrity and Report Set

Data Integrity

Report Set
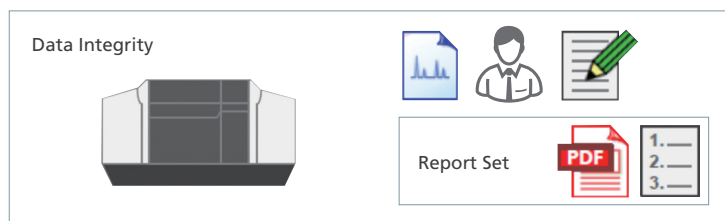
Data integrity refers to the completeness of data, with nothing missing or inconsistent. In other words, not only the data itself but also the metadata (the results of work that require human intervention, such as specifying conditions and analyzing analysis data) must be presented in a visible form, and verified together with the data. This is achieved by the Report Set.

What Is Shimadzu LabSolutions Report Set?

This function gathers operational information (operations and settings that require human intervention) distributed within the software, and collects it in a single report. Much like an electronic book, the content can be checked while turning the pages, which eliminates the need to check operations and settings by switching between windows and tab pages.
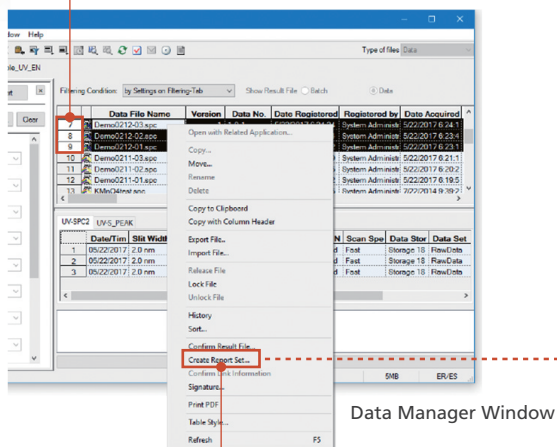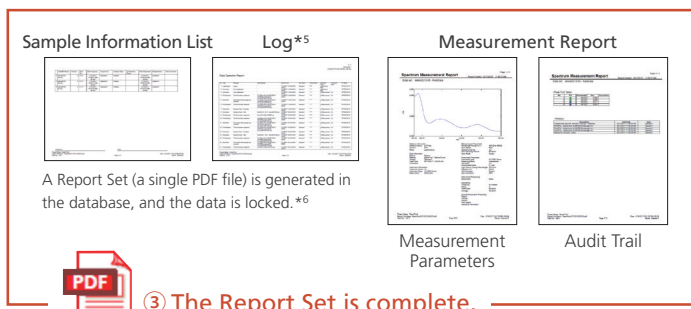

http://www.shimadzu.com/an/data-net/
labsolutions/reportset.html

Procedures for Creating a Report Set*1,*2 with a Shimadzu Spectrometer

The procedures for creating a Report Set with a spectrometer follow the sequence for chromatographs, so the procedures are just as simple as with a chromatograph.
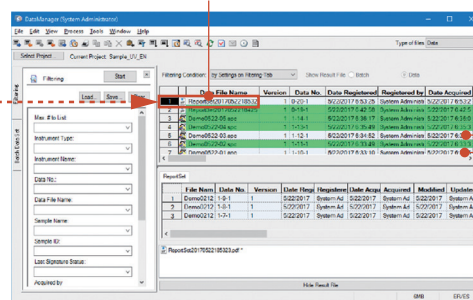
① Select a file.*3,*4

Data Manager Window

② Right-click, and select [Create Report Set].

Sample Information List   Log*5   Measurement Report

A Report Set (a single PDF file) is generated in the database, and the data is locked.*6

Measurement Parameters   Audit Trail

③ The Report Set is complete.

Data Manager Window

The confirmed and approved data is color coded, so orphan data can easily be found.

*1: As of February, 2020, the following functions (1) to (2) are not yet supported for UV, FTIR, and RF Report Sets.
   (1) ID assignment to measurement methods
   (2) Avoidance of duplicate printing of measurement methods for multiple data sets
*2: UV, FTIR, and RF Report Sets are supported by the LabSolutions CS network and LabSolutions DB standalone.
*3: In terms of file selection when creating report sets, for UV, RF photometric maesurement/quantitative measurement, if a single file is selected, a Report Set including any related files will be created.
   In contrast, with UV, FTIR, and RF spectral measurements, if multiple files are related, manually select those files.
*4: In sequential measurement, the report can be created from dataset batch. (A series of data report can be created)
*5: A log is recorded during measurements. If a postrun analysis is performed, a log will also be recorded during the postrun analysis.
*6: Locked files can only be unlocked by users with the relevant rights.

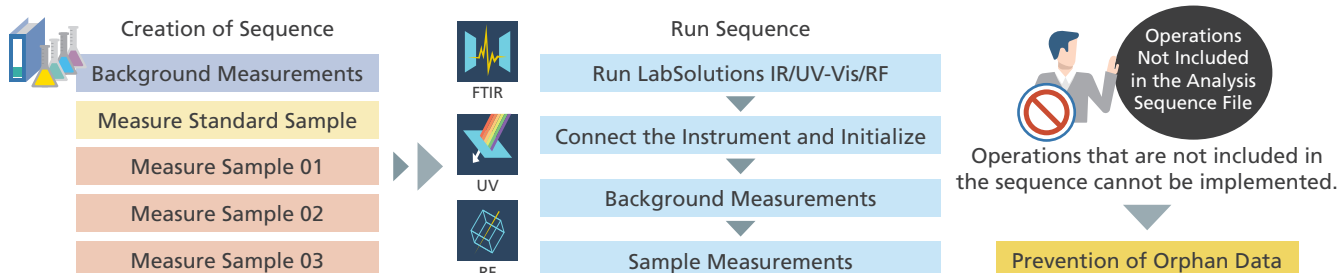# Analysis Sequence (Optional)

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.

Note This is only compatible with LabSolutions UV-Vis, the software that controls UV-Vis spectrophotometers. It is not compatible with UVProbe. Future compatibility with UVProbe is not expected. If compatibility is required, purchase LabSolutions UV-Vis, and then purchase Analysis Sequence separately.

Creation of Sequence
- Background Measurements
- Measure Standard Sample
- Measure Sample 01
- Measure Sample 02
- Measure Sample 03

FTIR / UV / RF

Run Sequence
- Run LabSolutions IR/UV-Vis/RF
- Connect the Instrument and Initialize
- Background Measurements
- Sample Measurements

Operations Not Included in the Analysis Sequence File

Operations that are not included in the sequence cannot be implemented.

Prevention of Orphan Data

Compatibility with Data Integrity for IR Microscopes (Optional)

The main application of IR microscopes is contaminant analysis, and compatibility with standards is not required. However, such instruments are often installed in the same laboratory as instruments used for confirmatory test applications. During inspections, it is necessary to explain the lack of compatibility with standards to inspectors. To avoid this troublesome process, the control software for IR microscopes for contaminant analysis applications is now compatible with data integrity.

The operations are simple. Run LabSolutions IR, the Shimadzu software used for confirmatory test applications. Click [AIM] for IR microscope measurements, which is built into the software. This will display the existing AIMsolution program. Then configure the various conditions, and start the measurements. After the measurements are finished, the data obtained is automatically transferred to the LabSolutions IR software, after which it is transferred up the line.

Note 1) Data integrity compatibility is not available when using the AIMsolution mapping software.
Note 2) The measurements are performed with AIMsolution. This is not compatible with Analysis Sequence.

Database Version (DB)

Client-server Version (CS)

Run LabSolutions IR from LabSolutions Manager Window
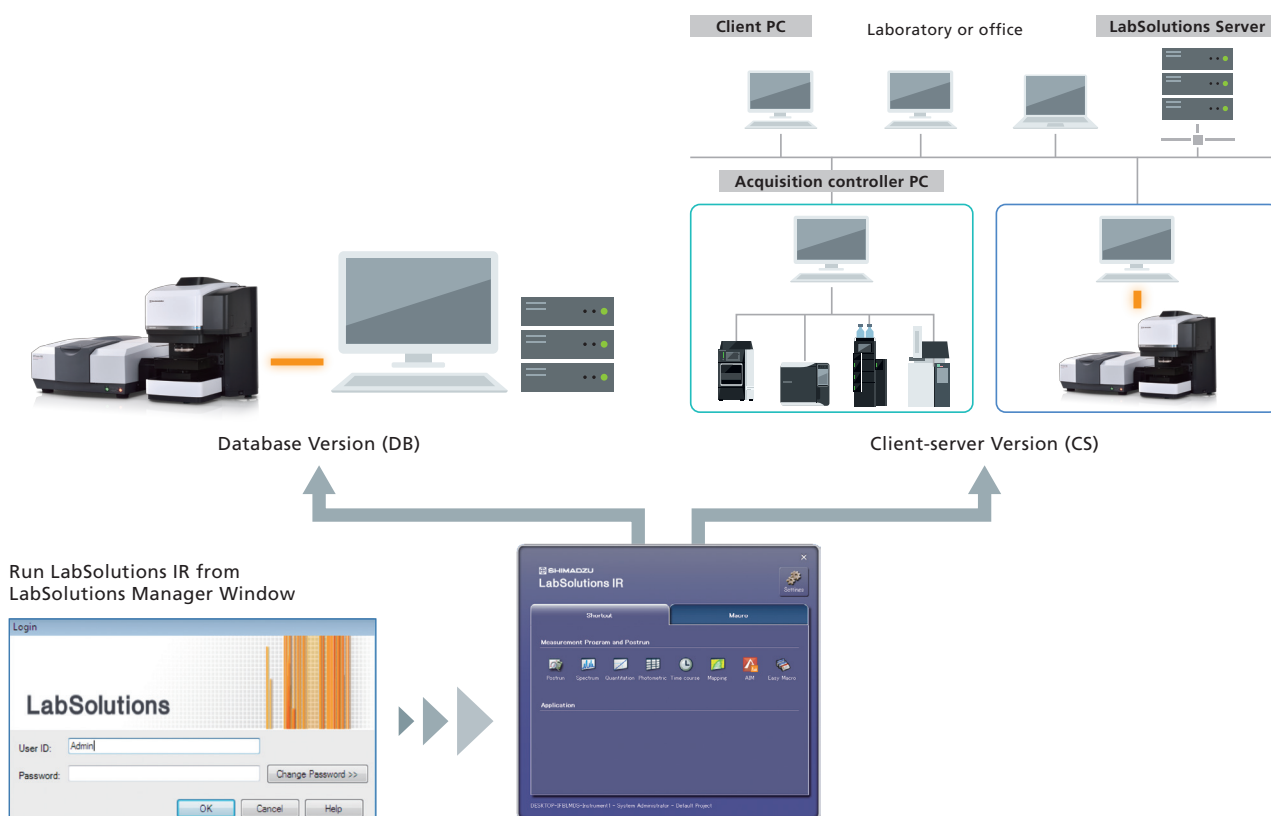
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