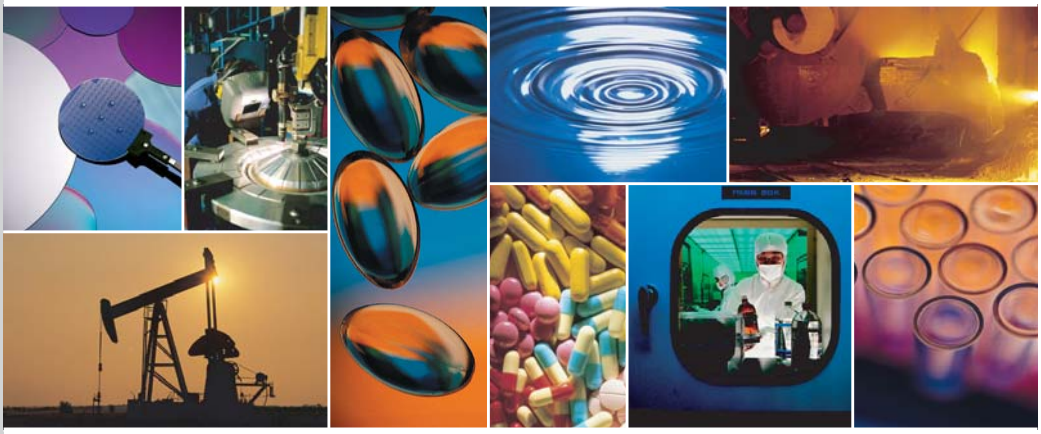
Antaris II User Guide



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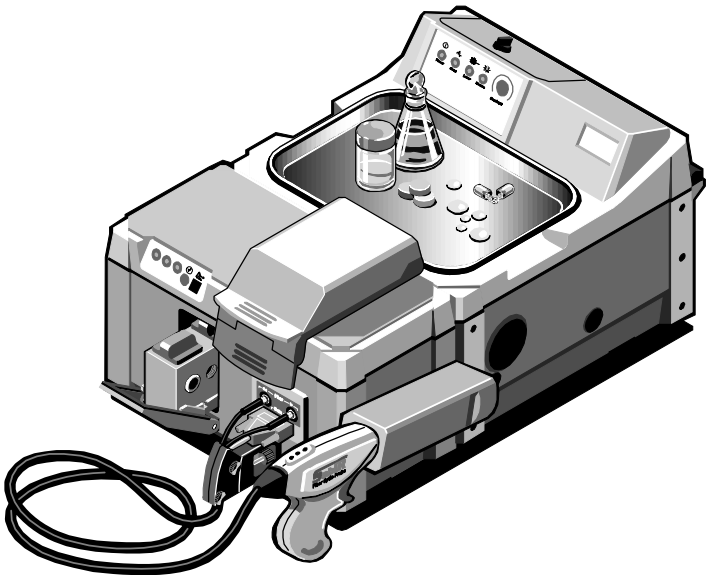
Chapter 1 Introduction

Congratulations on your purchase of an Antaris™ II analyzer from Thermo Fisher Scientific! The Antaris II is a dedicated *Fourier-transform near-infrared (FT-NIR)* system designed for the industrial environments of the pharmaceutical, chemical, polymer, and food and beverage industries.



Antaris II system

Note The Antaris II Method Development Sampling (MDS) configuration is shown above. Your system may look different depending on the sampling modules you have. ▲

This manual explains how to use the Antaris II analyzer and any of the following optional sampling modules: the integrating sphere module, the transmission module, the fiber optic module, and the tablet analyzer module. Also included is information on using RESULT software to run the analyzer, as well as chapters on how to operate, maintain, and service the system.

How to use this document

The printed and on-line documentation included with your system are designed to let you find the information you need quickly. We recommend first reviewing the contents and tabbed section names in this user's guide to become familiar with the document's content and organization.

See the "Antaris Sampling" chapter to learn how to collect a spectrum using the standard and any optional sampling modules that are included with your system. See the "Maintenance and Service" chapter when you have a question about setup, maintenance, or service procedures for your analyzer, such as:

- Cleaning the analyzer and sampling accessories.
- Checking and changing the desiccant.
- Changing replaceable parts.
- Installing an optional purge kit.
- Getting part number and ordering information.

Setup, maintenance, and service information is also provided in the on-line documentation provided with RESULT software. The on-line help also includes a detailed system warranty.

To access the on-line help, start RESULT Operation software and then choose Servicing The Antaris Analyzer from the Service menu.

Note If you cannot start RESULT Operation or access the Service menu, see your RESULT software administrator. ▲

If your system includes accessories, such as an autosampler, operating instructions came with them. You can store these documents in the "Accessories and Options" chapter. To learn about the software that runs your analyzer, see your *RESULT User's Guide*.

Document content

The tabbed chapters in this manual are described briefly below.

- **Chapter 1 Introduction**. This chapter gives an overview of the product's hardware and software components, including computer and software requirements. It also explains who to talk to about any questions or concerns about the product.

- **Chapter 2 Antaris Sampling**. This chapter gives instructions for collecting a spectrum using the standard and any optional sampling modules that are available for your system. It also includes detailed maintenance and service information for the optional module.

- **Chapters 3-6**. These chapters provide information about the sampling modules: the integrating sphere module, the transmission module, the fiber optic module, and the tablet analyzer module. The information in these chapters includes the features of the modules, instructions for setting up experiments and collecting data, tips for developing workflows, and troubleshooting information.

- **Chapter 7 Maintenance and Service**. This chapter provides detailed maintenance and service information for the Antaris II systems and their sampling modules.

- **Chapter 8 Accessories and Options**. This chapter is designed to hold operating instructions, including maintenance and service information, for any component options and accessories, whether those options and accessories were purchased with the system or afterwards.

- **Chapter 9 Antaris Updates.** This chapter is designed to hold the Antaris II Updates, which describe any changes made to the analyzer since this guide was last published.

- **Glossary**. Use the glossary to look up definitions for terms and abbreviations used in this document.

- **Index**. Use the index to quickly locate information on a specific topic.

Conventions used in this document

This manual includes safety precautions and other important information presented in the following format:

This symbol tells you that you can find more information in the on-line help system. To access the help system, choose Servicing The Antaris Analyzer from the Service menu in RESULT Operation software. See your RESULT software administrator if you cannot start RESULT Operation or access the Service menu.

Note Notes contain helpful supplementary information. ▲

Tip Messages like this contain a list of tips for using the feature being discussed. ▲

Notice Follow instructions labeled "Notice" to avoid damaging the system hardware or losing data. ▲

⚠ Caution Indicates a potentially hazardous situation which, if not avoided, may result in minor or moderate injury. It may also be used to alert against unsafe practices. ▲

⚠ Warning Indicates a potentially hazardous situation which, if not avoided, could result in death or serious injury. ▲

⚠ Danger Indicates an imminently hazardous situation which, if not avoided, will result in death or serious injury. ▲

Questions or Concerns

In case of emergency, follow the procedures established by your facility. If you have questions or concerns about safety or need assistance with operation, repairs or replacement parts, use the information below to contact Thermo Fisher Scientific. Outside the U.S.A., contact the local Thermo Fisher Scientific sales or service representative.

Phone: 1 800 642 6538 (U.S.A.) or
+1 608 273 5015 (worldwide)

Fax: +1 608 273 5045 (worldwide)

E-mail: techsupport.analyze@thermo.com

World Wide Web: http://www.thermo.com/spectroscopy

Product Safety

Before operating the Antaris II system, each person who plans to use a sampling module to collect data should read the operating precautions in this section to avoid damaging components or causing personal injury. Additional safety precautions are included where appropriate throughout this manual. Each person who plans to operate the system also should read the safety information provided in the Antaris II Site and Safety Information Guide. The guide is included in your manual set and is also available as a portable document format (PDF) file in your Thermo Scientific software. The guide is available in several languages. Contact our local office for information about the languages that are available.

⚠ Warning To prevent personal injury and damage to equipment, always follow the safety precautions in this manual and in the *Antaris II Site and Safety Information Guide* when you use the analyzer. ▲

Laser safety

The Antaris II sampling modules are Class I laser products. The accessible radiation levels are at or below Class I limits as defined by international standards and the United States Department of Health and Human Services. The laser source in the analyzer is a helium/neon (HeNe) laser head. A small amount of laser radiation is combined with the energy from the white light source in the analyzer. This energy is accessible through the integrating sphere window, the tablet analyzer base, and the fiber optic module connectors.

In the same way you are cautioned against staring at the sun or its bright reflection, do not stare at the beam that exits the integrating sphere window. Also, do not stare at the beam that exits the fiber optic connectors, at one end of a fiber optic cable while the other is connected to the module, or into the tip of a fiber optic accessory when it is connected to the module. If the tablet analyzer is connected to the instrument, do not open the tablet analyzer cover while the instrument is collecting a background or sample spectrum. If you are using the integrating sphere, the gold flag inside that blocks light from the source and the laser beam can open unexpectedly when a method is running. Do not stare at the integrating sphere window when a method is running.

Note For more information about laser safety and other safety issues, read the *Antaris II Site and Safety Information Guide*. This guide should be read thoroughly by any person who operates and/or maintains the instrument. ▲

Product Components

This section introduces the Antaris II analyzer and gives an overview of the product's hardware and software components. For information about hardware and software requirements, see the *Computer Requirements for Antaris Instruments Controlled by RESULT Software* document that came with your system.

RESULT software

RESULT is a dedicated analysis software package for industrial analyzers. RESULT is comprised of the following software applications:

- **Result Operation** is an intuitive, easy-to-use graphical interface for routine sample analysis. RESULT Operation uses the security features of the Microsoft® Windows® operating system, including user passwords, logons and digital signatures, to secure the system for routine operation, including data archiving and report generation. The software is compatible with standard readers and web browsers, allowing easy viewing of spectra, reports, and instructions, and complies with regulatory and validation requirements for production pharmaceutical, chemical, gas, and polymer analyses.

- **Result Integration** is a sophisticated yet easy-to-use development package for setting up controlled operating environments for routine sample analysis. RESULT Integration allows an analyst to integrate quantitative, qualitative, and spectral measurement methods with simple data collection, archiving, and reporting routines to create a custom analysis without the use of complicated programming or macro coding. RESULT Integration includes features for generating custom sample reports, and for attaching instructions or a standard operating procedure (SOP) to an analysis. The software's data simulation features allow the developer to create and test methods on non-production systems. Once a process is defined and thoroughly tested, it can be secured and then transferred from system to system for accurate, repeatable analysis results.

- **Result Data View** is a tool for viewing sequence data files collected from time-based experiments. You can use this application to display sequence spectra as well as the measured concentration values or other analysis results. The analytical data are presented on a time axis; selecting a data point displays the corresponding spectrum.

  RESULT is designed to work hand-in-hand with the Thermo Scientific *TQ Analyst™ method development software* for seamless method creation

and design. TQ Analyst is a sophisticated yet easy to use software package for developing analytical methods for mid-infrared, near-infrared and other spectroscopic applications. The software provides all the algorithms typically used for calculating component concentrations and classifying spectra based on a set of standards. You can also set up methods that simply measure spectral features and report the measured values. The software's extensive on-line help system, including training aids, context-sensitive help, and multiple wizards, helps you quickly learn the software and get up to speed developing accurate analytical methods.

RESULT is also compatible with other method development software packages used in the industry including:

- **PLSplus/IQ™** method development software for GRAMS/32® AI version 6.0 from Thermo Galactic Corp.
- **The Unscrambler®** version 7.6 (or greater) method development software from Camo ASA.
- **Pirouette®** version 3.04 or 3.11 (required for Windows XP) method development software from InfoMetrix®, Inc.

The RESULT *sequence module* allows real-time data collection and analysis for time-based experiments. For applications ranging from near-infrared reaction monitoring to FT-IR combustion gas analysis, RESULT provides all the tools needed for system control, data collection, reporting, and archival in real time.

On-line help

RESULT Operation provides a basic on-line help system that describes routine maintenance and service procedures for your analyzer. The help system includes system warranty information and a list of part numbers for ordering optional and customer-replaceable parts. The help system can be accessed from the Service menu in RESULT Operation software. See "RESULT Operation Software" in your *RESULT User's Guide* for more information.

Hardware and software requirements

For information about hardware and software requirements, see the *Computer Requirements for Antaris Instruments Controlled by RESULT Software* document that came with your system.

Antaris II FT-Near Infrared Analyzer

Your Antaris II analyzer is designed to be portable yet rugged, supplying accurate, repeatable data for industrial applications. This section describes the analyzer's major components, including the front and back panels and the standard and optional sampling modules. The system's basic internal components, such as the light source, laser, and detector, are also described.

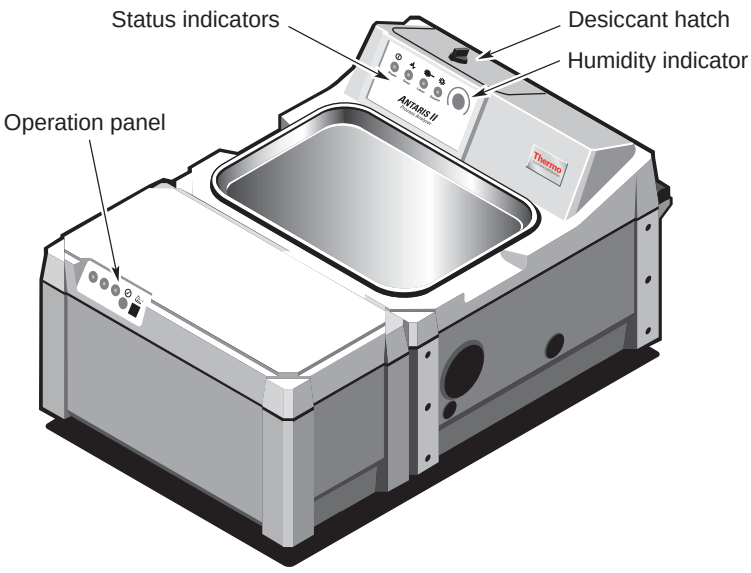
You can replace key parts of the analyzer, such as the laser, light source, and power supply. Instructions for replacing these parts are provided in the "Maintenance and Service" chapter of this manual.

Instructions for replacing the laser, light source, and power supply are also available on-line. Choose Servicing The Antaris II Analyzer from the Service menu in RESULT Operation software to access ordering information, step-by-step instructions, and videos for replacing parts.

Antaris II analyzers are sealed and desiccated to remove the effects of water from spectra and to prevent damage to electrical components from environmental humidity. An optional purge kit is available if your analyzer environment is excessively humid (above 95% non-condensing) or contaminated by routine use of potentially corrosive solvents or other agents. Purging (forcing dried air or nitrogen through the analyzer to eliminate water vapor and other airborne contaminants) will better protect the system's internal components under those conditions. We provide instructions for selecting a purge gas and installing the purge source and connectors in the *Antaris II Site and Safety Information Guide* included with your system.

Basic components

The following identifies the components on the outside of the analyzer.



Basic components of the Antaris II Analyzer

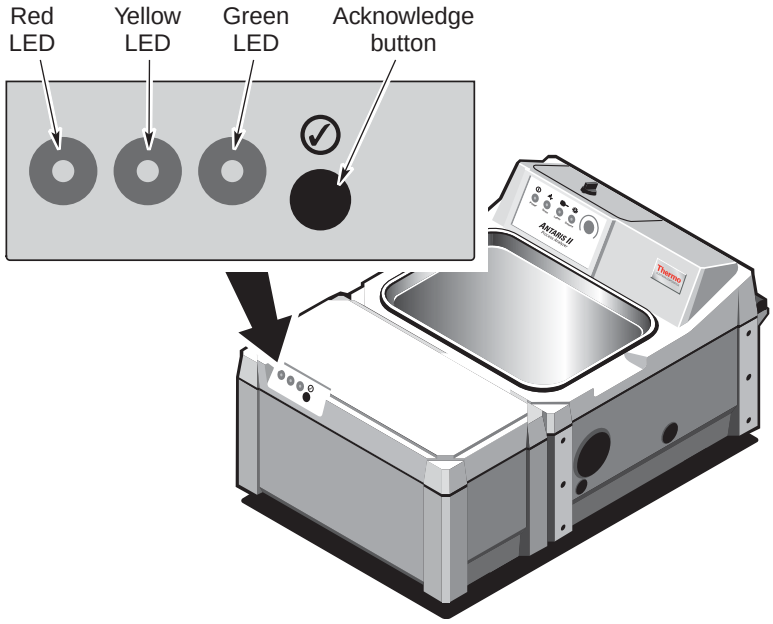
Humidity indicator – The humidity indicator lets you know when there is too much moisture inside the instrument. Check the indicator regularly (every two months when the analyzer is not in use) and change the desiccant packets if the indicator turns pink. See the "Maintenance and Service" chapter for instructions.

Desiccant hatch – The desiccant hatch provides access to the desiccant packet.

Status indicators – The status indicators show the current status of the analyzer. Here is a brief description of the function of each indicator:

Indicator	Description
Power	This indicator lights when the analyzer power is on and the power supply voltages are within specifications.
Scan	This indicator flashes with each scan of the interferometer.
Laser	This indicator lights when power is supplied to the laser and is operating within specifications.
Source	This indicator lights when the source is illuminated and is operating within specifications.

Operation panel – The operation panel contains indicators that alert the operator to take an action.



Antaris II operation panel

The green Acknowledge button allows the operator to initiate an action, such as the start of data collection. The *LED indicators* tell you the status of your collection without being directly in front of the computer screen. The following tables list the meaning of each indicator and indicator state:

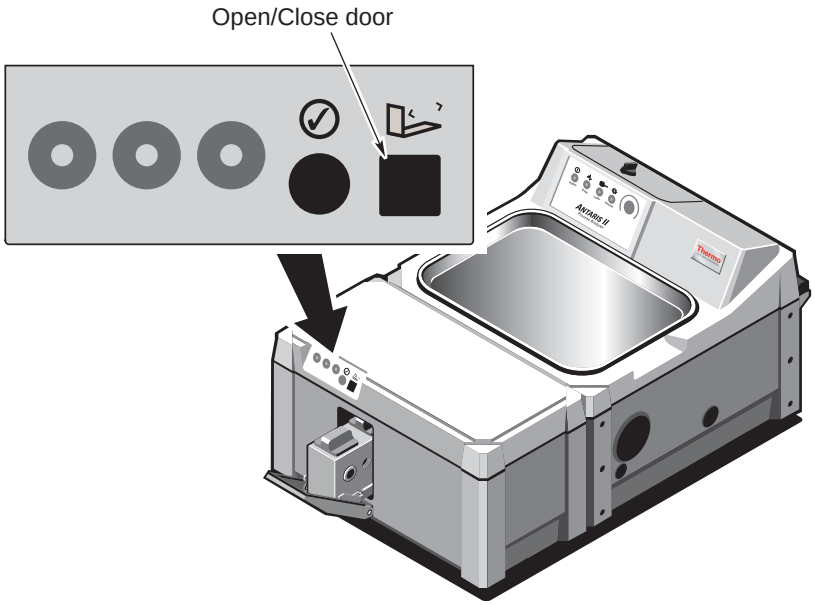
LED Indicators

Indicator	Meaning
Green	The system is waiting for a response from the operator.
Yellow	The instrument is collecting data.
Red	A failure occurred while running a workflow or other process.

LED States

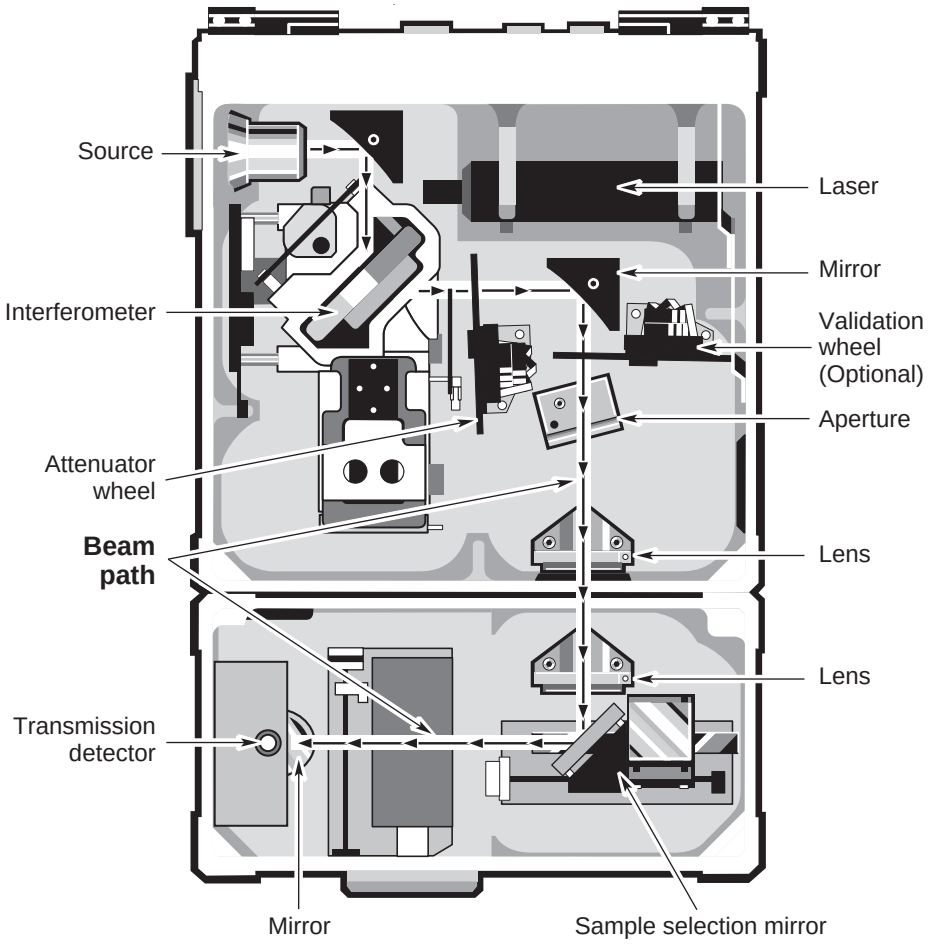
Indicator State	Meaning
Steady	The operator can respond to the indicator by pressing the green Acknowledge button on the instrument operation panel or by choosing a button in a software prompt at the computer.
Flashing	The operator is required to respond to the indicator by choosing a button in a software prompt at the computer.

If your system includes the *transmission sampling module*, the square black button opens and closes the door to the transmission module.



Internal components

The illustration below shows a top view of the optical layout of the analyzer with covers removed to reveal components.



Antaris II Internal Components

The system's internal components include:

Source – The near-infrared source in your Antaris II analyzer provides excellent throughput and durability. The source emits a beam of white light, which travels through the instrument and is selectively absorbed or reflected by the sample.

Interferometer – The light beam from the source is reflected into the *interferometer*, which combines all frequencies of the beam into one signal, called an *interferogram*. The interferometer contains a fixed mirror, a *moving mirror*, and a *beamsplitter*.

⚠ Caution Never stare into the laser beam or at its bright reflection. ▲

Laser – The laser is used as an internal calibrator in FT-NIR instruments because it emits light at a known and constant frequency. The laser helps control the moving mirror's position and signals the capture of data.

The laser source in the Antaris II analyzer is a helium/neon (HeNe) laser head, equipped with a neutral-density filter to help reduce power and reflections. The analyzer collects data at precise laser-calibrated points.

Mirrors and lenses – Antaris II analyzers use a combination of precision mirrors and lenses to focus and direct the near-infrared beam for optimum performance.

Aperture – The aperture is an opening that optimizes spectral line shape (*resolution*) by defining the number and direction of the infrared rays reaching the sample. The standard analyzer configuration uses a fixed aperture and provides resolution settings between 64 cm^{-1} and 2 cm^{-1}. An optional, two-position aperture is required to achieve maximum spectral resolution across the entire spectral range at the lowest (2 cm^{-1}) resolution setting. The software automatically selects the smaller aperture when the 2 cm^{-1} resolution setting is used and the two-position aperture is installed.

Detector – After being absorbed, reflected, or transmitted at specific frequencies by the sample, the infrared beam is focused onto the detector. The detector produces an electrical signal in response to the energy striking it. The signal is sent to the computer for processing.

Antaris II analyzers use detectors made from indium, gallium, and arsenide (InGaAs detectors) for collecting transmitted or reflected light. The transmission detector shown in the previous illustration is present in every analyzer configuration. It is used for collecting transmission data from the transmission sampling module, and for checking instrument performance. Each sampling module also has a dedicated InGaAs detector.

The standard InGaAs detector provides usable data in the range between 12,000 and 3,800 cm^{-1} (between 833 and 2,630 nm). See the "Antaris Sampling" chapter for specific detector ranges for each Antaris II sampling module.

Attenuator wheel – The detectors installed in the Antaris II analyzer are highly sensitive and can become saturated or produce a distorted signal if too much light reaches the detector element. The attenuator wheel provides two calibrated energy-limiting screens that can be used to lower the energy

sent to a sample. The screens are software selectable and have the following effect on the incident infrared beam.

Attenuator Screens in the Antaris II Analyzer

Screen	Percent of Incident Light Transmitted
None	100
B	6 – 10
C	2.5 – 3.5

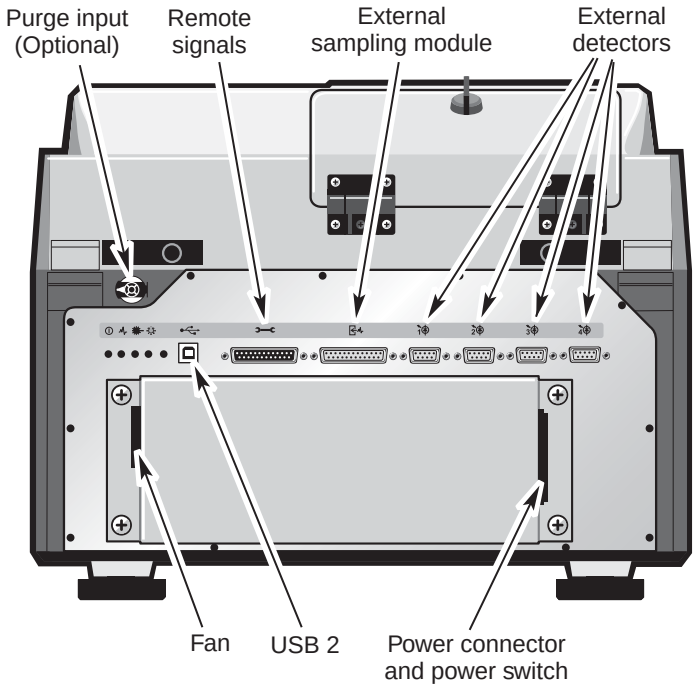
The wheel also includes a polystyrene sample combined with an energy limiting screen (C screen), which can be used to check instrument performance. The thickness of the polystyrene sample is 0.0325 inch.

Note The software's Optimize Gain feature can be used to determine the appropriate attenuator and gain settings for a particular sample. For details, see "Sample Specifications" in "Section 5 Workflow Events and Specifications" of your *RESULT User's Guide*. ▲

Validation wheel – The validation wheel is optional and comes only with ValPro. It contains six samples, including five glass transmission standards and a polystyrene sample. The five glass standards are calibrated to transmit approximately 2%, 10%, 20%, 40%, and 80% of the incident light beam. They may be used for instrument qualification using the optional *ValPro™ System Qualification package*. The polystyrene sample is calibrated to a thickness of 0.0325 inch, and can be used to validate instrument performance. The seventh wheel position is empty.

Rear panel

The illustration below shows the locations and uses of the connectors on the analyzer rear panel:



Antaris II Rear Panel

⚠ Caution Improper or unsafe cabling can damage your instrument and may create a safety hazard. Thermo Fisher Scientific is not responsible for damage or injury resulting from improper or unsafe cabling. ▲

Connector for power cord – Antaris II systems are powered by a power supply that is attached to the back of the analyzer. The power cord connects to this power supply and a wall outlet, power strip, or other AC power source. Always turn off the analyzer power before you connect the power cord to the analyzer or the AC power source.

Be sure to use an appropriate power cord for your electrical service. The power cord supplied with your analyzer is a 3-wire, grounded power cord, appropriate for use in the country listed as the shipping destination for the analyzer.

⚠ Warning Do not remove or defeat the ground prong on the power cord. If you use an extension cord, it must also have a protective conductor. ▲

Connector for cable from computer – The USB 2.0 data cable from the computer connects to this port.

Purge gas input connector (for optional purge) – This connector is used to install a source of purge gas if the analyzer is purged. Purging (forcing dried air or nitrogen through the analyzer to eliminate water vapor and other airborne contaminants) is recommended only if the analyzer environment is excessively humid (above 95% non-condensing) or contaminated by routine use of potentially corrosive solvents or other agents. We provide instructions for selecting a purge gas and installing the purge source and connectors in the *Antaris II Site and Safety Information Guide* included with your system. See the "Antaris II Sampling" chapter for instructions for setting purge pressure and flow.

⚠ Danger *Never* use a flammable gas or argon to purge the analyzer. Heat from the source or internal electrical components could ignite the gas. The purge gas must be free of moisture, oil, and other reactive or infrared-absorbing materials. We recommend using dry air supplied by a purge gas generator or pure air generator (available from Thermo Fisher Scientific), or dry nitrogen. ▲

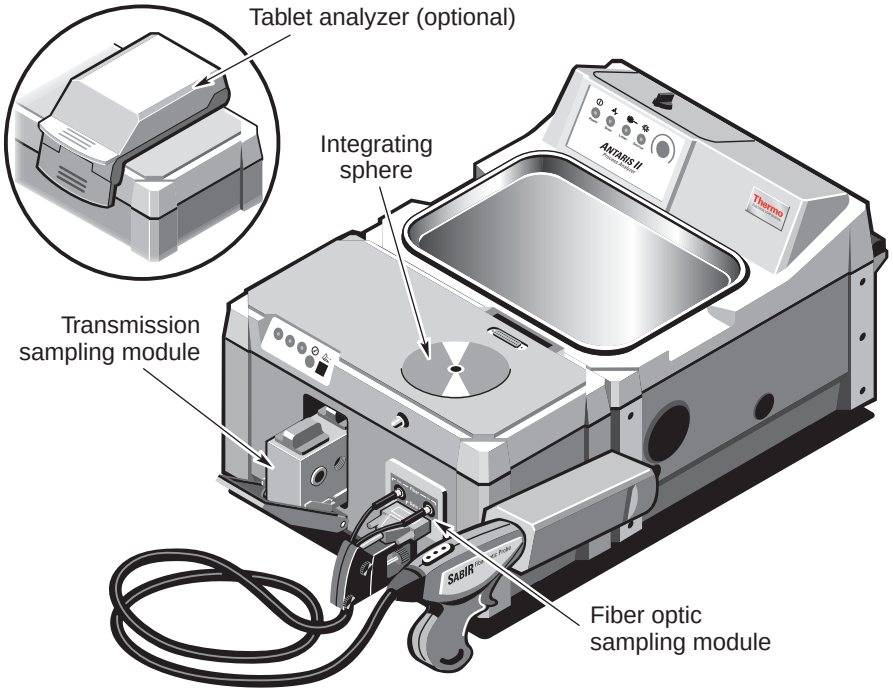
Connector for remote signals – This connector is used by Thermo Fisher Scientific customer support for diagnostic purposes.

Connector for external sampling modules – This connector is designed to carry the signal from an external sampling module.

Connectors for controlling external accessories – There are four accessory connectors. These connectors are designed to carry the signal from an external detector, or for communication cables from external accessories.

Sampling modules

The Antaris II can be configured as an application-specific system with any, or all, of the sampling modules that are described in this section. The Method Development Sampling (MDS) system is a preconfigured Antaris II system that includes the integrating sphere module, the transmission module, and the fiber optic module. This provides tools for analyzing most liquid and solid samples, ranging from films, powders, and tablets to free-flowing liquids, semi-solids, and pastes.



Antaris II Method Development Sampling (MDS) System

After choosing a sampling technique and defining the analysis process, the analysis can be transferred to other MDS or application-specific systems for routine sampling. Because every Antaris II sampling module and system uses the same optical components, alignment, and beam path, you can transfer your analysis to a different system without compromising on performance. The software recognizes and configures sampling modules automatically to simplify setup and minimize operator errors. Background measurements may be taken automatically using an internal background path or reference to ensure consistent sampling and repeatable results.

The next few pages describe the various sampling modules that are available for the Antaris II MDS System. For step-by-step instructions to collect data using one of the sampling modules described below, refer to the chapter with the corresponding name.

Integrating sphere sampling module – This sampling module is based on the standard diffuse-reflection sampling technique but uses a unique optical design, called an *integrating sphere*, to collect greater than 95% of the scattered NIR energy. This results in excellent sensitivity, robust calibrations, and high sample-to-sample repeatability. The durable sapphire

sampling window has a chemical-resistant seal for worry-free cleaning and maintenance.

The integrating sphere is ideal for measuring solids and powders. Sample materials may be measured directly or indirectly through packaging materials such as plastic bags, scintillation vials, and reagent bottles. Sample measurements are achieved by collecting the NIR energy that scatters off the surface of a powder or solid sample. An internal gold reference may be used for automatic background collections to ensure consistent sampling and repeatable results.

Transmission sampling module – Designed for quality control testing of raw materials, chemicals, polymers, surfactants, and formulations, the transmission sampling module provides quick transmission analysis of liquid samples in standard-size (0.5 mm to 1 cm thick) cuvettes, culture tubes, and card-mounted liquid cells, as well as transmission analysis of transparent solids and films. The 3-position sample holders allow automatic sample, background, and liquid reference collections, ensuring consistent sampling and repeatable results. A software-controlled internal heater ensures accurate, repeatable analysis for temperature-sensitive measurements (optional heated sample holder required).

Tablet analyzer sampling modules (optional) - The tablet analyzer sampling modules are convenient yet powerful tools for analyzing tablet samples. The module combines the Antaris II integrating sphere with a transmission detector to allow the collection of diffuse-reflection and transmission data from the same sample. This allows you to obtain tablet coating, ingredient, and uniformity information in one sample experiment at the same time.

The transmission detector collects the energy that passes through the tablet, providing standard transmission data for sample component analysis. Diffuse-reflection measurements are achieved by collecting the NIR energy that scatters off the surface of a tablet sample.

For more information

Additional information about your Antaris II analyzer is provided elsewhere in this and other documents in your manual set and in the on-line help for RESULT Operation software. A brief summary of this information is provided below.

Antaris II Site and Safety Information Guide – Read this important setup and safety information before using your analyzer.

Antaris II User's Guide – See the "Antaris Sampling" chapter for detailed information about collecting data using your Antaris II system.

RESULT User's Guide – For basic information about RESULT Integration, the development application for RESULT, read "Section 2 RESULT Integration Software." For information about RESULT Operation, the sample analysis application for RESULT, read "Section 3 RESULT Operation Software." For information about RESULT Data View, the application for viewing sequence data files, see "Section 4 RESULT Data View." For reference information about the development tools in RESULT Integration Software, see "Section 5 Workflow Events and Specifications." To learn about the administrative features of RESULT, see "Section 6 Software Administration." For information about using RESULT to collect and view calibration standards and build an analytical method, see "Chapter 4 Tools for Building Methods and Viewing Spectra" in "Section 2 RESULT Integration Software."

RESULT Updates – This guide describes any new features that were added to RESULT software since the *RESULT User's Guide* was last updated.

Servicing Antaris – Select "Servicing The Antaris Analyzer" from the Service menu in RESULT Operation software to access a detailed parts list, ordering information, and replacement procedures for the laser, light source, and power supply.

Release Notes – Your software CDs contain release notes for each software application. Release notes provide late-breaking news and helpful troubleshooting information. Look for the release note files in the Documents folder on your software CDs.

Technical bulletins, application notes, training classes, and newsletters provide more learning opportunities. See your Thermo Fisher Scientific customer support representative for more information.

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Chapter 2 Antaris Sampling

This chapter explains how to prepare your analyzer for operation, The following sections are included:

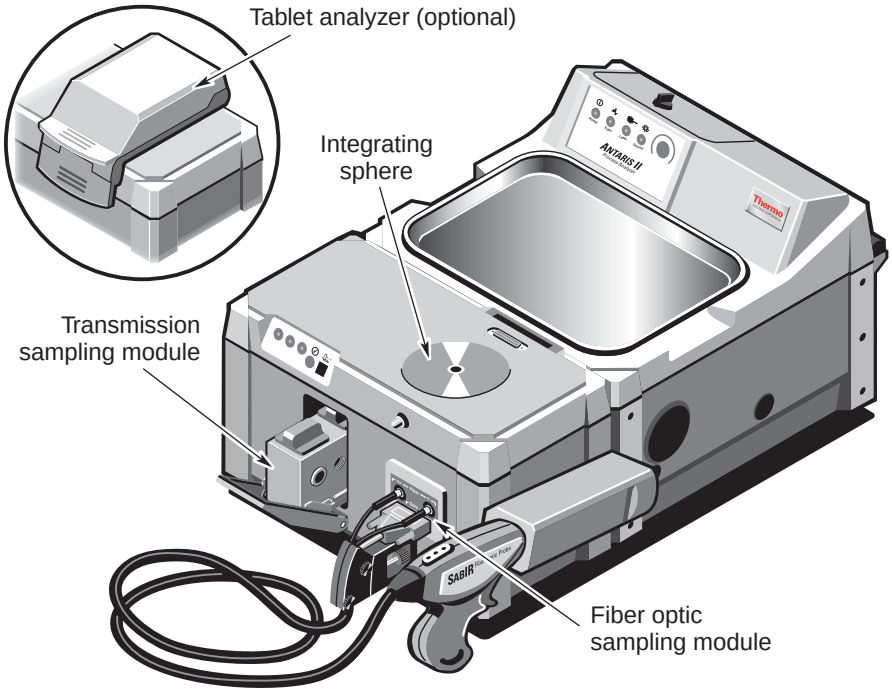
- **Introduction**. This section describes the system's configuration and lists the available sampling modules.
- **Operating precautions**. This section shows where to find information about maintaining personal safety while using the analyzer.
- **Getting started**. This section provides instructions for checking the analyzer desiccant, turning on the system components, and starting RESULT™ software.

Note For step-by-step instructions to collect data using one of the sampling modules, refer to the chapter with the corresponding name in this manual. ▲

Introduction

The Antaris II can be configured as an application-specific system with any, or all, of the sampling modules listed below. (These modules are described in the "Sampling modules" section of the "Introduction" chapter.) This provides tools for analyzing most liquid and solid samples, ranging from films, powders, and tablets to free-flowing liquids, semi-solids, and pastes. These multiple sampling platforms are designed to serve the advanced user responsible for selecting a sampling technique for a particular application and environment.

- Integrating sphere
- Transmission module
- Fiber optic module
- Tablet analyzer



Antaris II Method Development Sampling (MDS) system

Note For step-by-step instructions to collect data using one of the sampling modules, refer to the chapter with the corresponding name in this manual. ▲

After choosing a sampling technique and defining the analysis process, the analysis can be transferred to other MDS or application-specific systems for routine sampling. Because every Antaris II system uses the same optical components, alignment, and beam path, you can transfer your analysis to a different system without compromising on performance. The software recognizes and configures sampling modules automatically to simplify setup and minimize operator errors. Background measurements may be taken automatically using an internal background path or reference, ensuring consistent sampling and repeatable results.

Operating precautions

Before operating a sampling module, read the following operating precautions to avoid damaging components or causing injury to yourself.

Working with the integrating sphere

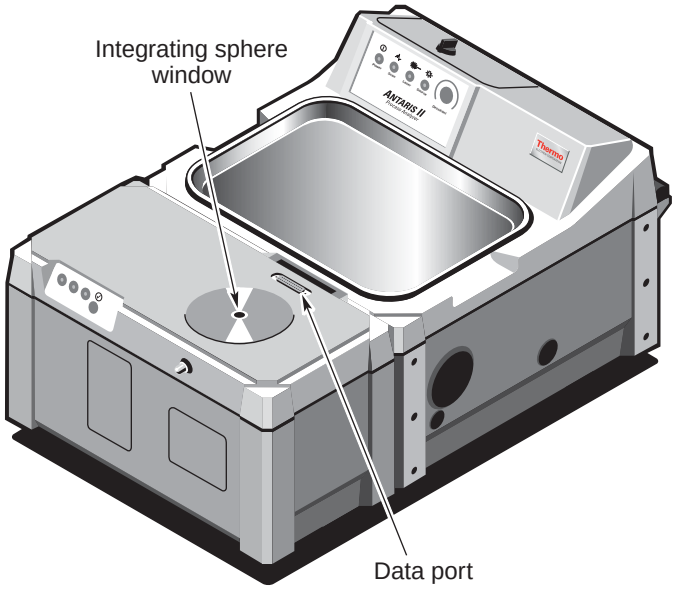
Observe the following precautions when working with the *integrating sphere sampling module:*

- Harsh solvents may weaken the seal around the window, and substances could then get into the integrating sphere. To clean the integrating sphere window, follow the instructions in the "Maintenance and Service" chapter.

- Do not pour liquids directly onto the integrating sphere window and sampling area. Pouring liquids directly onto the sampling area and integrating sphere window may weaken the seal around the window and substances could then get into the integrating sphere. Liquids poured directly onto the module could also spill into the electrical port on top of the module.

- Although the integrating sphere window is sapphire, very harsh, abrasive substances may scratch the integrating sphere window. When sampling abrasive substances, it is recommended that you put them in a glass vial or plastic bag.

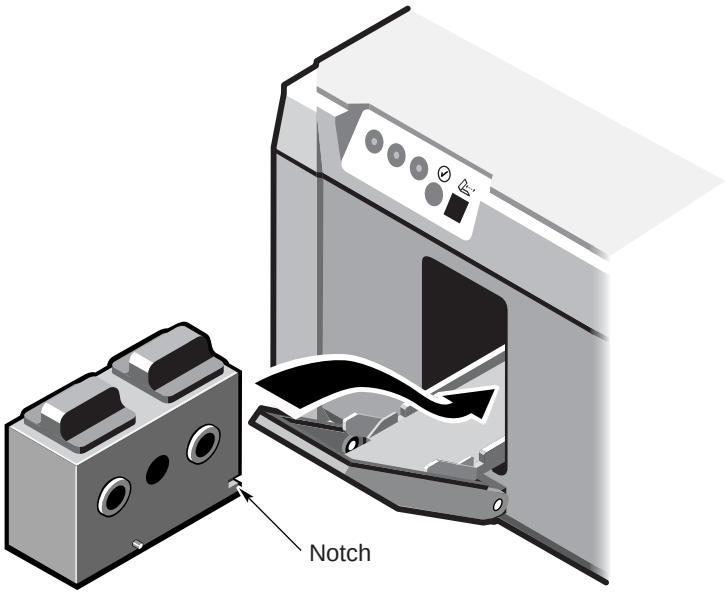
- Inspect the female connectors on the data port on the surface of the instrument on a regular basis. If the connectors are clogged or jammed, contact your Thermo Fisher Scientific service representative. Do not install a tablet analyzer if the connectors are clogged or jammed, and do not attempt to unclog the connectors yourself.



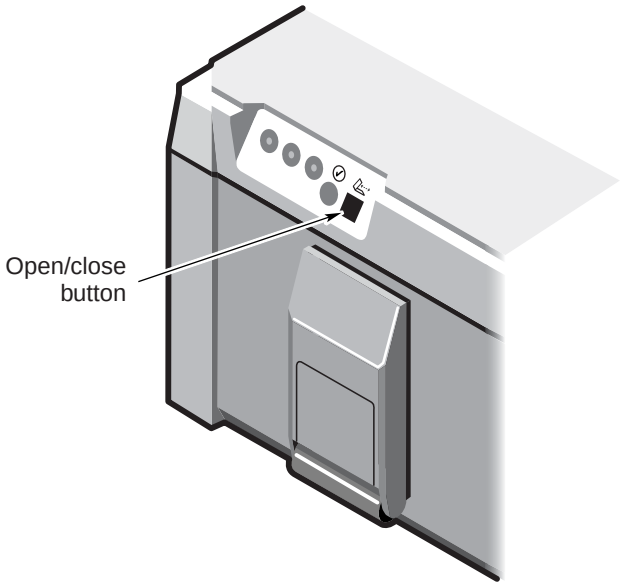
Working with the transmission module

Observe the following precautions when working with the *transmission sampling module:*

- The sample holders have notches in the back at the base. Always insert the sample holders so that these notches go in first.



- Before you open or close the transmission module door, make sure nothing is in the door's path.
- The height of a sample should not be over 3 inches (76 mm). Anything taller will not fit into the transmission module, and samples in glass containers may break when the transmission module door closes.
- If you are working with the heated samples, always wear protective gloves to prevent your hands and fingers from being burned.
- If you are working with samples of volatile liquids, follow standard laboratory safety practices. Do not heat any such liquid to its flash point, make sure the sample containers are capped, and always wear protective goggles and clothing.
- To avoid errors in data, do not manually open the transmission module door during data collection. (The open/close button is disabled during data collection.)



- To avoid exposure to *laser* radiation, do not put mirrors into the transmission module, and do not try to direct the laser out of the transmission module.

- If a cuvette/culture tube holder cap, or some other object, falls off in the transmission module, use extreme caution when removing it. Exit any workflow you are running, and do not touch any of the mirrors in the transmission module.

Working with fiber optic cables and the test fiber

Observe the following precautions when handling *fiber optic cables* and the *test fiber*:

- Optical fibers are delicate and expensive. Handle them gently. If you drop the cables, bend them tightly, or knock them against a hard surface, they may break or become damaged, which will reduce performance.

- Do not tightly coil fiber optic cables or the test fiber. The cables may be coiled loosely for storage; however, the radii of the coils should be at least:

  - 10 cm for the test fiber.

  - 30 cm for the SabIR diffuse-reflection probe.

For other fiber optic accessories, refer to the manufacturer's documentation.

- Do not touch the tips of the cables or test fiber with your fingers. If you must handle or clean the tips, use a clean cotton cloth or cotton balls. Do not use solvents to clean the tips of the cables or test fiber.
- Do not use tools to tighten connectors. Using tools to tighten connectors may damage the cables, connectors, or ports.
- When attaching the cables or test fiber to the ports on the instrument, do not over tighten the connectors. Over tightening may cause damage to the connectors or the *fiber optic ports*.
- Keep the protective caps on the ends of the cables, fiber optic ports, and test fiber at all times when they are not in use. This will help prevent damage to the connectors and protect the detector.

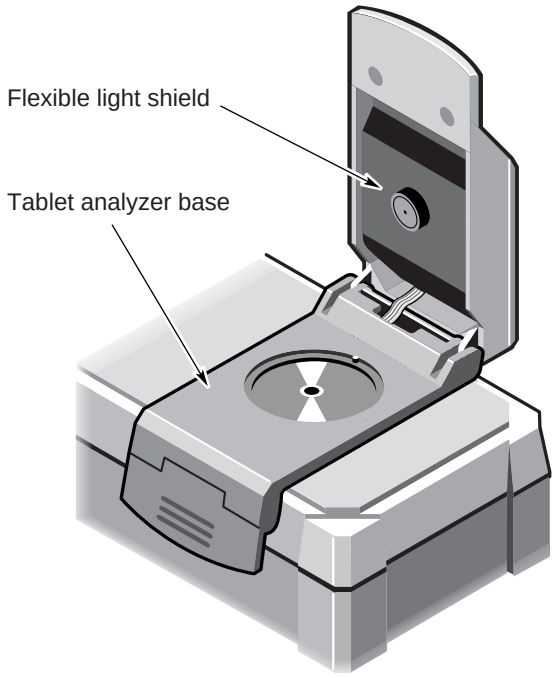
Working with the SabIR fiber optic probe

Observe the following cautions when using the SabIR fiber optic probe:

- Do not press the probe trigger while removing the probe from or inserting the probe into the holster. The probe may start data collection prematurely, which may affect your data. If you do press the probe trigger prematurely, you will need to stop and restart your experiment.
- Do not use the probe in extremely high or low temperatures. The probe is not intended for extended use in temperatures under 0°C or over 95°C. The probe is not intended for short use (two minutes or less) in temperatures under -25°C or over 120°C. Avoid rapid changes in temperature extremes (from 0°C to 100°C).
- Do not use the probe by itself with liquid samples. When sampling liquids, use the transflectance adapter available for the probe.
- Do not use the probe for sampling harsh chemicals, such as amyl alcohol, acetone, chromic acid, fluorine, and oleum. These harsh chemicals can degrade or soften the components in the probe tip.
- Avoid getting substances onto or into the probe housing.
- Do not use the probe in explosive environments.

Working with the tablet analyzer

Observe the following precautions when working with the *tablet analyzer sampling module*.



⚠ Caution Keep your fingers clear of the tablet analyzer base when installing the tablet analyzer. The tablet analyzer fits tightly onto the instrument and your fingers could get pinched if they are directly under the tablet analyzer when you are installing it. ▲

- Remove all sampling accessories, such as the universal tablet holder, from the tablet analyzer before installing or removing the tablet analyzer from the instrument. Shifting of removable objects inside the tablet analyzer may damage the tablet analyzer's internal components.

- To avoid damaging the flexible light shield, protective window, and/or detector, do not force the cover of the tablet analyzer closed if the sample material is too thick for the tablet analyzer to close normally.

- Always remove the tablet analyzer from the instrument before performing any maintenance task that requires you to open the main cover, such as replacing the laser.

- Be careful not to allow debris to get into the hole in the flexible light shield. This may cause damage to the window on the transmission detector and could affect spectral data.

- Do not allow liquids to get into the tablet analyzer, as this may damage the electronics.

- Before installing a tablet analyzer, inspect the female connectors on the data port on the surface of the instrument. If the connectors are clogged or jammed, contact your Thermo Fisher Scientific service representative. Do not install the tablet analyzer, and do not attempt to unclog the connectors yourself.

Getting Started

Follow the instructions in this section to prepare your Antaris II analyzer for operation. This section covers the following topics:

- **Turning on the system components**. This section provides instructions for turning the system components on and off.

- **Starting RESULT software**. This section demonstrates how to start RESULT software. RESULT is the Thermo Scientific dedicated analysis software package for industrial analyzers. You can use RESULT to collect data from any of the sampling modules available with your Antaris II system.

- **Setting optional purge.** This section demonstrates how to check the pressure regulator and flow meter on systems that are purged (optional).

- When you are finished preparing the analyzer and are ready to begin running samples using one of the Antaris II sampling modules, proceed to the chapter with the sampling module name.

Turning on system components

We recommend that you keep your analyzer on at all times, unless the building is subject to power outages or you need to perform a service or maintenance procedure. Leaving the system on keeps it stable and gives you the most consistent results. If you must turn the analyzer off, allow it to stabilize for at least one hour before collecting spectra.

⚠ Warning Always follow the safety precautions in this manual and in the Antaris II Site and Safety Information Guide that came with your system whenever you use the analyzer. ▲

Follow these steps to turn on the system components:

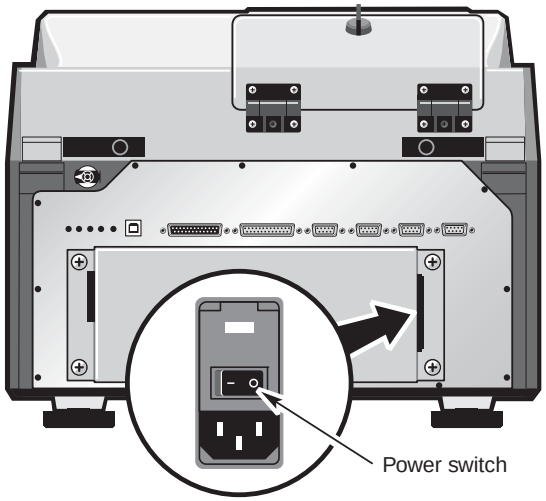
1. **If the power cord is not already connected to an AC power source, connect it.**

   Make sure the system components are turned off. Plug the power cord into the power supply on the back of the analyzer, and then plug the power cord into a wall outlet, a power strip, or another AC power source. (See "Rear panel" in the "Product Components" section of the "Introduction" chapter for information about the location of the power supply and the power cord connector.)

2. **Install any sampling accessories you plan to use.**

   This includes accessories such as a sample cup or tablet holder. See the chapter that describes the sampling module you plan to use for information about associated accessories.

3. **Turn on the analyzer by pressing the power switch on the power supply.**



I = On
O = Off

When you turn on the analyzer, the four status indicators—Power, Scan, Laser, and Source—flash in various sequences as the system runs through its diagnostic routines. When the routines are finished, the power, laser, and source indicators stay lighted. The scan indicator flashes with each scan of the *interferometer*. After you turn on the analyzer, let it stabilize for at least one hour before collecting spectra.

4. **Turn on the printer and then the computer.**

   Turn on the printer and computer as explained in the documentation that came with those components.

Note If the Power, Laser, or Source indicators flash or do not light at all, or if the Scan indicator does not light, turn the analyzer power off and then on. If that does not solve the problem, contact Thermo Fisher Scientific. ▲

Turning off system components

Reverse the order given in the preceding procedure when you turn off system components:

1. Turn off the computer.
2. Turn off the analyzer.
3. Remove any accessories.

Starting RESULT software

RESULT is the Thermo Scientific dedicated analysis software package for industrial analyzers. You can use RESULT to collect data from any of the sampling modules available with your Antaris II analyzer.

RESULT comprises the following software applications:

- **RESULT Operation.** This application provides an intuitive, easy-to-use graphical interface for routine sample analysis.
- **RESULT Integration.** This is a sophisticated yet easy-to-use development package for setting up controlled operating environments for routine sample analysis.
- **RESULT Data View** is a tool for viewing sequence data files. It is a companion to the RESULT sequence module, which allows real-time

data collection and analysis for time-based experiments. You can use the Data View application to display sequence spectra as well as the measured concentration values or other analysis results. The analytical data are presented on a time axis; selecting a data point displays the corresponding spectrum.

You may use the Quick Collect feature of either application to collect data from any of the sampling modules provided with your Antaris II analyzer, or you can set up a custom analysis in RESULT Integration and then transfer the analysis to RESULT Operation for routine operation. This section describes how to start both applications. For details on how to use the Quick Collect and other features of RESULT Operation or RESULT Integration, see the tabbed section with the corresponding name in your *RESULT User's Guide*. A tutorial on using Quick Collect to collect data using your Antaris II system is provided later in this section.

Starting RESULT Operation

Before you can log on to the computer workstation, you must receive a Windows® *user name* and password from your *Windows administrator*. If you are not a RESULT administrator, then the *RESULT software administrator* must also add your logon information to the RESULT user list.

After you log on the workstation, depending on how your workstation has been configured, RESULT Operation may start automatically.

To start RESULT Operation (if the software has not been configured to start automatically):

1. **Double-click the RESULT Operation shortcut on your workstation desktop.**

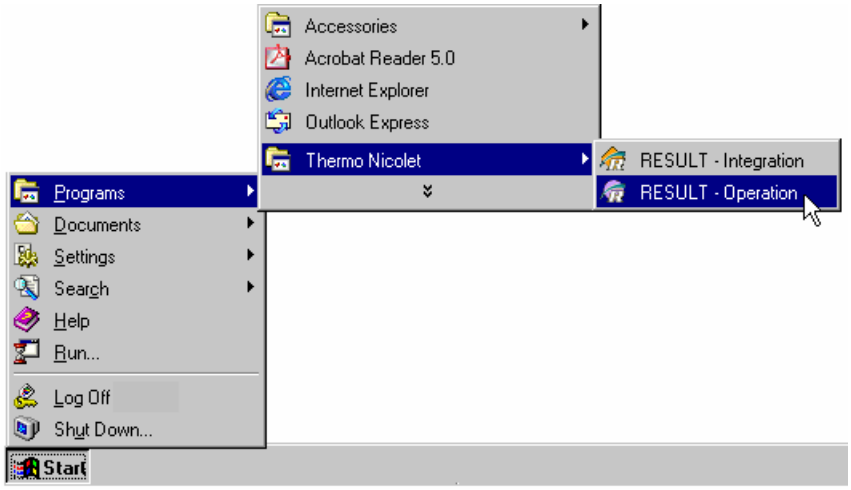
   -or-

   If the RESULT Operation shortcut does not appear on your desktop:

   - Open the Windows Start menu by choosing Start on the Windows taskbar.

   - Point to Programs in the Start menu.

- Point to the Thermo (or Thermo Nicolet) program group.
- Choose the RESULT Operation program.



Depending on how the software has been configured, RESULT may open a dialog box asking for your password.

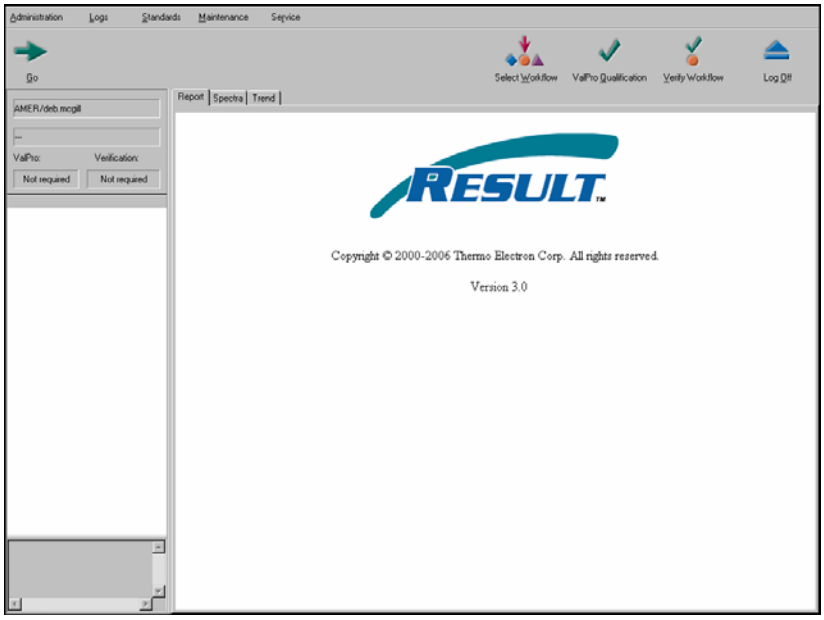
2. **Enter your Windows password, and then choose OK.**

   The password you entered must match your Windows password exactly, including the letter case.

Note You are given three attempts to enter your Windows password correctly. If, after the third attempt, the software cannot verify your Windows password, the software displays the following message:

See your *RESULT software administrator* if you are unable to start the software. ▲

If RESULT was able to verify that your password matches your Windows password, then the software will start, and the RESULT Operation main window will appear on the screen.



RESULT Operation main window

Starting RESULT Integration

Before you can log on to the computer workstation, you must receive a Windows *user name* and password from your *Windows administrator*.

To start RESULT Integration software:

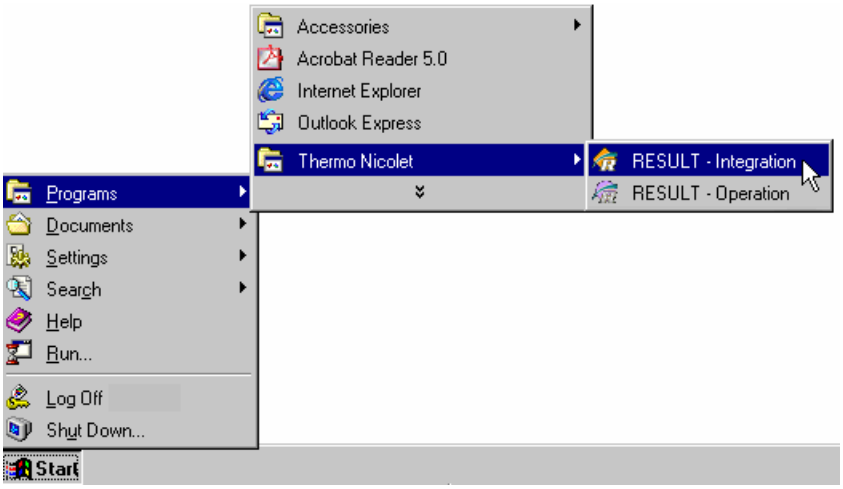
Double-click the RESULT Integration shortcut on your workstation desktop.

-or-

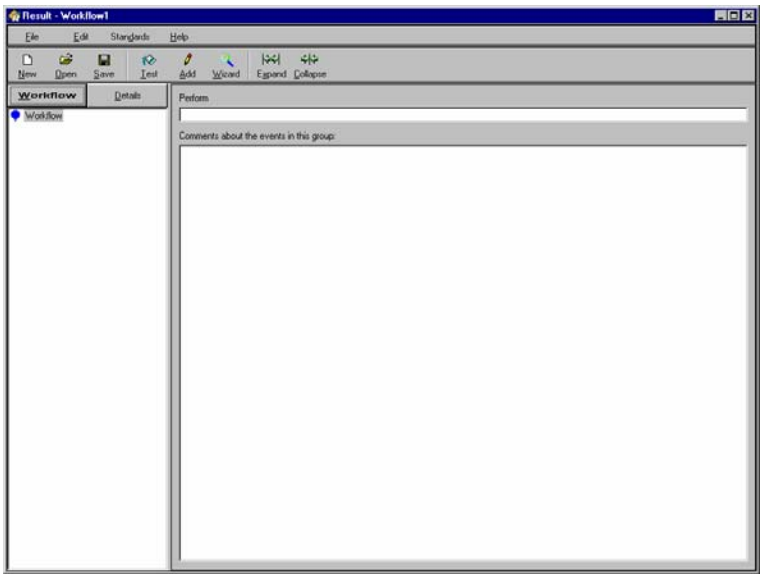
If the RESULT Integration shortcut does not appear on your desktop:

- Open the Windows Start menu by choosing Start on the Windows taskbar.

- Point to Programs in the Start menu.
- Point to the Thermo (or Thermo Nicolet) program group.
- Choose the RESULT Integration program.



After you have successfully started RESULT Integration, the RESULT main window appears on the screen.



RESULT Integration software main window

Available software diagnostics

With RESULT software, you can troubleshoot problems without affecting your production data by using any of the following features:

- **Quick Collect**. The Quick Collect feature, available in both RESULT Operation and RESULT Integration software, allows you to collect a spectrum of a background and/or sample without developing and running a workflow. Quick Collect is helpful to test repeatability or feasibility of measuring a sample. See "Chapter 5 System Maintenance" of "Section 3 RESULT Operation Software" in your *RESULT User's Guide* for more information about the Quick Collect feature.

- **Test Background, Test Sample, Test Measurement**. These three features are available in RESULT Operation software and allow you to test certain portions of a particular workflow to diagnose where a problem may reside. See "Chapter 5 System Maintenance" of "Section 3 RESULT Operation Software" in your *RESULT User's Guide* for more information about the workflow test features.

- **Running a workflow off-line**. This feature is available in RESULT Operation software, and allows you to run an entire workflow off-line, so the results do not affect production data. To use this feature, users and workflows need to be set up properly. See "Chapter 5 Managing Workflows" and "Chapter 6 Managing Users" of "Section 6 Software Administration" in your *RESULT User's Guide* for more information about this feature.

RESULT Operation software also contains diagnostics for checking the status of the instrument, running an instrument test, and aligning the instrument. See "Chapter 5 System Maintenance" of "Section 3 RESULT Operation Software" in your *RESULT User's Guide* for more information about these diagnostics.

Setting optional purge

If your analyzer is equipped with an optional purge kit, the pressure regulator should be set between 10 and 20 pounds per square inch (psi) and the flow meter should read approximately 20 standard cubic feet per hour (SCFH).

Note Read this section only if you purchased the purge option for your analyzer. ▲

If you need to adjust the flow rate, or if your application requires a different flow rate, follow the instructions provided in the "Maintenance and Service" chapter.

⚠ Danger *Never* use a flammable gas to purge the analyzer. Heat from the source or internal electrical components could ignite a flammable gas. The purge gas must be free of moisture, oil, and other reactive or infrared-absorbing materials. We recommend using dry air supplied by a purge gas generator or pure air generator (available from Thermo Fisher Scientific), or dry nitrogen. Other gases, even inert gasses such as argon (Ar), can damage the instrument. ▲

We recommend that you leave the purge on at all times (even when the instrument is powered off). This keeps the analyzer free of undesirable gases, protects the optics, and improves the system's thermal stability.

For information about installing purge equipment and inspecting and changing the purge gas filter, see the "Maintenance and Service" chapter.

To view this information from your computer, open the RESULT Operation application and choose "Servicing the Antaris analyzer" from the Service menu. Then view "Maintaining your analyzer" and look for the topics named above.

Where to go next

You are finished preparing the analyzer for operation. If you are ready to begin running samples using one of the Antaris II sampling modules, proceed to the chapter with the sampling module name.

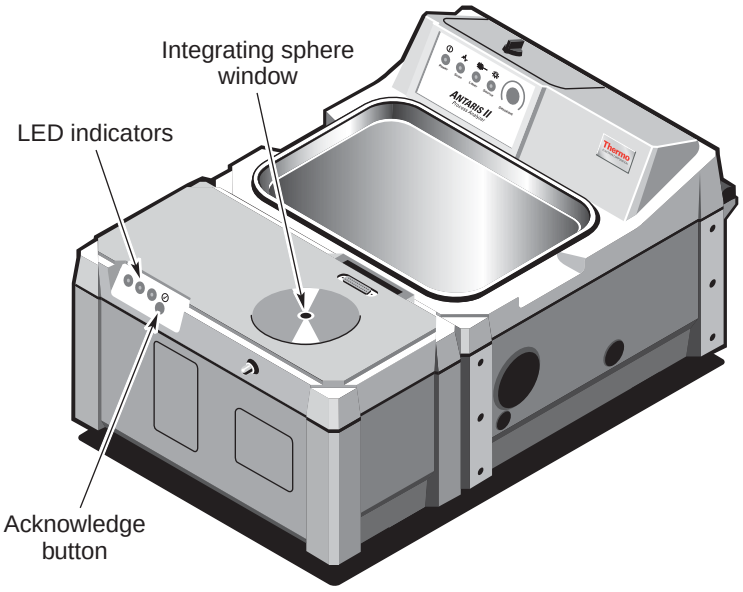
Chapter 3 Integrating Sphere Module

The Antaris II integrating sphere sampling module is a powerful, fast, and easy-to-use tool for diffuse-reflection sampling of solids and powders in the food and beverage, pharmaceutical, chemical, and polymer industries.

This chapter discusses how to test, use, and maintain the sampling module and optional sampling accessories. It also includes steps to conduct a simple diffuse-reflection experiment, information about typical spectra obtained using the integrating sphere, and some common problems with spectral data and suggestions for resolving them.

Introduction

The Antaris II integrating sphere sampling module is designed to work with Thermo Scientific RESULT Integration and RESULT Operation software to provide a powerful, fast, and easy-to-use system to analyze solids and powders using the *diffuse-reflection* sampling technique.



Antaris II integrating sphere sampling module

Module features

The important features of the integrating sphere module include:

- **Integrating sphere.** The high throughput *integrating sphere* has greater than 95% efficiency of collecting scattered energy when conducting a *diffuse-reflection* sampling experiment. The integrating sphere includes:
  - A scratch-resistant sapphire sampling window with a chemical-resistant seal.
  - Internal gold reference for automatic background collections.
  - A spectral range of 12,000 - 3,800 cm^{-1}.
  - Standard spectral resolution of 4 cm^{-1} or an optional resolution of 2 cm^{-1}.
  - InGaAs (Indium Gallium Arsenide) *detector*.
- **Sample accessory holder.** The sample accessory holder is specifically designed to hold Thermo Scientific sample cups and tablet holder accessories. The sample holder attaches to the top of the module and comes with two sample cup rings: a concentric (centering) ring that can be used with the micro- and macro-powder sample cups, and an eccentric (offset) ring that can be used with the macro-powder sample cups.
- **Optional tablet analyzers.** The sampling module can use either of the following tablet analyzers to perform transmission and diffuse-reflection sampling simultaneously:
  - **Standard tablet analyzer.** This analyzer is recommended for use with dense materials, such as opaque tablets, because it has a narrow band, high-sensitivity InGaAs detector, and covers a spectral range of 12,000-5,880 cm^{-1} (833-1,700 nm).
  - **Softgel tablet analyzer.** This analyzer is recommended for use with samples that are better transmitters, such as softgel capsules, paper, plastics, packaging materials, and polymers. It has a broad-band InGaAs detector and covers a spectral range of 12,000-3,800 cm^{-1} (833-2,630 nm).

  The tablet analyzers are similar to each other in appearance and can accommodate a sample up to 9.8 cm in diameter.

- **Optional tablet holder kit.** The tablet holder kit contains one *universal tablet holder* and two custom tablet holders that can be modified to exact tablet dimensions, along with a centering ring for the custom tablet holders. The tablet holder accessories can fit inside the sample cup holder.

- **Optional closed sample cups.** The closed sample cups come in packages of three sample cups. Each cup has a 1 mm or 3 mm low OH quartz window and can be used in conjunction with the sample accessory holder and sample rings.

- **Optional open sample cups.** The open sample cups come in packages of three sample cups. Each cup has a 4.78 mm or 12 mm low OH quartz window and can be used in conjunction with the sample accessory holder and sample rings.

- **Optional viscous liquid sampler.** The viscous liquid sampler (VLS) can be used to collect transflectance spectra from viscous liquids. If the system is equipped with a softgel tablet analyzer, the VLS can also be used for transmission analyses. The apparatus is designed to handle thick, concentrated samples with little mess and quick, easy cleanup. It fits on the sample accessory holder or the softgel tablet analyzer base.

- **Optional sample cup spinner.** The sample cup spinner is an accessory for the integrating sphere sampling module that allows multi-point reflection measurements of heterogeneous solids such as powders, granules and pellets.

- **MulitPro.** The MultiPro Autosampler is an accessory that allows you to automate near-infrared measurements of powders, tablets and softgel capsules using both transmission and diffuse reflection sampling techniques.

- **Autosampler RS.** The Autosampler RS is an accessory that allows you to automate near-infrared reflectance measurements of powders, solids and tablets. The Autosampler RS uses carousels that accommodate tablets and sample vials.

Testing the sampling module

RESULT Operation software contains an Instrument Check feature that runs an instrument performance test. Before running the performance test, turn on the instrument power and make sure the instrument has remained on for at least an hour to stabilize.

To run the instrument check:

1. **Log on to RESULT Operation software.**

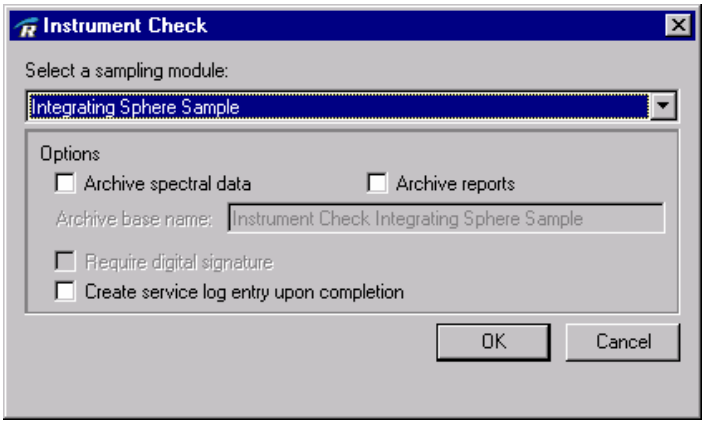
   See "Starting RESULT software" in the "Antaris sampling" chapter for instructions to log on to the software.

2. **Open the Maintenance menu from the Result Operation main window.**

Note If the Maintenance menu does not appear in the RESULT main window, then you cannot access the Instrument Check feature. See your *RESULT software administrator*. ▲

3. **Choose the Instrument Check option from the Maintenance menu.**

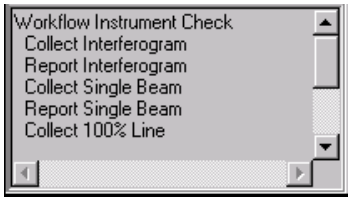
   The software will open the Instrument Check dialog box.



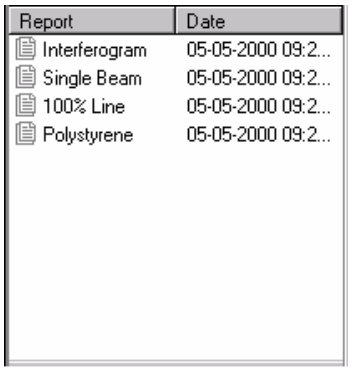
4. **If Integrating Sphere Sample is not already selected, select that option from the Select A Sampling Module drop-down list.**

5. **Choose OK to perform the check.**

   The software will start performing the instrument check. While the instrument check is running, the status indicator on the lower left side of the RESULT Operation main window will indicate the status of the instrument check.



   As each spectrum is collected, the software will create a report. The title of each report will appear in the report navigation frame.



   You can view a report by selecting the report name, and the selected report will open in the display area.

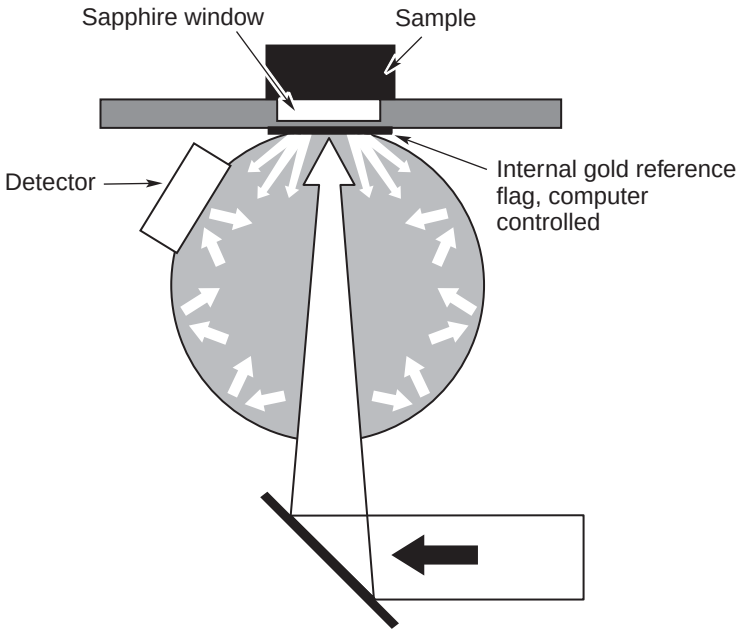
See "Chapter 5 System Maintenance" in "Section 3 RESULT Operation Software" of your *RESULT User's Guide* for information about archiving the test data, requiring digital signatures for the data, and creating a service log entry of the test. The "System Maintenance" chapter also contains example spectra with a description of each.

Diffuse-reflection sampling

Diffuse-reflection is a powerful technique for *Fourier transform* near infrared (FT-NIR) analysis of rough-surfaced solids, fine particles, and powders.

Diffuse-reflection measures the changes that occur in an infrared beam when the beam interacts with a particulate sample. When directed onto a surface, the infrared radiation will interact with the surface by alternately passing through it and reflecting. This causes the light to scatter, or "diffuse," as it makes its way through the sample.

Diffuse-reflection measurements are simplified by using an integrating sphere. The beam is directed into the sphere and travels directly through the center of the sphere, through the optical window, and into the sample.



Diffuse-reflection using the integrating sphere

The beam scatters off of the sample and the reflected light beams re-enter the sphere. The inside of the sphere is coated with diffuse gold, which collects the light beams and directs them into the detector.

Compatible sample types

The integrating sphere sampling module is designed for fast and easy sampling in the industrial environments of the pharmaceutical, chemical and polymer industries. The *integrating sphere* can measure a wide variety of samples. Because it uses *diffuse-reflection*, it is also useful for powders or "rough" solids. Samples can be analyzed by placing them directly on the integrating sphere window or through clear packaging materials, such as glass and plastic.

The following are some examples of sample types that can be used with the integrating sphere sampling module:

- Solids with a rough or diffuse surface, such as coated textiles, paper, wood, polymers, and plastics (especially plastics with a milky, opaque appearance).
- Powders in clear glass vials, clear plastic bags, or in Thermo Scientific sample cups.
- Tablets with reflective surfaces, either placed directly on the integrating sphere or in one of the tablet holder accessories.
- Suspense or opaque liquids and gels in glass or plastic containers.

Sample thickness or the amount of sample should be taken into consideration when using the *integrating sphere*. If a solid sample is too thin or if there is not enough of a powder sample, you may encounter problems with the spectra. See the "Common problems with spectral data" section of this chapter for more information.

Note Because clear gels and liquids are not reflective, it is not recommended that they be used with the integrating sphere. ▲

Your first experiment

This section goes through a simple experiment using the integrating sphere along with the Quick Collect feature in RESULT Operation or Integration software to produce a *diffuse-reflection spectrum*.

The Quick Collect feature in RESULT software allows you to collect a *background* and/or sample spectrum for investigation and sample setup without developing and running a *workflow*. Using Quick Collect is good practice to help you "get the feel" of sampling with the integrating sphere module before using the module in actual production workflows. Quick Collect also allows you to easily produce a spectrum without having to develop a workflow for a single collection *event*.

Before you begin

Before you begin the experiment:

- Power on the instrument and allow the instrument to stabilize for at least an hour (if the instrument has been powered off for more than 20 minutes).
- Have your sample material at hand. For the collection parameters in this experiment, it is recommended that you choose one of the following items for your sample:
  - 325 mg aspirin tablet; or
  - A piece of white bond paper or other paper, such as a Post-it® note.

Setting up the experiment

To set up the experiment:

1. **Start RESULT Operation or RESULT Integration software.**

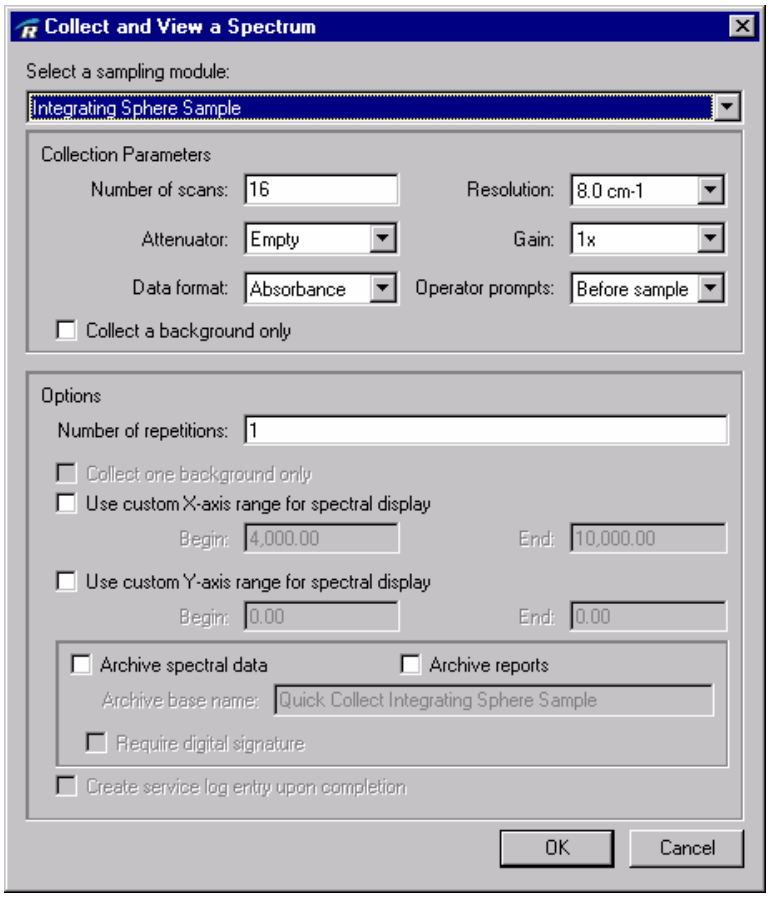
   See "Starting RESULT software" in the "Antaris sampling" chapter for instructions to log on to the software.

2. **Open the Quick Collect dialog box.**

   Select Quick Collect from the Tools menu in RESULT Integration or from the Maintenance menu in RESULT Operation.

Note If you are using RESULT Operation software and the Maintenance menu does not appear in the menu bar of the main window, then you cannot access the Quick Collect feature. See your RESULT software administrator. ▲

The Quick Collect dialog box should appear.



3. **If it is not already selected, select the Integrating Sphere Sample option from the Select A Sampling Module drop-down list.**

4. **For purposes of this experiment, confirm that the following collection parameters are set:**

Parameter	Setting
Number Of Scans	30
Resolution	8 cm^{-1}
Gain	1x
Attenuator	Empty
Data Format	Log (1/R)

5. **Select the None option from the Operator Prompts drop-down list.**

   This means that you will not be prompted to begin background or sample collection. Because the integrating sphere collects a background spectrum using an internal reference, no background prompts are needed.

6. **Do not change any other options for this experiment.**

   For more information about the other options in the Quick Collect dialog box, see "Chapter 5 System Maintenance" in "Section 3 RESULT Operation Software" of your *RESULT User's Guide.*

7. **Place the sample on the integrating sphere window.**

8. **Choose OK to begin the experiment.**

Collecting the background

The instrument will use the integrating sphere's internal reference to collect the background. The instrument contains a flag that will close beneath the integrating sphere's sapphire window so the light beam does not travel through the window.

You may hear the flag below the integrating sphere window "click" closed before the instrument begins collecting the background data. You can view the status of the background collection in the status indicator box in the software.

When the instrument has finished collecting the background, you may hear the flag inside the integrating sphere "click" open.

Collecting the sample

The instrument will automatically begin collecting sample data after it has completed collecting the background data. You can view the status of the data collection in the status indicator box in the software. When the instrument has finished collecting data, the software will display the spectrum in the display area.

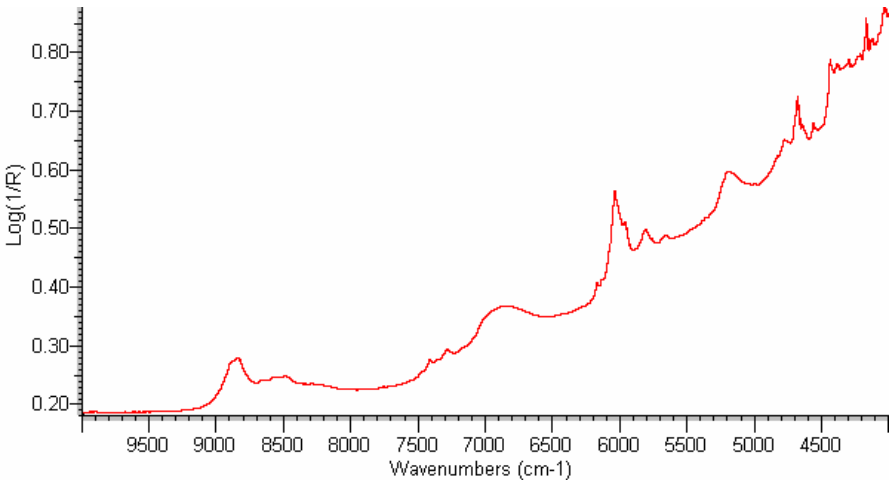
If the integrating sphere window collected any residue from the tablet, follow the instructions for cleaning these items in the "Maintenance and Service" chapter.

Typical diffuse-reflection spectra

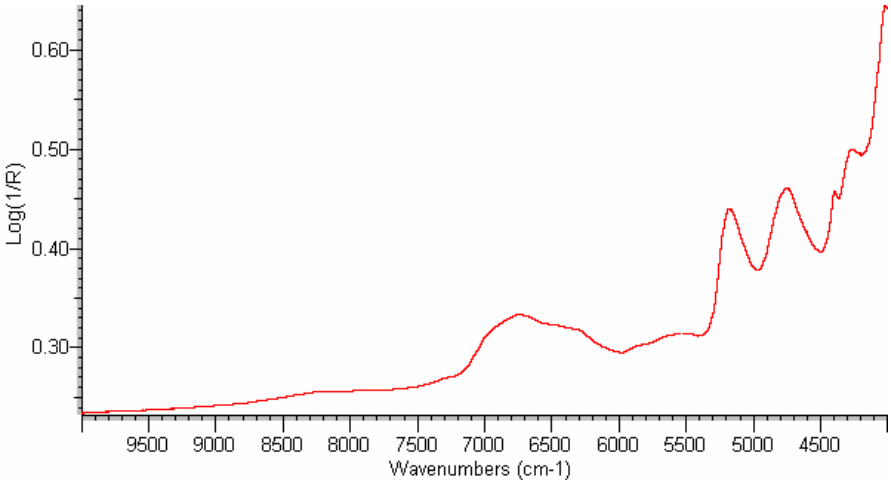
FT-NIR spectra produced by diffuse-reflection can have unique characteristics. Some problems with these characteristics are also discussed in the "Common Problems" section of this chapter.

Note The spectra shown in this section are only examples of the kinds of results you may obtain. The actual spectra produced from your experiments may vary greatly, depending on the sample material and preparation. ▲

The following spectra are representative of typical spectra taken using the integrating sphere sampling module:



Diffuse-reflection spectrum of 325 mg aspirin tablet



Diffuse-reflection spectrum of paper

The typical spectral range for a diffuse-reflection sample with the integrating sphere is 10,000 to 4,000 wavenumbers (cm^{-1}).

Collecting backgrounds

A *background* is a reference spectrum that accounts for the unique optics of the sampling module or accessory and the instrument. Each sample spectrum is ratioed against a background so that the final spectrum is free of these features. You can collect backgrounds using internal or external references, as directed by the workflow you are running.

The workflow you are running will direct how often to collect a background spectrum. The most recent background spectrum remains in memory and is compared against sample data until a new background spectrum is collected.

The "Common problems with spectral data" section of this chapter contains suggestions if a background spectrum is atypical from previously-collected background spectra.

For diagnostic purposes, you can collect a background using RESULT Operation software's Test Background or Quick Collect dialog box. The Test Background feature is helpful if you want to test background collection related to a particular workflow without affecting your production data. The Quick Collect feature is helpful if you want to test background collection independent of a workflow. The Quick Collect feature is also available in RESULT Integration software.

Using the internal reference

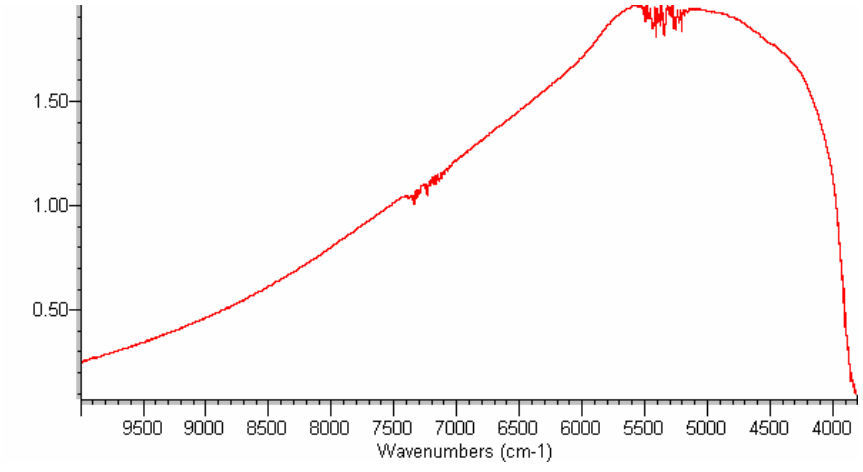
If collecting a background using the internal diffuse gold reference, it is not necessary to remove the sample material from the sampling area on the module (if the sample is already in place). The instrument contains an internal flag underneath the integrating sphere window which will close during background collection to prevent the light beam from traveling through the window.

Depending upon the workflow, you may or may not be prompted to begin background data collection. Because positioning a reference is unnecessary, the workflow may automatically collect background data without requiring any operator interaction.

If you are prompted to begin background collection, the green LED indicator on the instrument will be on when it is time to begin collection. If the indicator is steady, then you can begin collecting data by pressing the Acknowledge button on the instrument or responding to a prompt in the software. If the indicator is flashing, then you must begin collecting data by responding to a prompt in the software.

Before the instrument begins collecting background information, the flag under the integrating sphere window will “click” closed. The status indicator in the software will show you the status of the background collection. When the instrument has finished collecting the background data, the flag under the integrating sphere will “click” open.

A typical background spectrum using the internal diffuse gold reference should resemble the following:



Typical diffuse gold background spectrum with the integrating sphere

See the "Common problems with spectral data" section in this chapter if your background spectrum is not similar to the above spectrum, or if it is atypical from previous background spectra.

Using an external reference

If the workflow you are running includes collecting a background spectrum using an external reference, then the workflow should prompt you when to begin background collection.

Some examples of materials that can be used as an external background reference include:

- Diffuse gold.
- Spectralon, which is a very diffuse substance with high reflectance.
- Ceramic.

Note Once a material is selected for a background reference, make sure to use the same material each time you run the workflow. ▲

Your workflow or an instruction document attached to the workflow should have information about preparing and positioning the background reference. See "Chapter 2 Running Workflows" in "Section 3 RESULT Operation Software" of your *RESULT User's Guide* for more information about viewing instructions attached to workflows.

The green indicator on the instrument will be on when the instrument is ready to begin collecting the background. Your workflow or an instructions document should contain steps for preparing the reference material and instrument for background collection.

Depending on whether the green LED indicator is flashing or steady, press the Acknowledge button on the instrument's operational panel or choose the appropriate response in a software prompt when you are ready to begin collecting the background data.

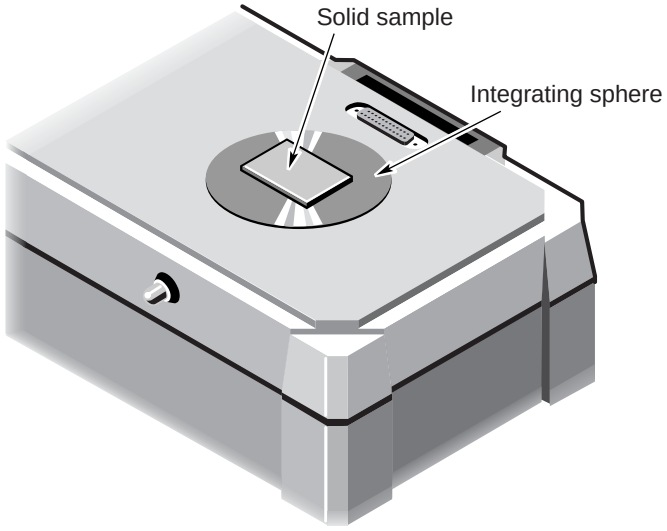
The status indicator in the software will display the status of the data collection. Do not move the reference material from the integrating sphere window until the instrument has finished collecting the data.

Preparing samples

This section contains information preparing samples and accessories for use with the integrating sphere for diffuse-reflection experiments

Sampling solids

You can conduct *diffuse-reflection* experiments on solids using the integrating sphere. When sampling a solid, place the solid over the top of the sapphire window on the integrating sphere.



Sampling a solid using the integrating sphere

You can also sample solids through clear packaging materials, such as glass vials, plastic bags, or plastic wrap. If you are sampling a particularly abrasive solid, it is recommended that you put the solid in a clear glass container or plastic bag to avoid scratching or damaging the surface of the integrating sphere window and sampling area.

Sampling powders

Like solids, you can sample powders through clear packaging materials such as glass vials or plastics. When sampling powders through packaging materials, follow the same sampling instructions used for sampling solids.

If you are using glass vials, use the kind with a flat bottom, and place the bottom of the vial on top of the integrating sphere when collecting data. You should fill the vial to a depth of at least 4-5 mm to produce a good spectrum.

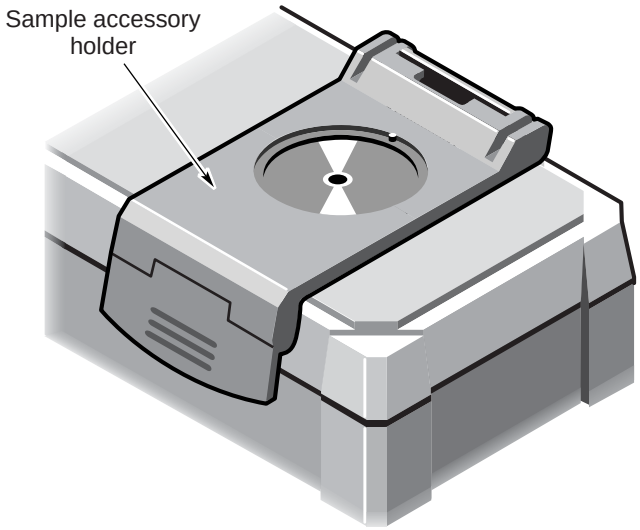
Using sampling accessories

Thermo Fisher Scientific offers a number of sampling accessories for sampling powders and tablets with the integrating sphere sampling module to assist you in conducting precise and repeatable sampling experiments. This section covers using the Thermo Scientific sample accessory holder in conjunction with Thermo Scientific sample cups and sample cup rings, the universal tablet holder, and custom tablet holders.

Note The sample cups and sample cup rings, the universal tablet holder, and the custom tablet holders can be used with the tablet analyzer as well as the sample accessory holder. The instructions that follow work for all of these. ▲

Using the sample accessory holder

The sample accessory holder can be used in conjunction with Thermo Scientific sample cups and sample cup rings, the universal tablet holder, and custom tablet holders.



Sample Accessory Holder

The sample accessory holder comes with concentric (centering) and eccentric (offset) rings that can be used in conjunction with Thermo Scientific sample cups. More information about the sample cup rings is included in “Using Sample Cups” later in this chapter.

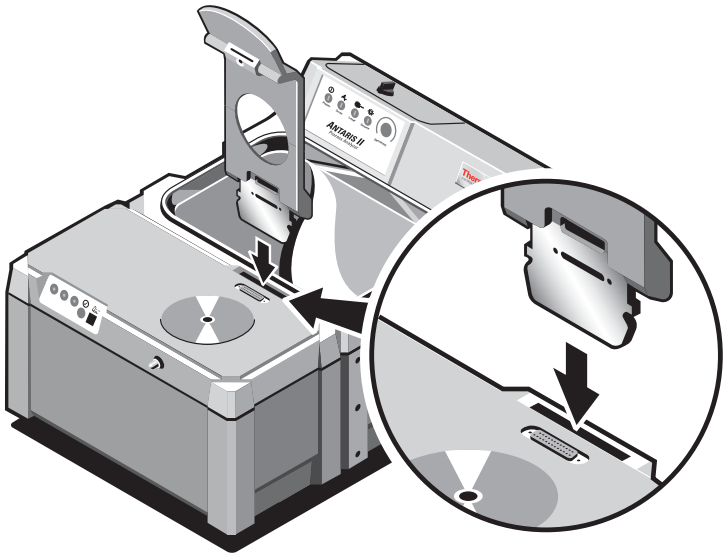
Installing the sample accessory holder

To install the sample accessory holder:

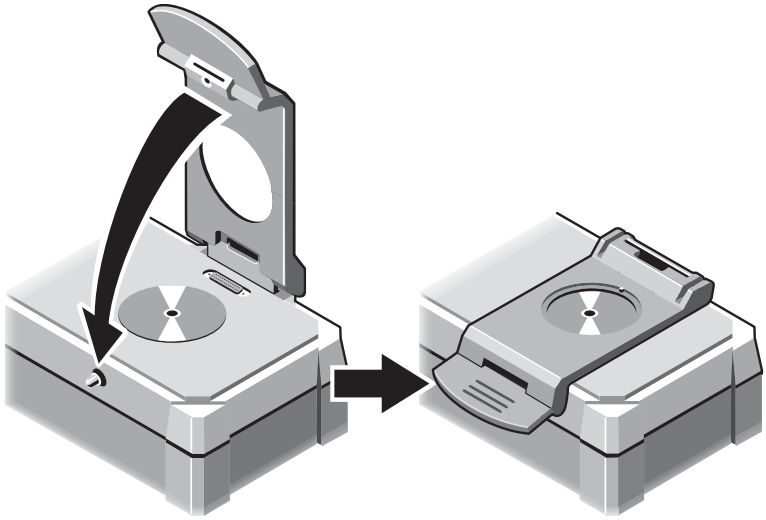
1. **With both hands, hold the sample accessory holder upright, with the bottom facing you.**

   The silver connection hinge should be facing downward.

2. **Insert the connector hinge into the slot on the top of the instrument.**



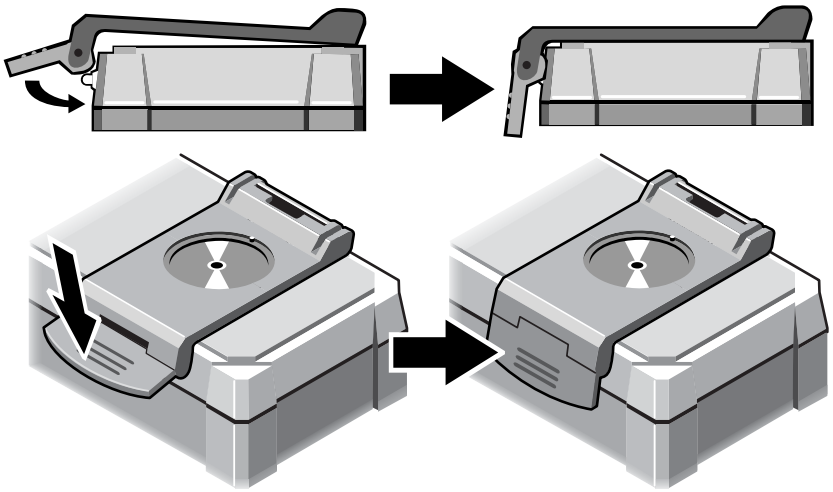
3. **Slowly and gently set the holder down on the top of the instrument.**



⚠ Caution The sample accessory holder fits tightly onto the instrument. To avoid pinching your fingers, keep your fingers clear of the bottom of the holder when pressing on the latch. ▲

4. **Firmly press down on the latch on the sample accessory holder.**

   If the latch does not close or it will not lie flush against the instrument, or if the sample accessory holder is not resting flatly on top of the instrument, remove the holder and attempt to install it again.



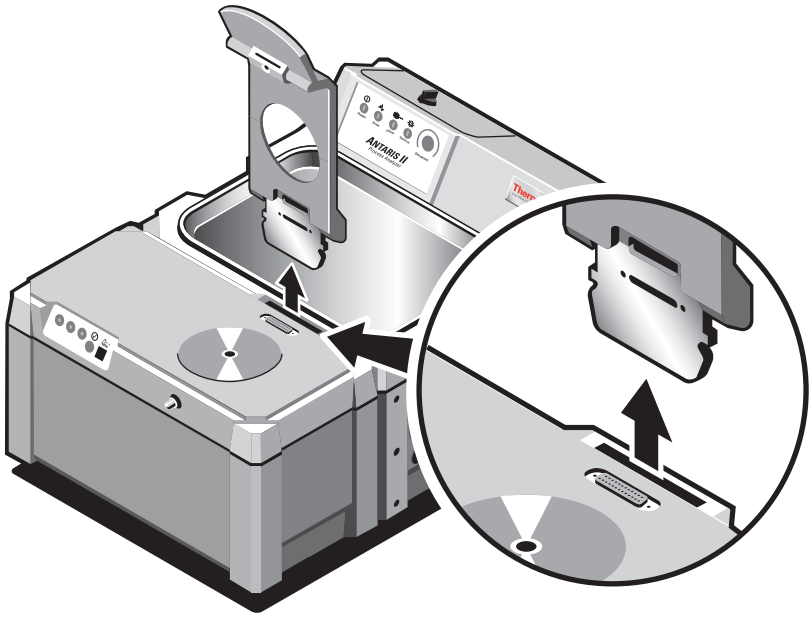
Removing the sample accessory holder

The sample accessory holder can remain on the instrument at all times unless it is necessary to remove it to sample large items using the integrating sphere or to replace internal parts in the instrument.

To remove the sample accessory holder:

1. **Remove all sampling materials and accessories from the sample accessory holder, and release the latch.**

2. **Lift the sample accessory holder until it is perpendicular with the instrument, and then carefully pull up on the sample accessory holder.**



Using sample cups

The optional Thermo Scientific sample cups and sample cup rings can be used in conjunction with the sample accessory holder to conduct diffuse-reflection experiments. Powders can be sampled leaving the sampling cups open or by using the sample cup lids. The sample cup lids contain an internal press to assist in powder-packing consistency. The sample cup kits are available in two sizes:

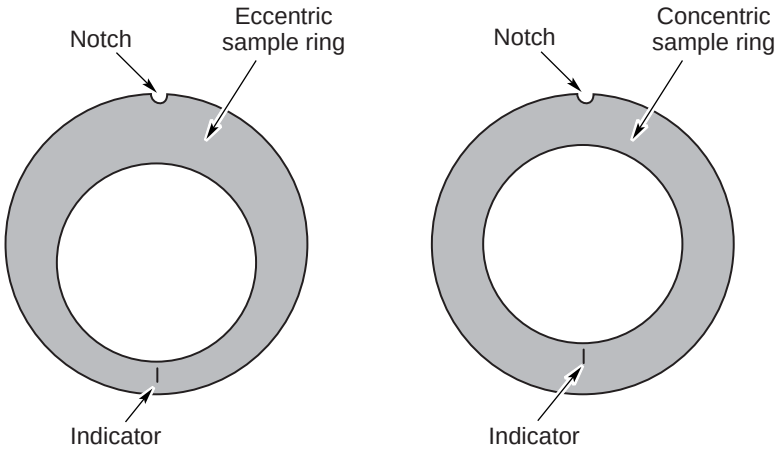
- **Optional closed sample cups.** The closed sample cups come in packages of three sample cups. Each cup has a 1 mm or 3 mm low OH quartz window and can be used in conjunction with the sample accessory holder and sample rings.

- **Optional open sample cups.** The open sample cups come in packages of three sample cups. Each cup has a 4.78 mm or 12 mm low OH quartz window and can be used in conjunction with the sample accessory holder and sample rings.

Note The sample cups and sample cup rings, the universal tablet holder, and the custom tablet holders can be used with the tablet analyzer as well as the sample accessory holder. The instructions that follow work for all of these. ▲

Note It is not recommended that the sample cups be used for sampling gels or liquids, as these types of substances may be difficult to remove and clean from the sampling cups. ▲

When used in conjunction with the sample cup rings, the sample cups allow you to run multiple collections of a powder in different sampling positions. The concentric ring opening is centered around the integrating sphere window and can be used with both the micro- and macro-powder sample cups. The eccentric ring is offset around the integrating sphere window, and can be used with the macro-powder sample cup to conduct experiments covering all areas of the sample surface.



Sample cup rings

Note Do not use the micro-powder sample cups with the eccentric sample ring. In some sampling positions around the ring, the micro-powder sampling window will not be aligned with the optical window on the instrument and you will be unable to collect spectra of the sample from those positions. ▲

Preparing a sample

To prepare powders for analysis using Thermo Scientific sample cups:

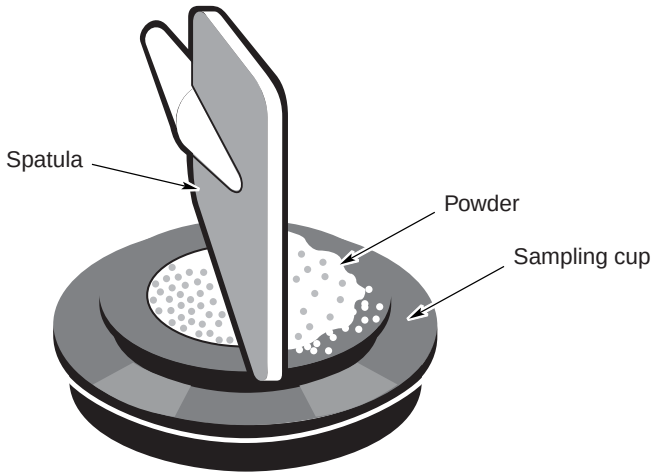
1. **Place the sample cup on a flat surface.**

   To catch any powder residue, place a clean cloth or paper towel underneath the sample cup.

2. **Fill the sample cup with the powder until it is overflowing.**

   You can *tamp* the powder cup to help the particles settle into the cup consistently, and then add more powder to the cup so it is overflowing.

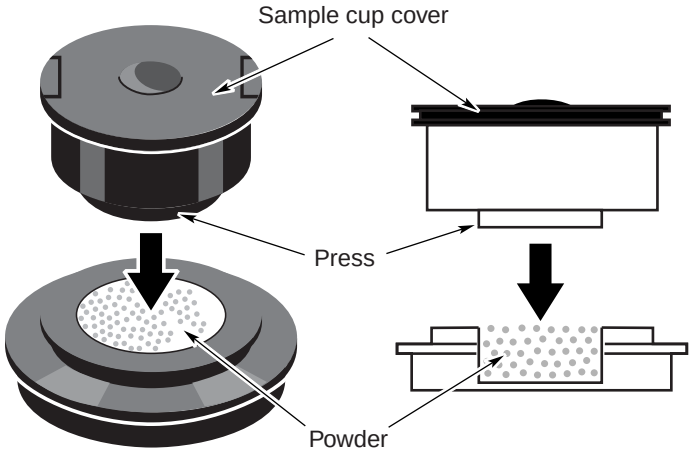
3. **Use a spatula or flat edge to level off the top of the sample cup.**



4. **If using the sample cup cover, gently place the cover on the sample cup.**

   The cover is properly attached to the cup when you hear it "click" in place.

   It is recommended that you use the sample cup cover when sampling powders, to ensure that the powders are packed consistently. The sample cup covers contain a spring-loaded press that will pack down the powder when the cup is closed.



Using the sample cups

The sample accessory holder can be used in conjunction with the sample cups and sample cup rings when doing multiple data collections to ensure sample uniformity.

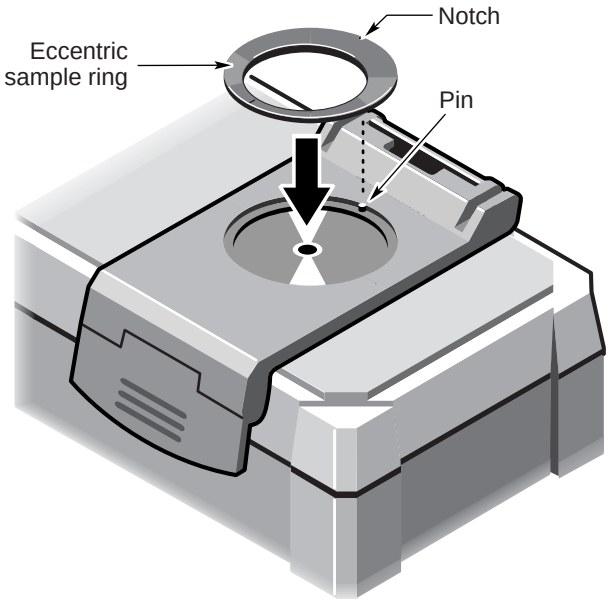
Note The sample cups and sample cup rings also can be used with the tablet analyzer. See "Installing a tablet analyzer" in the "Tablet Analyzer Module" chapter for more information. ▲

To use the sample cups and sample cup rings:

1. **If the sample accessory holder is not installed, install the sample accessory holder.**

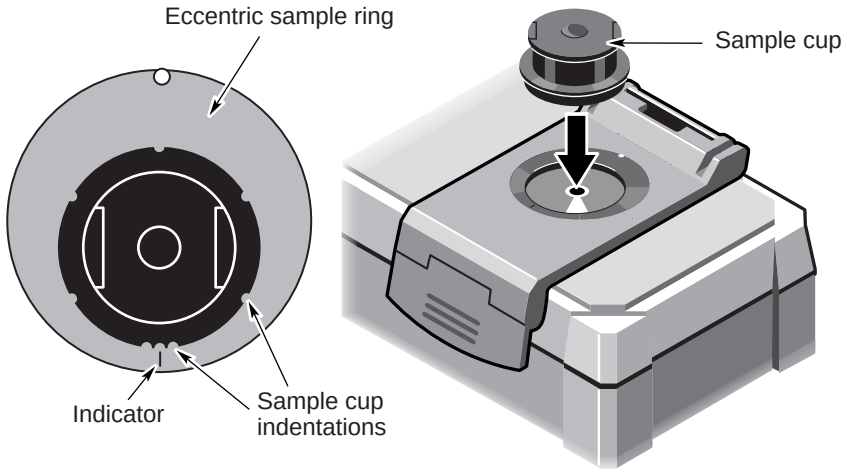
   See "Installing the Sample Accessory Holder" earlier in this chapter for instructions.

2. **Insert a sample cup ring in the sample accessory holder or the tablet analyzer base.**



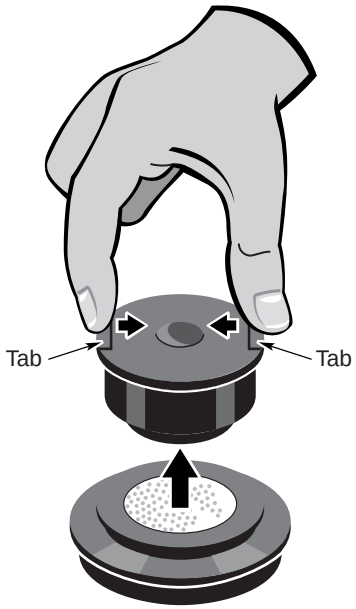
   Align the notch in the sample cup ring with the pin in the sample holder to secure it in place.

3. Insert the sample cup into the sample ring.



The sample ring has an indicator that can be aligned with indentations at 60° increments around the circumference of the sample cups. Use the alignment indicators to ensure consistency when conducting experiments on multiple samples. When performing multiple data collections on a sample, you can use these indicators, in conjunction with the indentations in the sample cups, to rotate the sample to repeatable positions. When you have finished your experiment, remove the sample cup and sample cup ring from the sample accessory holder before removing the holder.

To open a sample cup, press the tabs on the sides of the cover and lift. (See the "Maintenance and Service" chapter for cleaning instructions.)



Using tablet sampling accessories

Thermo Fisher Scientific offers a universal tablet holder and custom tablet holders that can be used in conjunction with the sample accessory holder to help ensure proper and consistent tablet positioning when conducting experiments on multiple samples. For more information, see "Using the universal tablet holder" in the "Tablet Analyzer Module" chapter.

Tips for developing workflows for the integrating sphere

When developing workflows using RESULT Integration software, there are some factors you want to take into consideration to make sampling with the integrating sphere sampling module as efficient as possible. Sample parameters and specifications are highly dependent on the sample type, the amount of time available to collect data, and the level of interest in different spectral characteristics. This section contains recommendations for starting points when specifying collect event parameters, sample specifications, and background specifications.

See "Section 5 Workflow Events and Specifications" in your *RESULT User's Guide* for more information about the items mentioned in this section.

Collect event parameters

A collect event in RESULT Integration software instructs the instrument to collect a spectrum of a sample. The following table contains the recommended starting points for sample collection parameters for the integrating sphere sampling module:

Parameter	Integrating Sphere Setting
Number Of Sample Scans	30
Data Format	Log (1/R)
Background Frequency	Every Hour

- **Number Of Sample Scans**. To start, try using 30 scans. You can then decrease the number of scans to the smallest number that can still produce tolerable signal-to-noise (determined by error of prediction or pre-defined limit) if sampling time is at a premium. If using a higher resolution, the spectra will contain more spectral noise, so you may need to increase the number of scans to better distinguish sample features from noise.

- **Background Frequency.** If collecting samples only periodically, then collecting a background before every sample is recommended. If collecting many samples at a time, then collecting a background every hour should be sufficient.

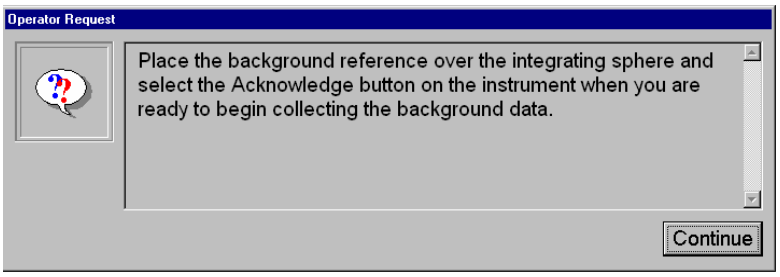
Operator prompts

When developing a workflow in RESULT Integration software, the collect event allows you to include operator prompts for both sample and background collection.

Notice When creating sample collection prompts, make sure your prompts include specific information for the application. If the operator is required to reposition the sample (for example, if you've created a repeat loop in a workflow to sample powders in a sample cup) it is recommended that you prompt the operator each time the sample needs to be repositioned, and include the number of degrees the sample should be rotated. ▲

For background prompts, because no preparation is necessary to collect a diffuse-reflection background spectrum using the integrating sphere's internal reference, no prompts are necessary before performing this function.

However, if using an external reference for background collection, it is recommended that you include a detailed operator prompt to ensure that the background data is collected properly. The following is an example prompt for collecting backgrounds:



Sample specifications

In RESULT Integration software, a sample specification is used to specify advanced collection parameters to optimize the workflow based on a sampling technique. Sample specifications are attached to collection events in workflows. The following table contains the recommended starting points for sample specifications:

Specification	Integrating Sphere Setting
Attenuator	Empty
Resolution	8 cm^{-1}
Gain	1x
Spectral Range	10,000-4,000 cm^{-1}

- **Gain and Attenuator**. You may want to begin with a Gain setting of 1x and an Attenuator setting of Empty. This setting will be appropriate for the majority of samples. If you want to increase the gain, you can utilize RESULT Integration software's Optimize Gain feature.

  For more information about using the Optimize Gain feature, see the Sample Specification information in "Section 5 Workflow Events and Specifications" of your *RESULT User's Guide*.

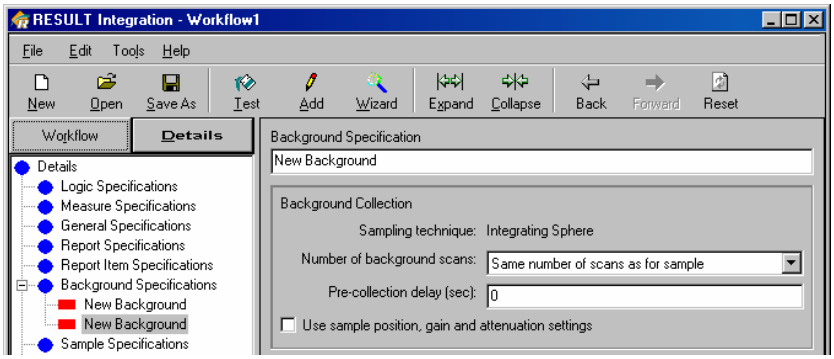
- **Resolution**. Try 8 cm^{-1} as a starting point. You can increase the number of scans to improve signal-to-noise ratio. You can also improve the signal-to-noise increase by increasing the resolution (e.g., from 8 cm^{-1} to 4 cm^{-1}) if required by your sample. You can try a lower resolution to trade off resolution for signal-to-noise.

Background specifications

The settings in the Background Specification are affected by whether you will be using an external or internal reference for background collection.

If you plan to use an external reference for a diffuse-reflectance background, make sure to select the Use Sample Position, Gain, And Attenuation Settings check box in the Background Specification of your workflow. This check box defines the Attenuator setting used for background collection. When the check box is selected, the software uses the Attenuator setting that is shown on the sample specification. When the check box is cleared, the background will be collected with the internal gold reference (reference flag in closed position). The default gain setting

will be 1x, and the default attenuator setting will be C screen.



A good starting point for the Number of Background Scans parameter is Same Number Of Scans As For Sample.

Common problems with spectral data

Before using the instrument for precise quantitative analysis, evaluate the effects of temperature and sample contact on spectral features. Other items that may influence spectra are bad backgrounds; the amount of noise; improper collection of a sample; sample particle size, homogeneity, and concentration.

If you encounter a problem, before you do anything else, check the following items:

- Make sure the sample is properly positioned over the integrating sphere window (and in the sample accessory holder if it is being used) when collecting the sample data.
- Make sure the integrating sphere window is not dirty. If there is residue on the window, follow the instructions in the “Maintenance and Service” chapter to clean the window.

Problems with background spectra

If a background spectrum you collected is atypical from previously-collected backgrounds or from the typical spectrum described in the “Collecting the Background” section of this chapter and you were using an external reference, the problem may be one of the following:

- The sample material could have been run as the background.
- The reference was moved while the instrument was collecting data.
- The reference is dirty. Clean it or replace it, if necessary.

For the above problems, or if you were using the instrument's internal reference, you should take test backgrounds using either the Quick Collect (not associated with a workflow) or Test Background (following the steps for background collection in a workflow) features in RESULT Operation software before running the workflow again in production.

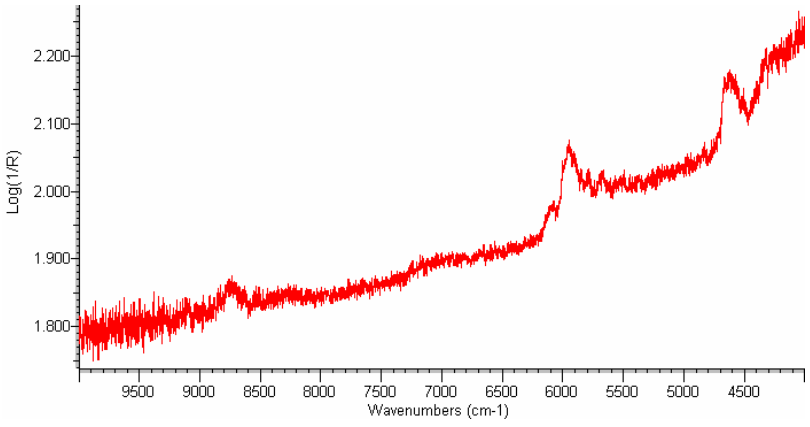
If using the internal reference, and backgrounds become atypical from prior backgrounds, you may want to run the instrument status and instrument check features to see if there may be a problem with the instrument. See "Chapter 5 System Maintenance" in "Section 3 RESULT Operation Software" in your *RESULT User's Guide* for more information about running the instrument status and instrument check features.

Problems with sample spectra

Several factors may affect a sample spectrum. Before deeming the sample as "bad," collect the sample data again either by running the workflow off-line, using the Test Sample feature, or using the Quick Collect feature in RESULT Operation software.

High noise

A spectrum that contains a high amount of *noise* will resemble the following:

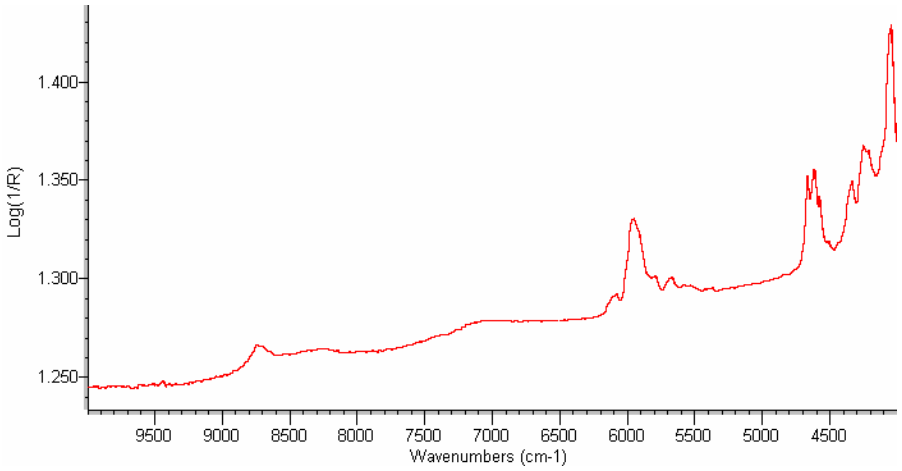


Ascorbic acid spectrum with high noise using the integrating sphere

As shown above, the high level of noise is represented as very small peaks in a spectrum. If you experience this problem, you may want to increase the number of scans or lower the resolution to decrease the amount of noise in the spectrum. You can also try increasing the detector gain. Finally, check to make sure any attenuation screens that are in place are needed. If they are not needed, remove them.

Offset baseline

A spectrum with an offset baseline may resemble the following:



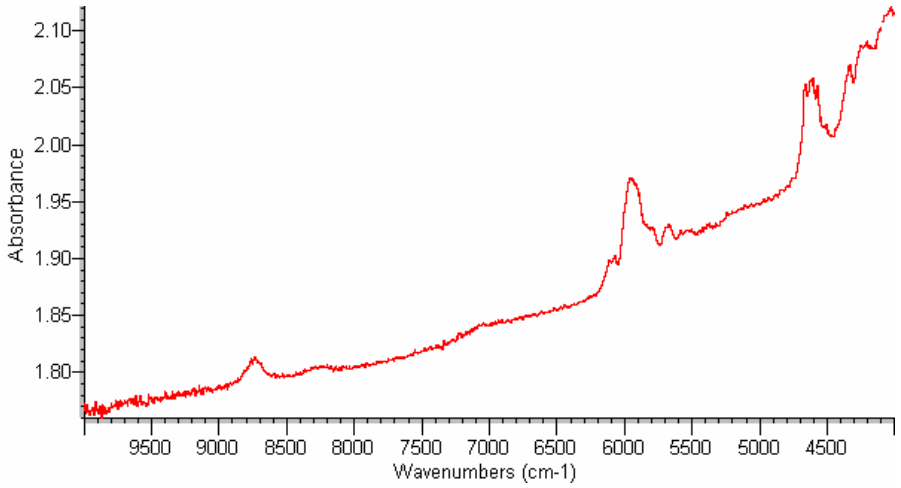
Aspirin spectrum with baseline offset using the integrating sphere

As shown above, the spectrum baseline started at 1.250 Log(1/R). Some spectra may normally have a baseline that does not start at zero, depending on your sample material, preparation, and positioning. However, if the baseline of your spectrum is not consistent with previous spectra, one of the following may have occurred:

- The sample material may be too thin.
- The sample material did not completely cover the integrating sphere window.

Samples not appropriate for diffuse-reflection

Some samples may not be diffuse enough to use with the integrating sphere. An example spectrum of a smooth sample may resemble the following:



Thin polystyrene film spectrum showing insufficiently diffuse features using the integrating sphere

As shown above, the baseline is high (above 1.8 absorbance units). Very little light was diffused and reflected back into the integrating sphere. The spectral features are relatively small. For this type of sample, you may want to try another sampling technique, such as transmission.

Sample particle size, homogeneity, and concentration

Particle size, *homogeneity*, and concentration all affect the quality of spectra. Changes in particle size can affect scattering and may have ramifications on the effective pathlength. This can cause differences in *band* intensity and baseline shape.

The quality of your spectrum will be most affected if there are extreme differences in particle size throughout the sample (for example, a sample containing particles smaller than 3 microns and above 500 microns).

Homogeneity can affect reproducibility. The degree of heterogeneity in a sample should be taken into consideration when determining the number of collection event repetitions to include when creating a workflow, so you can achieve a representative spectrum of the sample. The spectral data will probably be of good quality, but each individual spectrum may not be representative of the sample as a whole.

Concentration does not affect *signal-to-noise* in a spectrum. Signal-to-noise can, however, become more of a factor when working with lower concentrations of a sample.

To keep these types of problems at a minimum, when developing workflows, consider adding repeat loops to your workflows to collect data from samples in different sampling positions. If sampling powders, consider using the Thermo Scientific sample cups along with the cup covers to ensure consistent powder packing for each experiment.

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Chapter 4 Transmission Module

The Antaris II transmission sampling module is a powerful, fast, and easy-to-use tool for raw material identification, quality measurements, and sample *component* analysis in the pharmaceutical, chemical, polymer, and food and beverage industries. The module allows you to analyze *samples* of liquids and solids using *near-infrared transmission spectroscopy*.

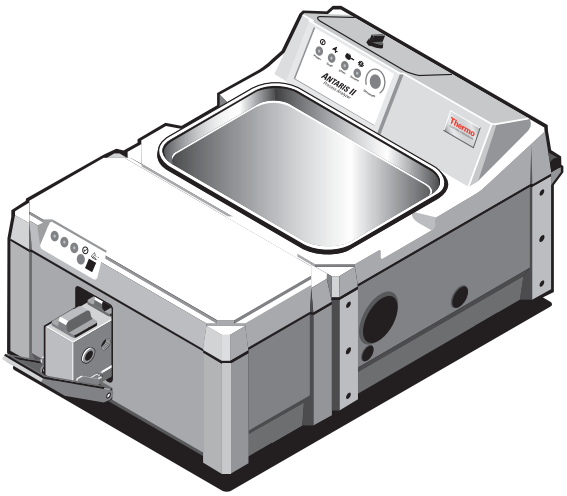
This chapter discusses how to use and maintain the *transmission module*. It also includes steps to do simple transmission experiments, information about typical spectra obtained using transmission techniques, some common problems with transmission spectra and suggestions for resolving them.

Introduction

Near-infrared spectroscopy has typically used transflection (transmission through a sample coupled with reflection from a mirror-like substrate) as a standard technique, but the *near-infrared* region actually lends itself very well to true transmission spectroscopy. Pathlengths are relatively long, and you can often run thick samples, particularly packaging materials, without pressing them or dissolving and casting them as films. Further, since glass absorbs little near-infrared radiation, you can use inexpensive glass *vials* and *culture tubes* for sampling. This makes sample preparation easy and helps prevent cross contamination since the tubes can be discarded after being used. Sampling with glass containers also allows you to analyze heated sample materials, so you can obtain high quality spectra from liquids rather than solids, which tend to scatter near-infrared radiation.

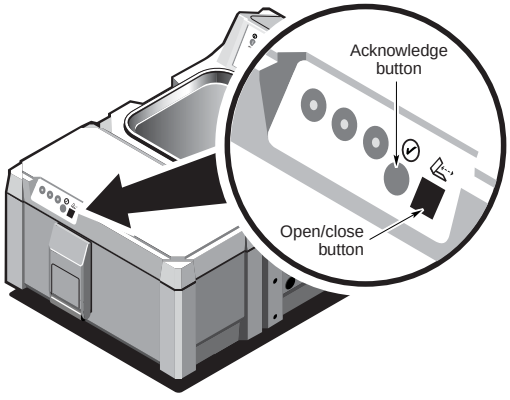
Module features

The Antaris II transmission sampling module is designed to work with the Thermo Scientific *RESULT™ software* to provide a powerful, fast, and easy-to-use system to analyze liquids, transparent solids, and thin films by transmission.



The features of the transmission module include:

- An extended range *InGaAs detector*.
- A *spectral range* of 12,000 – 3,800 cm^{-1} (2,631 - 833 nm).
- A sampling compartment that accommodates *three-position cuvette/culture tube holders* for liquids and *three-position sample card holders* for transparent solids and thin films.
- Compatibility with the heated version of the three-position cuvette/culture tube holder (the heating capacity ranges from 25 °C to 50 °C at ± 0.5 °C and from 50 °C to 100 °C at ± 1.0 °C).
- A square black button to the right of the Acknowledge button that allows an operator to open and close the transmission module door without using the software.



Testing the sampling module

RESULT Operation software contains an Instrument Check feature that runs an instrument performance test. Before running the performance test, power on the instrument and make sure the instrument has remained on for at least an hour to stabilize.

To run the instrument check:

1. **Log on to RESULT Operation software.**

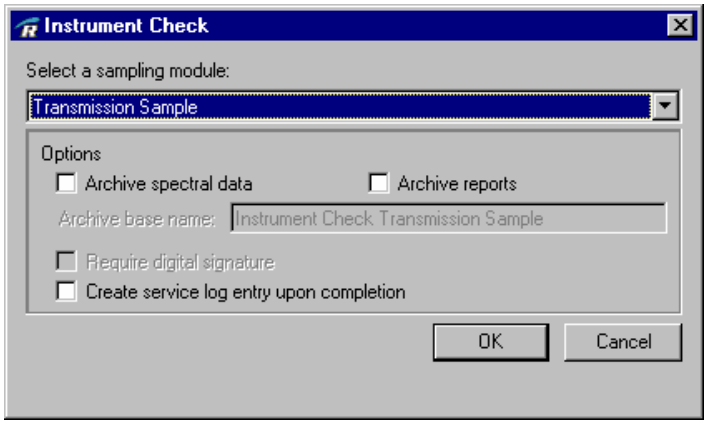
   See "Starting RESULT software" in the "Antaris sampling" chapter for instructions to log on to the software.

2. **Choose the Maintenance menu from the Result Operation main window.**

Note If the Maintenance menu does not appear in the RESULT main window, then you cannot access the Instrument Check feature. See your *RESULT software administrator*. ▲

3. **Choose the Instrument Check option from the Maintenance menu.**

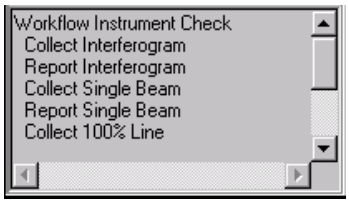
   The software will open the Instrument Check dialog box.



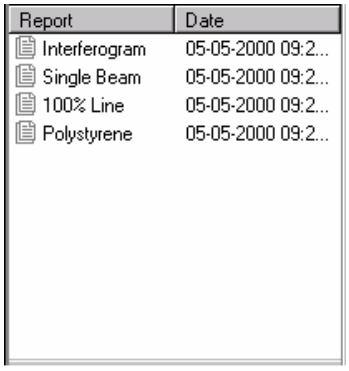
4. **If Transmission Sample is not already selected, select that option from the Select A Sampling Module drop-down list.**

5. **Choose OK to perform the check.**

   The software will start performing the instrument check. While the instrument check is running, the status indicator on the lower left side of the RESULT Operation main window will indicate the status of the instrument check.



   As each spectrum is collected, the software will create a report. The title of each report will appear in the report navigation frame.



   You can view a report by selecting the report name, and the selected report will open in the display area.

   See "Chapter 5 System Maintenance" of "Section 3 RESULT Operation Software" in your *RESULT User's Guide* for information about archiving the test data, requiring digital signatures for the data, and creating a service log entry of the test. The "System Maintenance" chapter also contains example spectra with a description of each.

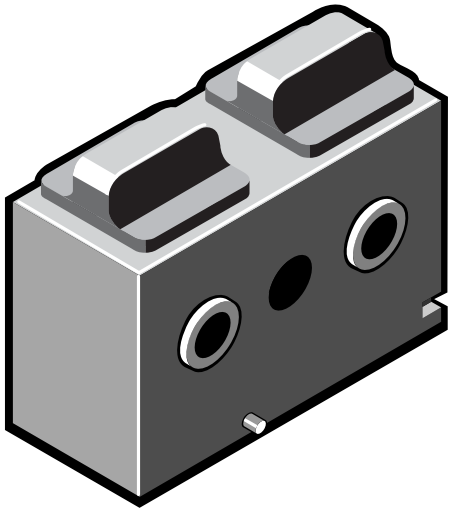
Transmission sampling techniques

Transmission sampling is fast and easy because little or no *sample* preparation is required. Transmission spectroscopy measures the percentage of light transmitted through a sample. When using the transmission module, the *infrared beam* is directed through an *interferometer* (or modulator), then through the sample and onto a dedicated *detector*.

Compatible sample types

The transmission module is designed for *samples* of liquids (heated or unheated), transparent solids, and thin films. The following is important information about analyzing these types of samples with the transmission module:

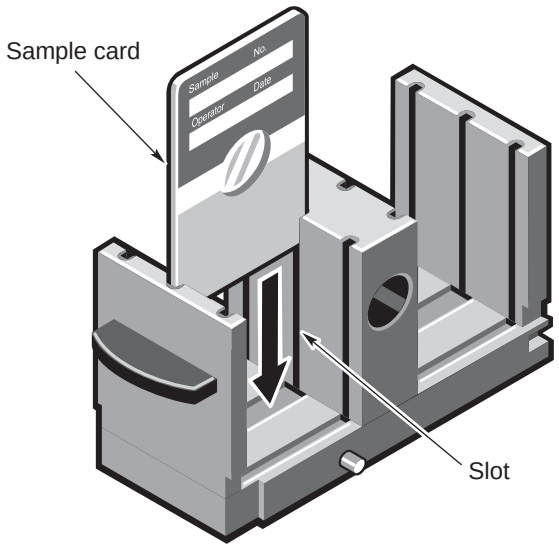
- Liquids are contained in clear glass *culture tubes* and *vials*, or *cuvettes* made of either glass or quartz. To sample a liquid you place the cuvette, culture tube, or vial in the *three-position cuvette/culture tube holder* (also called the sample tube holder).



Note You can use culture tubes and vials made of plastic, but this is not recommended. Plastic absorbs *near-infrared* radiation and will affect your data. If you choose to use plastic sample containers, be sure you know what the effects are so you can account for them in your results. ▲

Liquids that are heated for analysis can be held in the same containers as unheated liquid samples. To heat and maintain the elevated temperatures of liquids during sampling, you use the heated version of the three-position cuvette/culture tube holder (also called the heated sample tube holder).

- Transparent solids and films are held in sample cards. To sample a transparent solid or film mounted in a sample card, you slide the card into a slot in the three-position sample card holder (also called the sample card holder).



Note The sample holders are referred to as having three positions because they have both a front and a rear position where samples can be collected, and there is an opening in the center through which backgrounds can be collected. In addition, the sample card holder has three slots for *sample cards* in both the front and back positions. The middle slot brings the sample closest to the focal point of the *beam*, but the front and back slots allow a larger area to be sampled, which can reduce *channeling* and *fringing*. (For more information, see "Problems with bad sample spectra" later in this chapter.) ▲

Note Blank sample cards are available from Thermo Fisher Scientific. See your on-line parts list for more information. To open your on-line parts list, choose Servicing Antaris from the Maintenance menu in RESULT Operation software, and look for the topic on ordering parts. ▲

Your first experiment

This section goes through a simple experiment using the *transmission module* with the *Quick Collect* feature in *RESULT software* to produce a transmission *spectrum* of a liquid.

The Quick Collect feature in RESULT software allows you to collect the spectrum of a *sample* without creating a workflow. Using Quick Collect is good practice to help you "get the feel" of sampling with the transmission module before using the module in an actual production workflow.

This experiment involves configuring the RESULT Integration or RESULT Operation software, inserting a sample into the sample holder, installing

the sample holder in the transmission module, collecting a background, and collecting the *sample spectrum*.

Before you begin

The following details need to be taken care of before you start the experiment:

- Power on the Antaris II and allow it to stabilize for at least an hour.
- Select a sample that is liquid at the ambient temperature.
- Place your sample liquid in a cuvette, culture tube, or vial. (For more information about preparing samples, see the "Preparing samples" section of this chapter.)

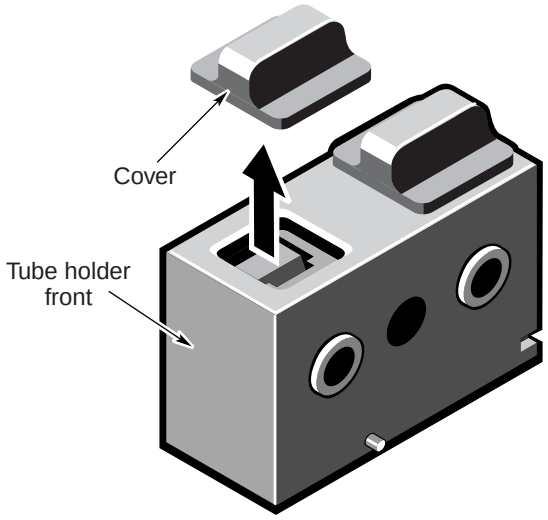
Inserting the sample into the sample holder

Once your sample is prepared, you must insert it into the sample tube holder.

To insert the sample:

1. **Remove the cover from the front position of the sample tube holder.**

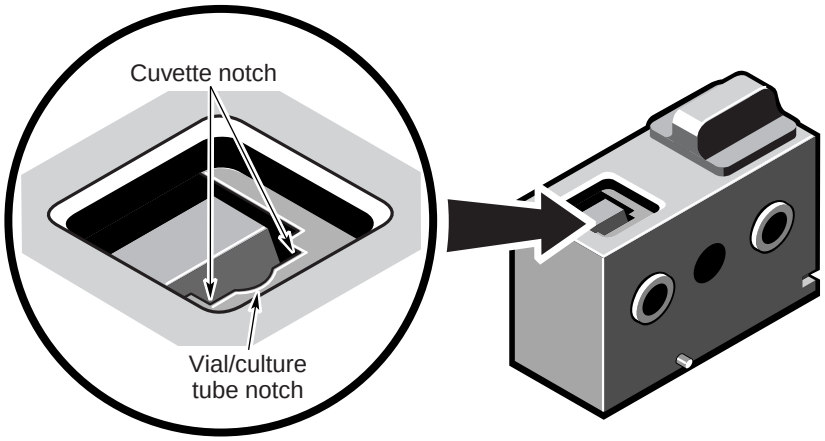
   When you are using the Quick Collect feature, you must put samples in the front sample position. Samples in the rear position cannot be analyzed when using Quick Collect.



⚠ Caution To avoid breaking your cuvettes, culture tubes, or vials, and possibly injuring yourself, be very gentle and use only a moderate amount of force when inserting or seating samples into the sample tube holder. ▲

2. **Slide the culture tube, vial, or cuvette into the notch in the opening at the top of the sample tube holder.**

   The notch for vials or culture tubes is triangular. The notch for cuvettes is wider and rectangular.

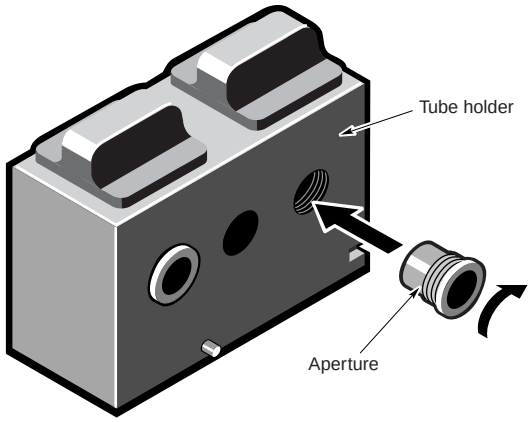


3. **Make sure the sample is firmly seated.**

   If a sample feels loose or free to move in the sample tube holder, move it carefully back and forth and apply gentle downward pressure. The sample will slip further into the sample tube holder until it stops and feels firmly held. (You will be able to move culture tubes and vials from side to side, but they will always snap back into position when properly seated.)

4. **If you are using a culture tube or vial, screw an aperture into the front position opening (if an aperture is not already in place).**

   The aperture should fit all the way into the opening where the beam passes through the sample holder and into the sample. For more information, see "Using apertures with liquid samples" later in this chapter.



Installing the sample holder

Once you have inserted a sample into the sample tube holder, you must install the sample holder in the transmission module.

To install the sample holder:

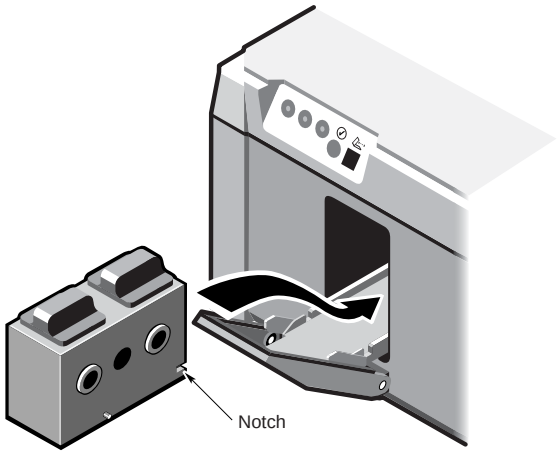
1. **Open the door of the transmission module.**

   Make sure the yellow indicator light on the instrument is not on, and then press the black button on the analyzer operation panel.

2. **Gently push down the transmission module door until it is level.**

3. **Place the sample tube holder on the sample track.**

   There are notches in the back of the sample tube holder. Always put the end with these notches into the transmission module first.



4. **Gently slide the sample tube holder forward until the pins on the side of the holder slide up and into the slots in the sample track.**

   You will hear the click and feel the sample tube holder stop when it is in place.

⚠ Caution Always verify that the area around the transmission module is clear before opening or closing the transmission module door. ▲

5. **Close the transmission module door.**

   Press the black button on the Antaris II operation panel to close the door.

Setting up the experiment

After you have installed the sample tube holder in the transmission module, you need to set up the RESULT Integration or RESULT Operation software.

To set up the software:

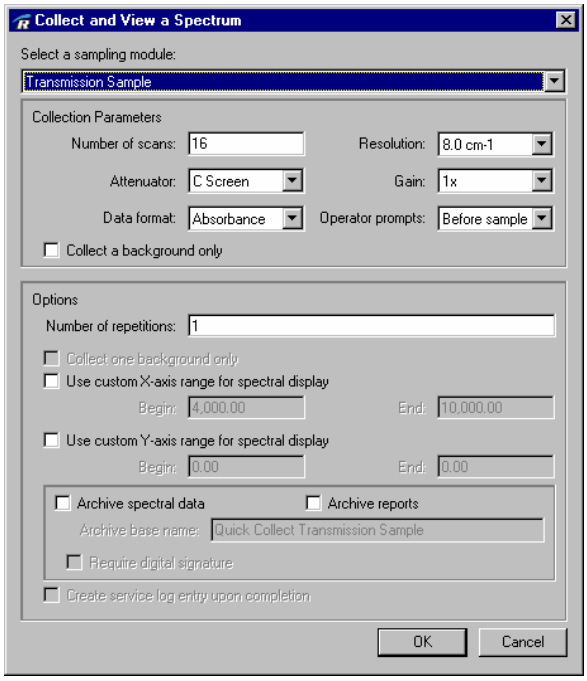
1. **Start the RESULT Integration or RESULT Operation software.**

   See "Starting RESULT software" in the "Antaris sampling" chapter for instructions to log on to the software.

2. **From the software's main window, choose the Quick Collect option from the Tools menu in Result Integration or from the Maintenance menu in Result Operation.**

Note If you are using RESULT Operation and the Maintenance menu does not appear in the *menu bar* of the main *window*, you cannot use the Quick Collect feature. See your *RESULT administrator*. ▲

   The Quick Collect dialog box should appear.



3. **Select the Transmission Sample option from the Choose A Sampling Module drop-down list.**

4. **For purposes of this experiment, enter the following Collection Parameters:**

Parameter	Setting
Number Of Scans	16
Resolution	8 cm^{-1}
Attenuator	C screen
Gain	1x
Data Format	Absorbance
Operator prompts	Before sample

5. **Do not change any other options for this example experiment.**

For information about the other options in the Quick Collect dialog box, see "Chapter 5 System Maintenance" of "Section 3 RESULT Operation Software" in your *RESULT User's Guide*.

6. **Choose OK, and respond to the prompt to begin the background and sample collections.**

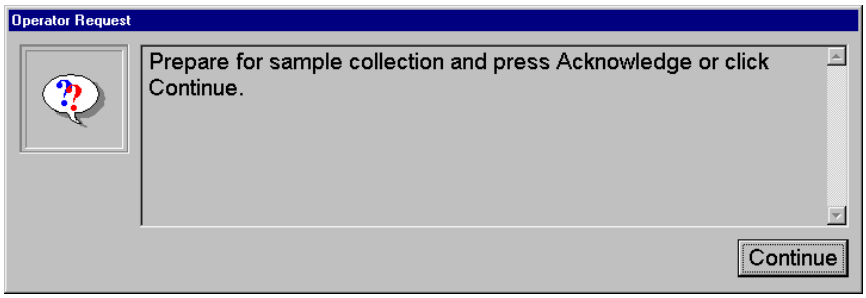
   See the following sections for more information about collecting the background and collecting the sample.

Collecting the background

In this experiment, you put the sample tube holder in the transmission module before setting up the software. In some experiments, this is not the case, and a *prompt* must be created to tell the operator when to insert the sample tube holder for the background collection. In this example, however, the background collection is automatic. Simply choose OK in the Collect And View A Spectrum dialog box. You can monitor the progress of the background collection in the status indicator box in the lower left corner. (For additional information about collecting backgrounds, see the "Collecting backgrounds" and "Tips for developing workflows" sections of this chapter.)

Collecting the sample

After the background has been collected the following prompt appears.



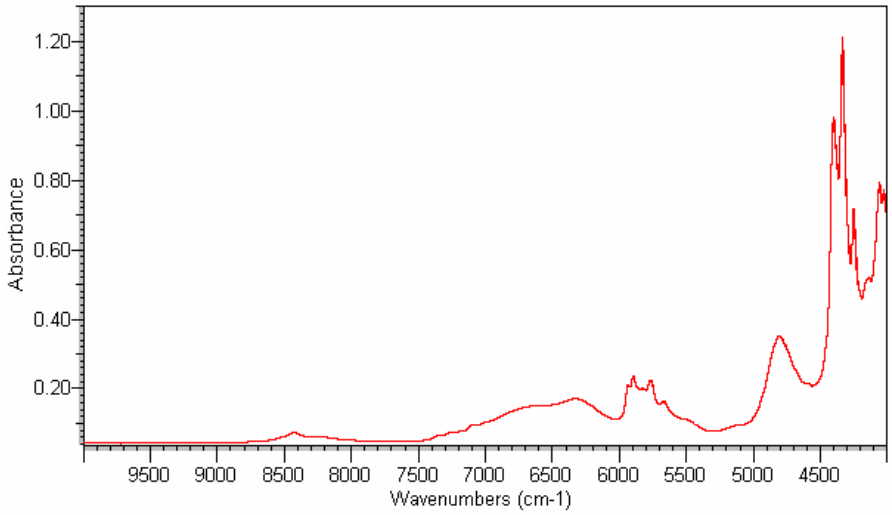
This prompt allows you to make sure you are ready to collect the *sample*. The sample tube holder is already in the transmission module, but in some experiments this is not the case, and a prompt is necessary to tell the operator when to insert the sample tube holder for the sample collection. For this experiment, however, you can press the green Acknowledge button or choose Continue when you are ready. You can monitor the progress of the sample collection in the status indicator box. When the collection is finished, the sample spectrum is shown in the *display area*.

Typical transmission spectra

FT-NIR spectra collected by *transmission* have unique characteristics. These characteristics were taken into consideration by Thermo Fisher Scientific when making recommendations for collection parameters using the transmission module. (Some problems associated with transmission spectra are discussed in "Common problems with spectral data" later in this chapter.)

A typical transmission spectrum for a liquid

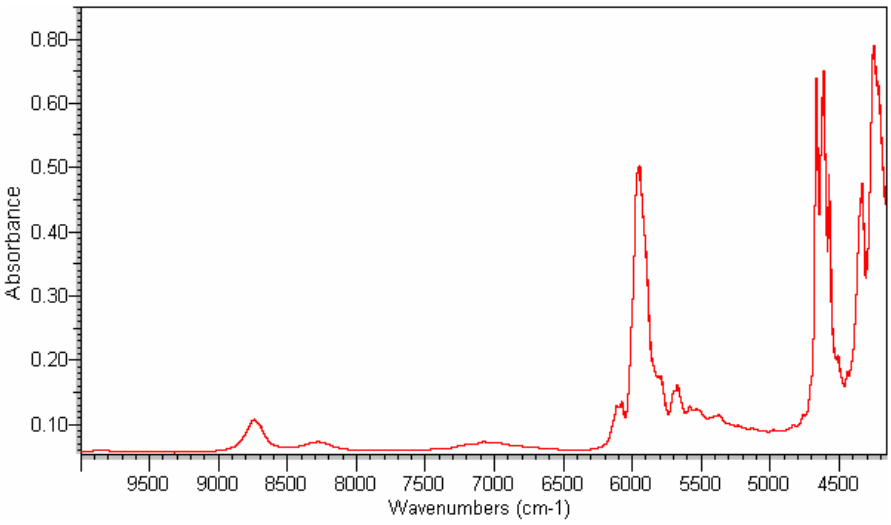
The following is an example of a liquid sample *spectrum* collected with the transmission module. The spectrum is of ethyl alcohol held in a 0.5 mm pathlength cuvette.



Transmission spectrum of ethyl alcohol

A typical transmission spectrum for a solid

The following is an example of a transparent solid sample spectrum collected with the transmission module. The material used to obtain the spectrum was a polystyrene sample (0.83 mm thick) held in a *sample card*.



Transmission spectrum of polystyrene

Note These spectra are only representative of the kinds of results you might obtain. The spectra you obtain will vary because you will be analyzing different samples, and your sample preparation and collection may not be the same as what was used for these examples. ▲

Taking backgrounds with Quick Collect

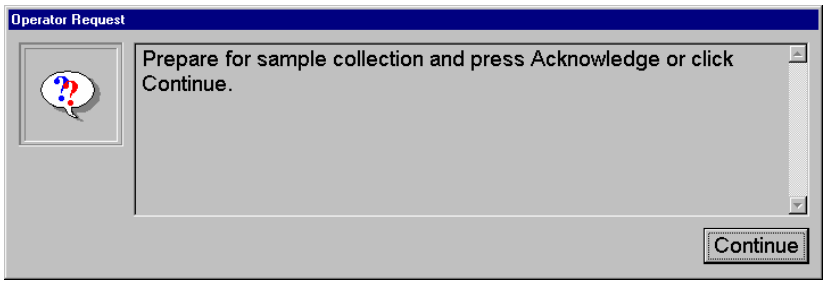
A *background spectrum* measures the response due to current environmental conditions and the instrument itself. Once the *sample spectrum* is collected, it is divided by the background, a process called *ratioing*, which removes the spectral effects recorded by the background. The result gives you a final *spectrum* where the *peaks* are due solely to the *sample*.

When using the *Quick Collect* feature with the *transmission module*, backgrounds are commonly taken by collecting through the open space in the center of the sample holder. A useful option, however, is to include a *reference* in a background spectrum. References are sample *components* that cause peaks you do not want in your final sample spectrum. For example, when you collect the spectrum of a sample that uses a solvent, the peaks caused by the solvent are part of the sample spectrum. A convenient way to eliminate those peaks, however, is to collect the background through the pure solvent held in the same kind of container your sample is held in. This makes the spectrum of the solvent part of the background, so when your sample spectrum is ratioed against the background, the peaks associated with the solvent are eliminated as part of the ratioing process.

Taking a background without a reference

If you are not including a reference, the Quick Collect feature automatically takes the background before collecting the sample. The following are collection parameters you can set to affect how a background without a reference is collected:

- **Operator prompts**. You can set the Operator Prompts list box to either None or Before Sample. (The Before Both option is used only when collecting a *reference background spectrum*.) When you choose None or Before Sample, no prompt is given before the background is taken, and the collection is made through the center opening. If you choose the Before Sample option, however, the following prompt will appear after the background has been collected.



  This allows you to make sure you are ready before collecting the sample spectrum. When you are ready, choose Continue or press the green Acknowledge button to start the sample collection.

- **Collect a background only**. To collect a background spectrum, select this checkbox. The background collection is made through the opening in the center of the sample holder, the resulting spectrum is displayed, and no sample spectrum is collected.

Taking a background with a reference

When using the Quick Collect feature, no collection is made through the rear sample position, so you must use the front sample position to collect both reference backgrounds and sample spectra.

To collect a reference background with Quick Collect and transmission module sampling:

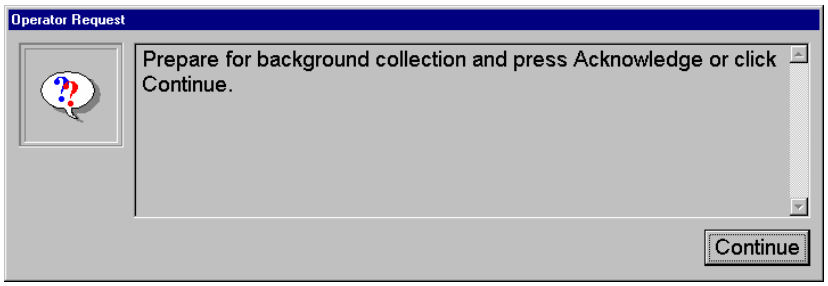
1. **Insert your reference sample into the front position of the sample tube holder, and install the sample holder in the transmission module.**

For more information, see "Inserting the sample into the sample holder" and "Installing the sample holder" in "Your first experiment" earlier in this chapter.

2. **In the Collection Parameters field, set the Operator Prompts list box to Before Both.**

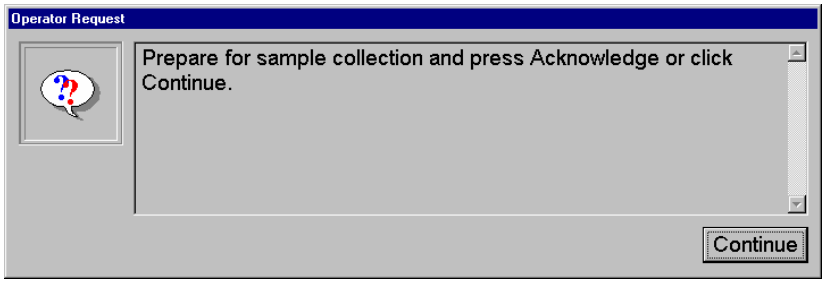
   This causes the background to be collected through the front sample position, and it also causes prompts to be issued before the background is taken and before the sample is collected. These prompts are important because after the background has been collected, you must remove the reference from the front sample position and replace it with your sample.

3. **Choose OK, and the following prompt appears.**



4. **Place your reference material in the front sample position, if you have not placed it there already, and you are ready to collect the background. Choose Continue or press the green Acknowledge button.**

   After the reference background is collected, the following prompt appears.



5. **Remove the reference from the front sample position, and replace it with your sample.**

   You do not have to remove the sample holder from the transmission module to move samples into and out of the front position. (For more information, see "Inserting the sample into the sample holder" in the "Your first experiment" earlier in this chapter.)

6. **Choose Continue or press the green Acknowledge button.**

   When the sample spectrum has finished collecting, it is shown in the display area.

Collecting backgrounds with an aperture

If you use an *aperture* to collect a sample spectrum, the background must also be taken through an aperture. To do so, you can install an aperture in either the front or rear sample position and collect both the background and the sample from that position. You can also install apertures in both the front and rear sample positions, and then collect the sample from one position and the background from the other position. You cannot, however, install an aperture in the opening in the center of the sample holder. Even if you are not including a *reference*, when you use an aperture you must collect the background from either the front or rear sample position.

When collecting backgrounds with an aperture, *prompts* are needed for both the background and sample collection and should include instructions to make sure the apertures are in place. (For more information about using apertures, see "Using apertures with liquid samples" in the "Preparing samples" section of this chapter.)

Preparing samples

The *transmission module* is designed to *sample* liquids (unheated or heated), transparent solids, and thin films in the industrial environments of the pharmaceutical, chemical and polymer industries.

Preparing liquid samples

The following are examples of containers you can use to hold liquid samples:

⚠ Caution To avoid injuring yourself or damaging your samples or the transmission module, make sure your *cuvettes*, *culture tubes*, and *vials* do not exceed the heights specified below. If a sample is broken off in the sample holder, use caution when removing it. If you cannot remove it safely, call Thermo Fisher Scientific for assistance. ▲

- Liquid samples can be contained in glass vials and culture tubes that are 4 to 12 mm in diameter and no more than 76 mm (3 inches) in height.
- Liquid samples can also be contained in cuvettes made of quartz or glass that are 10 mm in width, no more than 50 mm in height, and have a pathlength of 0.5 to 10 mm.

⚠ Warning To avoid personal injury or damage to the transmission module, always follow standard laboratory safety practices when preparing liquid samples. Do not heat any volatile liquid to its flash point, make sure the sample containers are capped, and always wear protective goggles and clothing. ▲

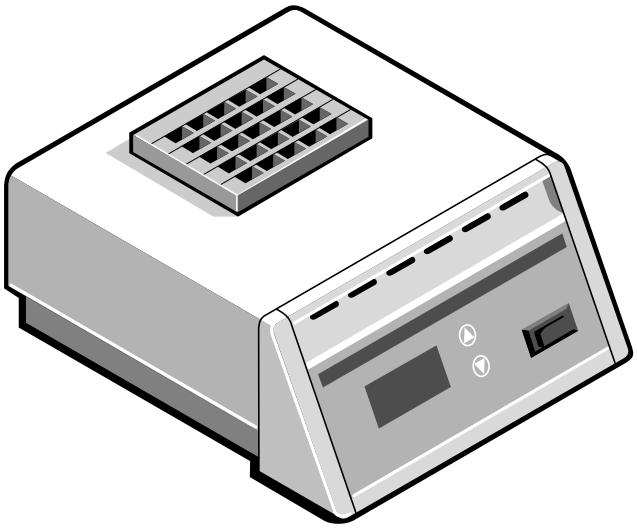
To prepare a liquid for sampling, simply place it in the appropriate container: a cuvette, a culture tube, or a vial. Follow standard laboratory safety practices, and be sure to place a cap on the container if your sample is a volatile liquid.

Once your sample is prepared, you can insert it into the sample tube holder. For more information, please see "Inserting the sample into the sample holder" in "Your first experiment" earlier in this chapter.

Preparing heated liquid samples

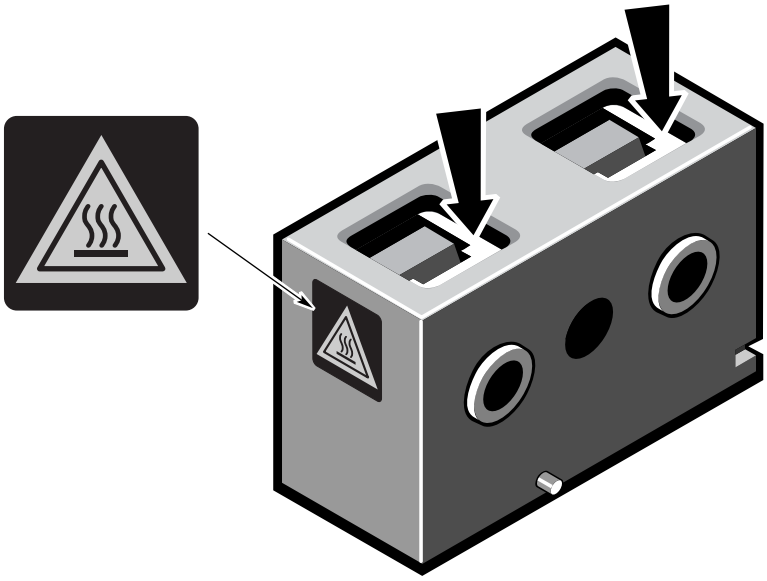
Heated liquid samples are analyzed using the heated version of the sample tube holder and can be pre-heated before inserting them into the heated sample tube holder. (Pre-heating is not necessary, but it is recommended because it eliminates having to wait for the sample holder to heat your sample.)

To pre-heat samples, you should use a *block heater*. A block heater heats a removable sample block that has spaces for cuvettes, culture tubes, or vials of varying sizes. (The example shown below is a standard block heater offered by Thermo Fisher Scientific. Your model may be different.)



Block heater from Thermo Fisher Scientific

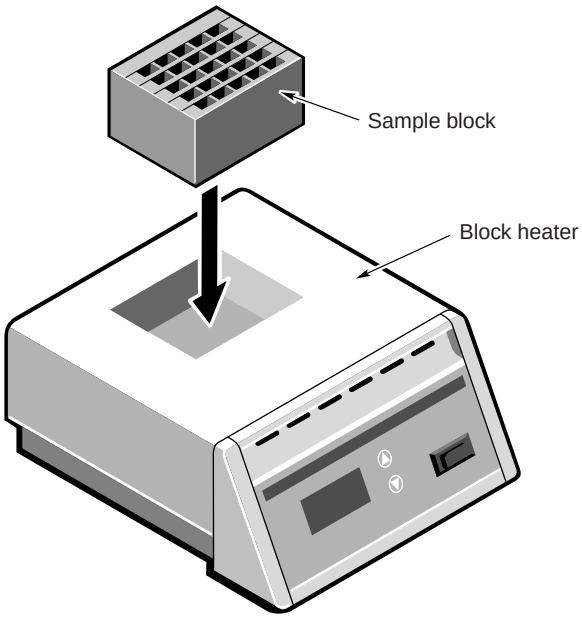
⚠ Warning To avoid burning your fingers or hands, always wear protective gloves when handling any object (such as a block heater, sample block, or sample) that is heated above 85 °C. If gloves or other protection is not available, allow at least 15 minutes for heated objects to cool down before handling them. ▲



The following instructions explain how to use a block heater to pre-heat liquid samples.

1. **Place your cuvettes, culture tubes, or vials in a sample block.**

2. **Place the sample block in the block heater.**



3. **Turn on the block heater and set the desired temperature.**

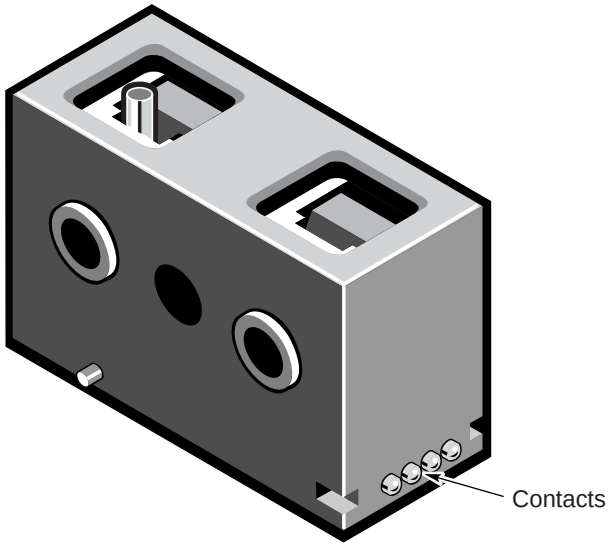
   See the manufacturer's instructions for your block heater for details on how to do this.

4. **Allow your sample(s) to reach the desired temperature.**

   Once your sample is at the desired temperature, place the sample in the heated sample tube holder. (For an estimate of the time it takes to heat the heated sample tube holder, see "Setting the heated sample tube holder temperature" below.)

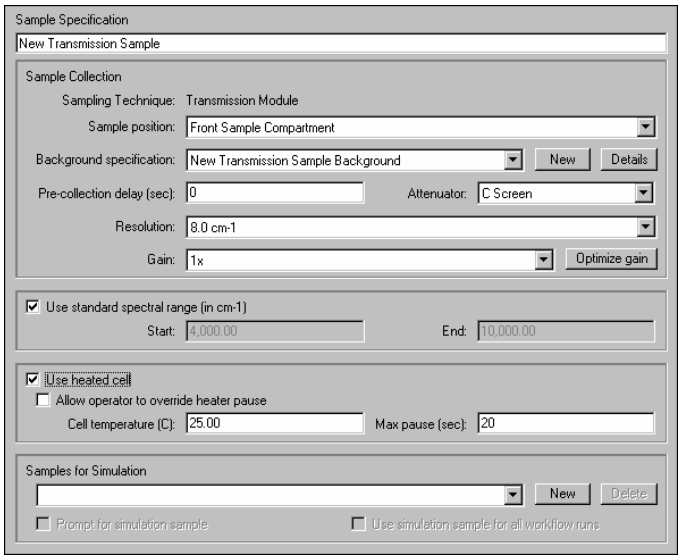
Setting the heated sample tube holder temperature

To analyze heated liquid samples, you use the heated sample tube holder, which contains heating elements and controls that allow you to maintain a sample at a specific temperature.



To set the temperature of the heated sample tube holder:

1. **Go to the Sample Specification screen in RESULT Integration software.**



2. **Select the Use Heated Cell checkbox.**

3. **Enter the temperature you wish to maintain in the Cell Temperature field.**

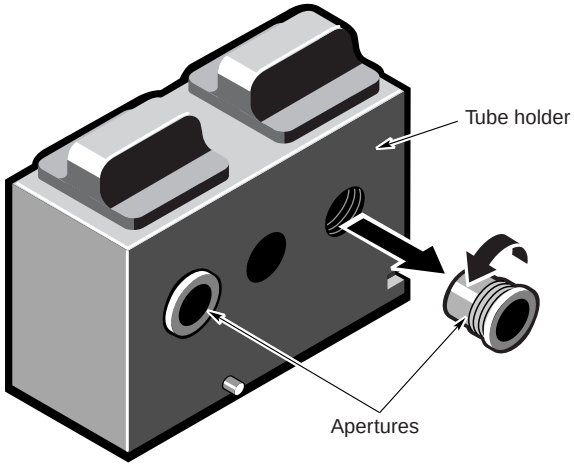
When you place a heated sample tube holder in the transmission module, the heating process occurs in two stages. The sample tube holder heats first, and then it heats the sample to the temperature you set. For more information about this process, see "Specifications for heated samples" in the "Tips for developing workflows" section of this chapter.

The following table gives the time it takes to heat the heated sample tube holder to the given temperatures:

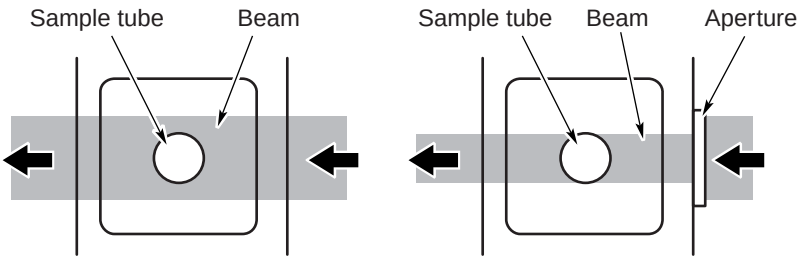
Temperature	Time to Heat
30°C	1-5 minutes
60°C	5-10 minutes
90°C	15-20 minutes
100°C	20-25 minutes

Using apertures with liquid samples

The front and rear positions in the sample tube holder (either heated or unheated) have removable *apertures* that restrict the *beam* that passes through the sample.



Although they can be removed, you should leave the apertures in your sample tube holder except when you are using *cuvettes* or when your experiment requires the apertures to be taken out. This is particularly important when you use *culture tubes* and *vials*. An aperture cuts down the size of the beam from 7mm to 4mm, which ensures that all of the beam passes through the sample. Without an aperture the beam size is larger than the diameter of the tube or vial, which can affect baselines and give false readings due to *lensing* problems. (For additional information, see "Collecting backgrounds with an aperture" in the "Tips for developing workflows" section of this chapter.)



Note One situation where you might want to remove the apertures is when you are performing *quantitative analysis*. Quantitative measurements generally work better when the sample is exposed to the entire beam, but this is largely dependent on your sample. (You should design an experiment to test whether you get the best results with or without an aperture.) If you remove the apertures for sampling, you must remember to remove them for both the sample and the background collection. If you remove the apertures for one and not the other, you will see inconsistencies in the baselines.

In addition, when doing quantitative work, you can place your sample in a cuvette. Cuvettes often provide better quantitative accuracy because they are less susceptible to positioning errors (which you can estimate by making repeated collections of the same sample). Cuvettes also allow the beam to pass through a larger amount of sample and do not suffer from the effects of the curvature of vials and culture tubes. (For more information, see "Problems with bad sample spectra" later in this chapter.) ▲

Preparing transparent solids and thin films

To analyze a transparent solid or thin film in the *transmission module*, samples are usually mounted in *sample cards* that are 2 inches (5.1 cm) wide by 3 inches (7.6 cm) tall. The center of the opening where the sample is held must be 1.5 inches (3.8 cm) from the bottom of the sample card.

You can purchase self-adhesive cards that meet the required dimensions from Thermo Fisher Scientific. For ordering information, please refer to the parts list in the on-line help for Antaris II.

Mounting a sample in a sample card

Mounting a sample of a transparent solid or a thin film is a simple process that involves cutting a piece of the sample and securing it in a sample card.

To mount a transparent solid or film sample:

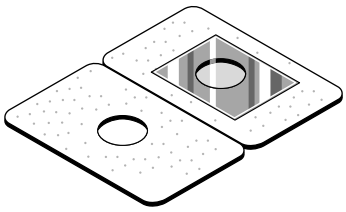
1. **Cut a representative sample of the film you want to analyze.**

   The sample should not extend beyond the edges of the card, but it must be larger than the hole in the card.

2. **Place a new, unfolded sample card on a flat surface, and remove the backing from the adhesive.**

3. **Place your sample on the opposite side of the card so that the film covers the hole completely.**

   To help prevent errors in data collection, make sure there are no wrinkles in the area of the film visible through the hole.

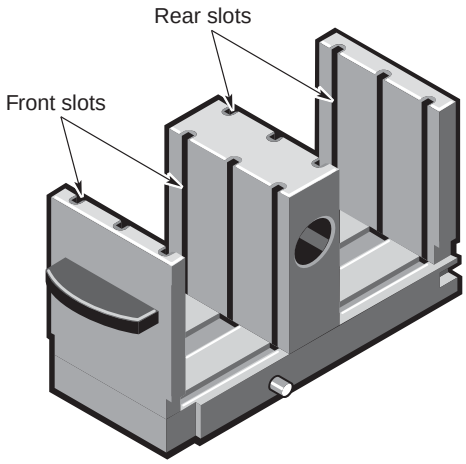


4. **Gently fold the card to secure the film.**

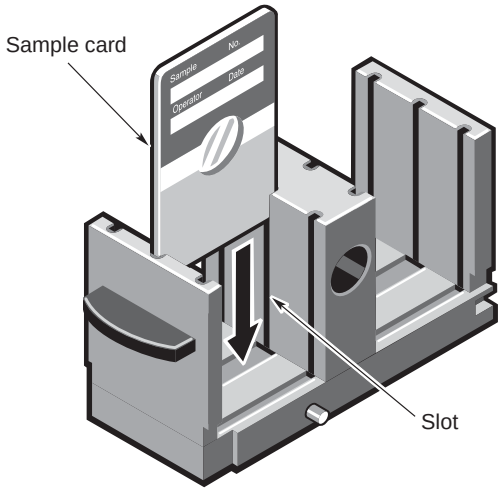
   You can trim the film if it extends beyond the edge of the card.

Inserting a sample card into the sample card holder

Transparent solids and thin films are placed in the *three-position sample card holder* for sampling.



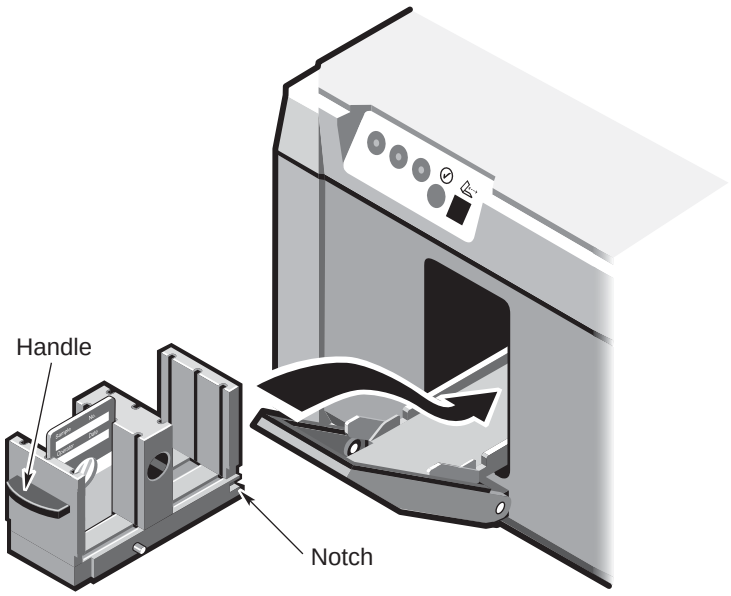
There are three slots in the front and rear positions in the sample card holder. To insert a sample card, simply slide it into a slot.



At the middle slot, the diameter of the *beam* is 7 mm, and at both the front and back slots, the beam diameter is 10.35 mm. Normally, you should use the middle slot because it brings the sample closest to the focal point of the beam. (Sample shapes can vary widely, however, so you may need to experiment with the other slots to see which one brings your sample nearest to the beam's focal point.)

Installing the sample card holder

Installing the sample card holder in the transmission module is basically the same as installing the sample tube holder. The main difference is that the sample card holder has a handle you can use to place the unit on the *sample track*.



For more information, see "Installing the sample holder" in "Your first experiment" earlier in this chapter. Be sure to follow all cautions and warnings presented there.

Tips for developing workflows for the transmission module

When developing *workflows* using *RESULT Integration software*, there are some factors you want to take into consideration to make sampling with the *transmission module* as efficient as possible. Sample parameters and specifications are highly dependent on the sample type, the amount of time available to collect data, and the level of interest in different spectral characteristics. This section contains recommendations for starting points when specifying collect event parameters, sample specifications, and background specifications.

See "section 5 Workflow Events and Specifications" of your *RESULT User's Guide* for more information about the items mentioned in this section.

Collect event parameters

A collect event in RESULT Integration software instructs the instrument to collect a spectrum of a sample. The following table contains the recommended starting points for sample collection parameters for the transmission module:

Parameter	Setting
Number Of Sample Scans	30
Data Format	Absorbance
Background Frequency	Every hour

- **Number Of Sample Scans**. To start, try using 30 scans. You can then decrease the number of scans to the smallest number that can still produce a tolerable signal-to-noise ratio (determined by error of prediction or pre-defined limit) if sampling time is at a premium. When using a higher resolution, the spectra will contain more spectral *noise*, so you may need to increase the number of scans.

- **Background Frequency**. If collecting samples only periodically, then collecting a background before every sample is recommended. If collecting many samples at a time, then collecting a background every hour should be sufficient.

Operator prompts

When adding a Collect *event* to a workflow, you may want to consider including *operator prompts* to assist the operator in properly collecting the data. This is particularly important when collecting both a *reference background spectrum* and a sample spectrum from the same position in the sample holder (for more information, see *Background Specifications* in this chapter). Some example prompts include:

- Place the reference in the front sample position, and press the black button to close the transmission module door. When the door is closed, press the green Acknowledge button to collect the background spectrum.

- Remove the reference and place the sample in the front sample position. Press the black button to close the transmission module door, and then press the green Acknowledge button to collect the sample spectrum.

Sample specifications

When specifying collection details in a workflow, the *sample specifications* are highly dependent on sample types, the amount of time available to run collections, and the level of interest in different spectral characteristics. However, the recommendations in this section can give you a starting point when deciding the collection parameters to use in workflows:

Parameter	Setting
Attenuator	C screen
Resolution	8 cm^{-1}
Gain	1x
Spectral Range	10,000-4,000

- **Gain and Attenuator**. You may want to use RESULT Integration's Optimize Gain feature to determine the appropriate gain and attenuator settings for your sample. If you use the Optimize Gain feature, the software will collect the sample material using each possible combination of gain and attenuator specifications to find the *specifications* that produce the best results. If you choose not to use this feature, you may want to begin with the default Gain setting of 1x and an Attenuator setting of "C Screen." (For more information about using the Optimize Gain feature, see the Sample Specification information in "Section 5 Workflow Events and Specifications" of your *RESULT User's Guide*.)

Note Always use the Optimize Gain with the most transmissive samples to avoid saturating the detector. ▲

- **Resolution**. Try 8 cm^{-1} as a starting point, You can increase the resolution (e.g., from 8 cm^{-1} to 4 cm^{-1} or 2 cm^{-1}) if required by your sample and then increase the number of collections to provide a larger signal-to-noise ratio. You can try 16 cm^{-1} or 32 cm^{-1} to trade off resolution for an improved signal-to-noise ratio.

If you are using heated samples, you will also need to specify the following parameters in the sample specification for the transmission module:

- **Use Heated Cell**. Select this box to use the heated sample tube holder.

- **Cell Temperature**. Use this box to set the temperature of the heated sample tube holder. You can set the heated sample holder to maintain your sample at any temperature between 25 °C and 100 °C.

- Do not heat the sample tube holder higher than 100° C, and you cannot set the temperature below the internal temperature of the instrument. The heated sample tube holder cannot maintain a temperature lower than that of the surroundings.

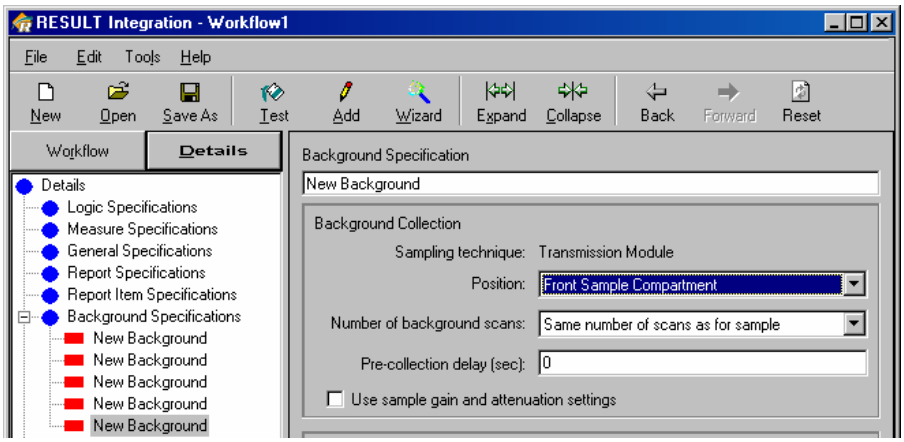
- **Heater settle time**. The transmission module can be set to allow a specified amount of time for the temperature of the heated sample tube holder to stabilize once the target temperature has been achieved. The amount of time that is appropriate is dependent on the nature of your sample and the temperature you want to maintain. You can set this parameter by entering a time in the Max Pause (Sec) text box in the Sample Specification.

- **Allow operator to override heater pause**. This option allows an operator to take a collection without waiting for a sample tube holder to reach the specified temperature. If temperature is critical to the analysis, the quality of your data may be affected by using this option.

Background specifications

When collecting a background through a workflow, it is common to collect through the open space in the center of the sample holder. A useful option, however, is to collect a *background* using a *reference*. References are sample *components* that you do not want to analyze but are mixed with the sample. For example, when you collect the spectrum of a sample that uses a solvent, the peaks caused by the solvent are part of the sample spectrum. A convenient way to eliminate those peaks, however, is to collect the background through a portion of the solvent held in the same kind of container your sample is held in. This makes the spectrum of the solvent part of the background, so when your sample spectrum is ratioed against the background, the peaks associated with the solvent are eliminated as part of the ratioing process.

For background collections, a good starting point for the Number of Background Scans parameter is Same Number Of Scans As For Sample. The following sections contain information about other aspects of background specifications based on whether or not you are using a reference and an aperture.



Backgrounds without a reference

The following are considerations for setting the background specifications when you are not using a reference:

- In the Background Specification, set the Position list box to Background Position. This causes the background collection to be made through the opening in the center of the sample holder.
- In the Operator Prompts field in the collection event, there is no need to create an operator prompt to be issued before the background collection, but you should create a prompt to be issued before the sample collection. If the experiment uses the sample card holder, the prompt should indicate which slot the sample card should be placed in.
- Backgrounds can be collected with the same Attenuator setting that is used for the samples or with the software default setting. The Use Sample Position, Gain, And Attenuation Settings check box on the background specification defines the Attenuator setting used for background collection. When the check box is selected, the software uses the Attenuator setting that is shown on the sample specification. When the check box is cleared, the software uses the default Attenuator setting. The default setting depends on the sampling module used for background collection and, in some cases, the type of background specification. If the Use Sample Gain And Attenuation Settings check box is not selected, the default gain setting will be 1x , and the default attenuator setting will be C screen for transmission.

Backgrounds using a reference

The following are considerations for setting the background collection events when you are including a reference:

- In the Background Specification field, set the Position list box to either Front Sample Position or Rear Sample Position. This specifies the location where the background collection will be made. It doesn't matter which option you select, but if you choose the same position for both the background and the sample collection, you must remember to remove the reference and insert your sample after the background collection is finished. It is often easiest to place your reference in the rear position and your sample in the front position. This keeps you from having to remove your reference before collecting the sample, and you can move samples in and out of the front position without taking the sample holder out of the transmission module.

- Backgrounds can be collected with the same Attenuator setting that is used for the samples or with the software default setting. The Use Sample Position, Gain, And Attenuation Settings check box on the background specification defines the Attenuator setting used for background collection. When the check box is selected, the software uses the Attenuator setting that is shown on the sample specification. When the check box is cleared, the software uses the default Attenuator setting. The default setting depends on the sampling module used for background collection and, in some cases, the type of background specification. If the Use Sample Gain And Attenuation Settings check box is not selected, the default gain setting will be 1x , and the default attenuator setting will be C screen.

In the collect event, go to Operator Prompts and create prompts to be issued before the background collection and before the sample collection. This is particularly important when the workflow requires a reference background and the sample to be collected from the same position—the operator must be informed when the reference should be removed and the sample should be inserted. (If the experiment uses the sample card holder, the prompts should also indicate which slot the sample cards should be placed in.).

Backgrounds using an aperture

If you use an aperture to collect a sample spectrum, the background should also be taken through an aperture. When using apertures, you can take the background from the same position as the sample (the location where the aperture is installed) or you can insert the same type of aperture in the

position where the background collection will be made. You cannot, however, install an aperture in the center opening, so when using apertures, you must collect the background from either the front or the rear sample position.

For additional information about using apertures, see "Using apertures with liquid samples" in the "Preparing samples" section of this chapter.

Additional workflow considerations

An additional factor you may want to take into consideration when specifying collection details in a *workflow* is adding repeat trees to your workflow. When collecting a sample, one source of error can be the way the sample is positioned. To help ensure that sample positioning does not affect the repeatability of sample results, you may want to add repeat events to your workflow. This allows an operator to take multiple readings of a sample in order to check the consistency of results.

Common problems with spectral data

Before using the *analyzer* for precise *quantitative analysis*, evaluate the effects of temperature on spectral features. Other factors that may influence spectra are bad backgrounds, natural variations in *sample* position, inconsistent use of *references* in the background, and inconsistent use of *apertures*.

If you encounter a problem, before running any other diagnostics or deciding that backgrounds or samples are "bad" you may first want to check the following items:

- Make sure your sample is firmly seated in the sample holder.
- Make sure the sample holder is properly installed in the transmission module.

For more information, see "Inserting the sample into the sample holder" and "Installing the sample holder" in "Your first experiment" earlier in this chapter.

Problems with background spectra

If a *background spectrum* you collected is atypical from previously-collected backgrounds, the reason may be related to one or more of the following:

- If you use apertures, you should use them consistently. You have to use an aperture to take all of the backgrounds in an experiment or you

- You must also use references consistently. You cannot include a reference in some backgrounds in an experiment and leave it out of others. If you do, you will see discrepancies in your background spectra and results.

- If a reference material becomes contaminated or damaged, the backgrounds that use that reference may change. When this happens, you must replace the reference, but you have to test the replacement to make sure it is the same as the original.

- Do not change the attenuator position unless it is necessary for your sample. Using different attenuator positions for background collections may cause variations in your results.

Problems with sample spectra

Several factors may affect a *sample spectrum*. Before deeming the *sample* as "bad," collect the sample again in a diagnostic mode, either by running the *workflow* off-line, using the Test Sample feature, or by using the *Quick Collect* feature in *RESULT Operation software*.

The following are factors that may affect the quality of your spectral data:

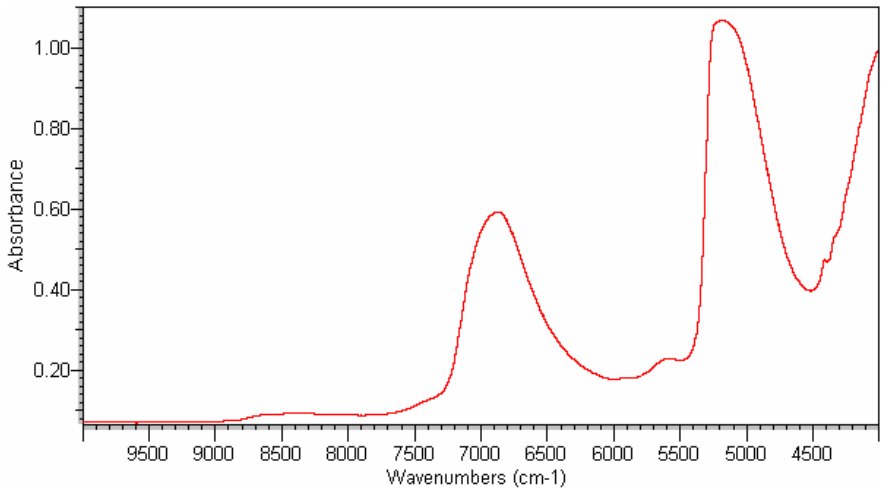
- If you are using the *three-position sample card holder*, always place your samples in the same position to help ensure repeatability. The sample card holder has three slots for *sample cards* in both the front and back positions. The middle slot brings the sample closest to the focal point of the beam, but it also allows the smallest area of the sample to be collected. This can cause a greater degree of *fringing* (the effect caused by constructive and destructive interference of internally reflected waves from parallel surfaces), which occurs when the surface of your sample is extremely flat. By using one of the slots in front of, or behind, the middle slot you can sample a larger area, which may help reduce fringing.

- Variations in positioning can affect the quality of your spectra, so try to be consistent in the way you position your samples. If positioning variations affect your results, perform repeat collections to determine the magnitude of the changes.

- If you use different attenuator positions for the background collection and the sample collection, you may see slight shifts in the baselines of your sample spectra.
- Variations in cuvettes, culture tubes and vials can affect your spectra. To quantify the magnitude of these effects, perform repeat collections using different cuvettes, culture tubes, or vials.
- The curvature of culture tubes and vials can cause a *lensing* effect that interferes with high accuracy measurements. Cuvettes are flat and do not suffer from this effect, so when taking measurements that require high accuracy, cuvettes are recommended over vials or culture tubes.
- Using an aperture for the background collection and not for the sample collection (or vice versa) will cause variations in your results. Always use apertures consistently.
- If you are analyzing a heated sample, make sure all collections are done at the same temperature. Inconsistencies in temperature can cause significant variations in *peak* intensities and shifts in the X-axis.

Broad/rounded spectral bands

A spectrum that has spectral *bands* that are broad and rounded may resemble the following:



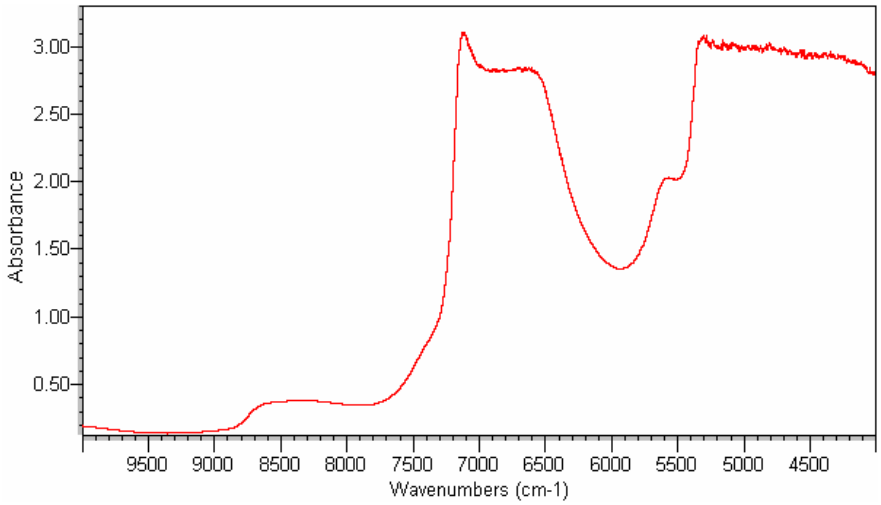
Water spectrum with broad, rounded bands using the transmission module

If you experience a problem with broad and rounded peaks, you may want to try increasing the resolution or using a sample container with a shorter pathlength.

Note Spectra of water in NIR tend to have broad, rounded bands even if you increase resolution or use a shorter pathlength when sampling. ▲

Spectral bands are too big

A spectrum that has spectral bands that are too big may resemble the following:

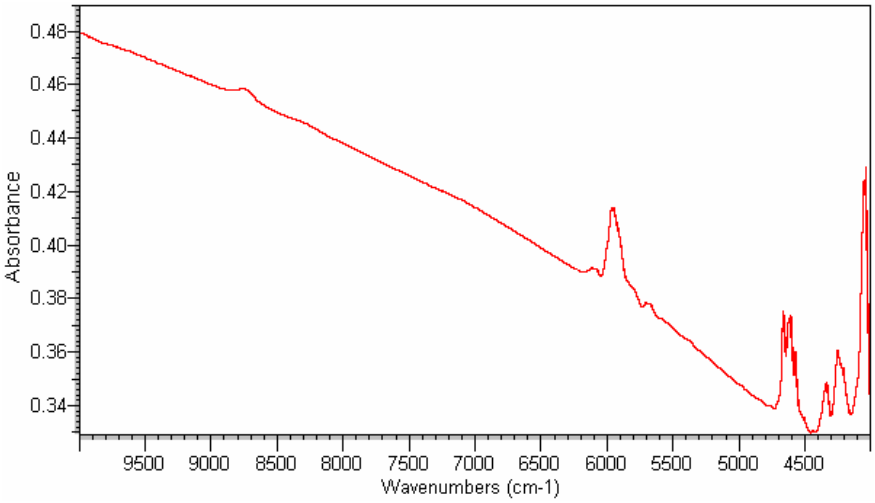


Water spectrum with totally absorbing bands using the transmission module

If you experience a problem with sample bands being too big, you may want to try decreasing the pathlength of the sample.

Spectral bands are too small

A spectrum that has spectral bands that are too small may resemble the following:

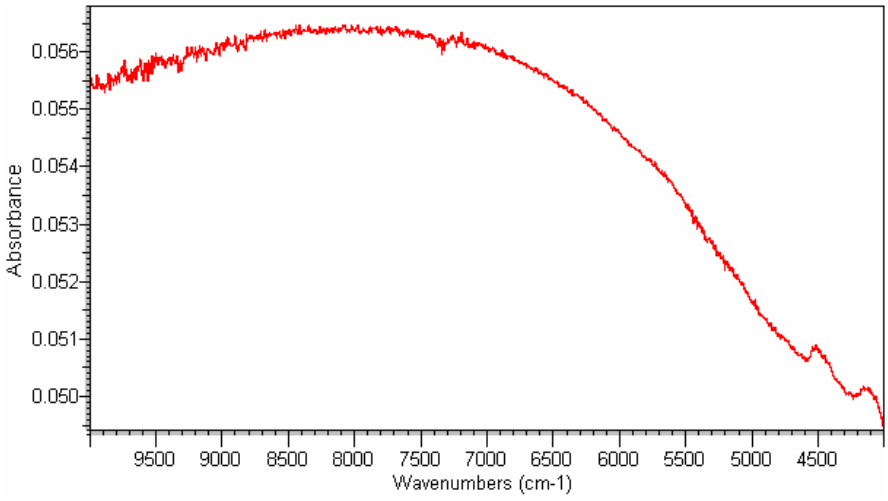


Thin polystyrene spectrum with bands that are too small using the transmission module

If you experience a problem with sample bands being to small, you may want to try using a thicker sample.

Severely curved baseline

A spectrum that has a severely curved baseline may resemble the following:



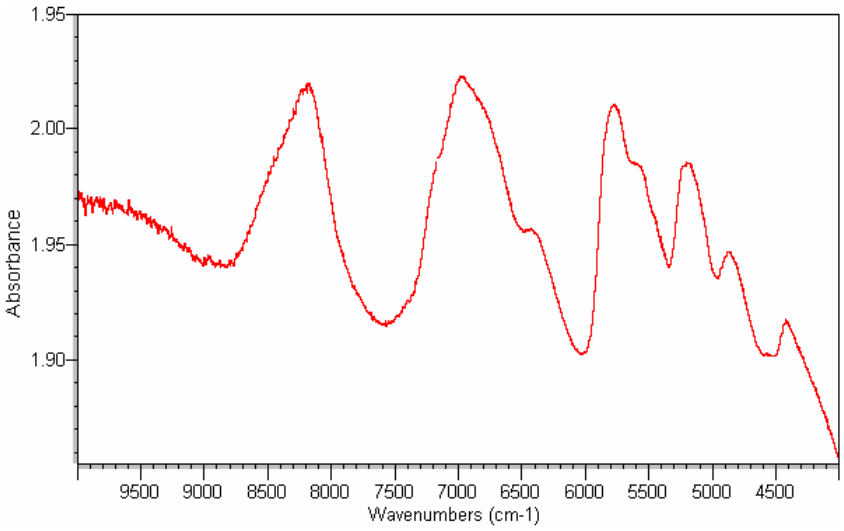
Spectrum with curved baseline using the transmission module

A severely curved baseline is often caused by the scattering of particles. If you experience this problem, check your sample for transparency. You also may want to try one of the following:

- Using a sample container with a different pathlength.
- Using reflection to collect your sample.
- Using spectral processing to reduce the effect of scattering on your results. (For more information, see the *TQ Analyst User's Guide*.)

Tilted and offset baseline

A spectrum that has a tilted and offset baseline may resemble the following:



Wax spectrum with tilted, offset baseline using the transmission module

A tilted and offset baseline is often caused by particles scattering and absorbing the transmitted light. Possible solutions include:

- Using a sample container with a shorter pathlength. (If you are using a vial or culture tube, you could try using a cuvette instead.)
- Using reflection to collect your sample.
- Using spectral processing to reduce the effect of scattering on your results. (For more information, see the *TQ Analyst User's Guide*.)

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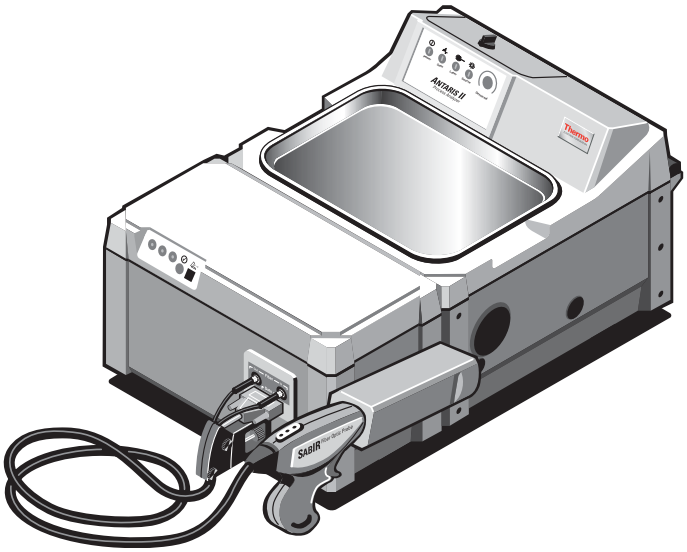
Chapter 5 Fiber Optic Module

The Antaris II fiber optic sampling module provides remote sampling for raw material identification, quality measurements, and sample component analysis in the chemical, pharmaceutical, polymer, and food and beverage industries. The fiber optic module contains standard SMA connectors and is compatible with many fiber optic probes in the industry, such as the Thermo Scientific SabIR™ probe.

This chapter discusses the important features of the fiber optic module, and includes information about testing the module and setting up and conducting experiments. The final section in this chapter discusses using the fiber optic module with the SabIR probe.

Introduction

The Antaris II fiber optic sampling module is designed to work with Thermo Scientific RESULT Integration and RESULT Operation software to provide easy, remote sampling of solids, powders, and liquids used in the pharmaceutical, chemical, and polymer industries.



Antaris II system with fiber optic sampling module and SabIR probe

The module's *multi-lens optics* send a near-infrared *beam* into the optical fiber and efficiently focus the returned light onto the dedicated InGaAs (Indium Gallium Arsenide) *detector*. The module has standard SMA connectors and is compatible with fiber optic probes that use various sampling techniques.

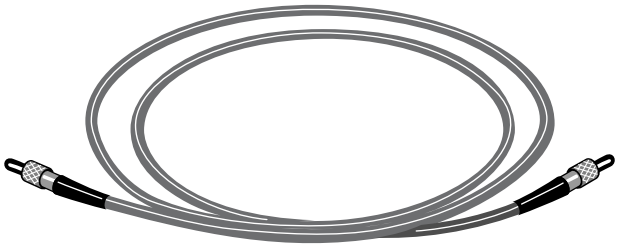
Module features

The important features of the fiber optic module include:

- Remote start capabilities.
- A *test fiber* that can be used to test the instrument's performance.
- A spectral range of 12,000-3,800 cm^{-1} (833-2,630 nm).
- Standard SMA connectors for compatibility with fiber optic sampling accessories, such as the Thermo Scientific SabIR diffuse-reflection probe and fiber optic dip probe.
- A strain relief mechanism that was designed specifically for the SabIR diffuse-reflection probe. The strain relief mechanism can be attached to the instrument to help lessen strain on the fiber optical cables of sampling accessories. See "Connecting the strain relief to the module" in the "Using the SabIR diffuse-reflection probe" section of this chapter for more information about attaching and using the strain relief mechanism.

Testing the sampling module

The fiber optic module includes an optical *test fiber* which can be used to perform an operation test without attaching a fiber optic sampling accessory. The test fiber is a troubleshooting tool and can be used to determine if any problems exist with the sampling module or a fiber optic accessory.



Optical test fiber

The test fiber can be used along with the Instrument Check feature in RESULT Operation software to perform an instrument test of the module optics and *detector*.

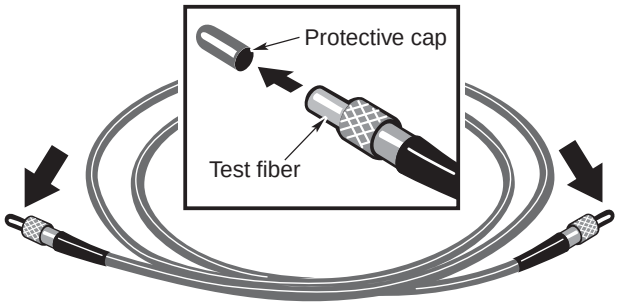
Connecting the test fiber to the sampling module

The test fiber can be easily connected to the fiber optic sampling module. It is not necessary to power off the instrument before connecting the test fiber.

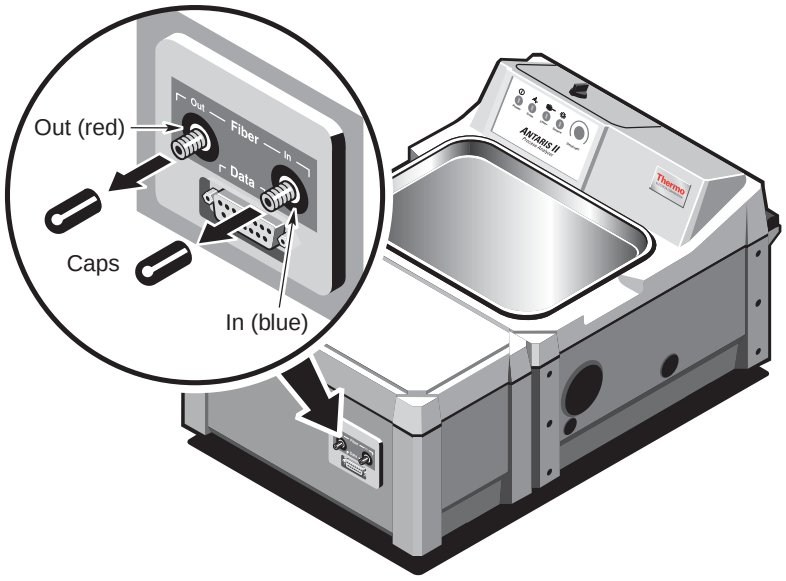
Note Do not discard the protective caps from the test fiber or the fiber optic sampling module. The caps should be put back on to the fiber optic connectors when the test fiber and/or module are not in use. ▲

To connect the *test fiber* to the fiber optic module:

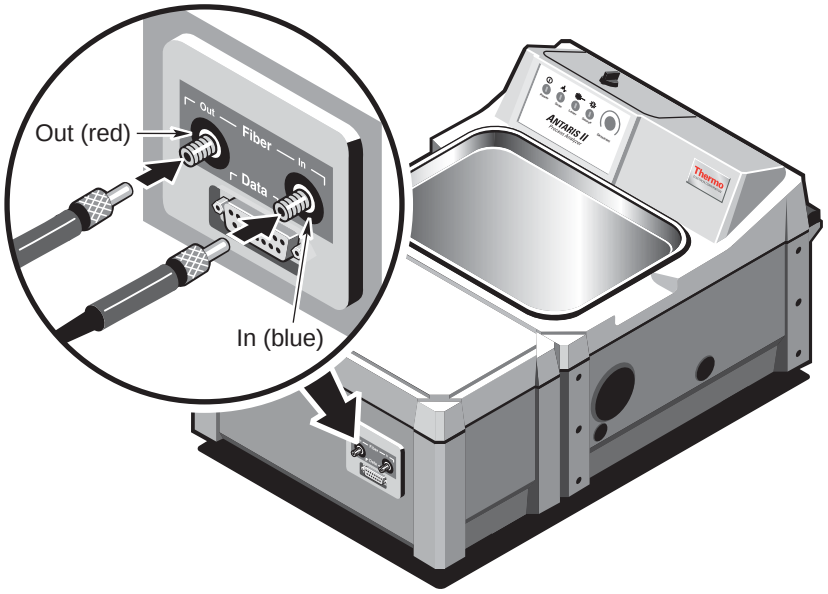
1. **Remove the protective caps from the ends of the test fiber.**



2. **Remove the protective caps from the In and Out *fiber optic ports*.**



3. **Connect both ends of the test fiber to the In and Out ports on the instrument.**



Note Either end of the test fiber can be connected to either of the ports. ▲

Notice Do not use tools to tighten the thumbscrews. Do not over tighten the screws. Using tools or over tightening may damage the ends of the test fiber or the connectors on the module. ▲

⚠ Warning Do not stare into the fiber optic connectors or into the non-terminated end of the test fiber when the instrument is running. ▲

4. **Hand tighten the *thumbscrews* on the test fiber connectors until they are finger tight.**

   The test fiber is now connected. If the instrument has not been powered on, power on the instrument and let the instrument stabilize for approximately one hour before using the test fiber. See "Getting Started" in the "Antaris Sampling" chapter if you need instructions for turning on the instrument.

Performing an instrument check

RESULT Operation software contains an Instrument Check feature that runs an operation test. Before running the test, attach the test fiber and power on the instrument. If the instrument has been powered off for more than 20 minutes, allow the instrument to stabilize for at least an hour before perform an instrument check.

To run the instrument check:

1. **Log on to RESULT Operation software.**

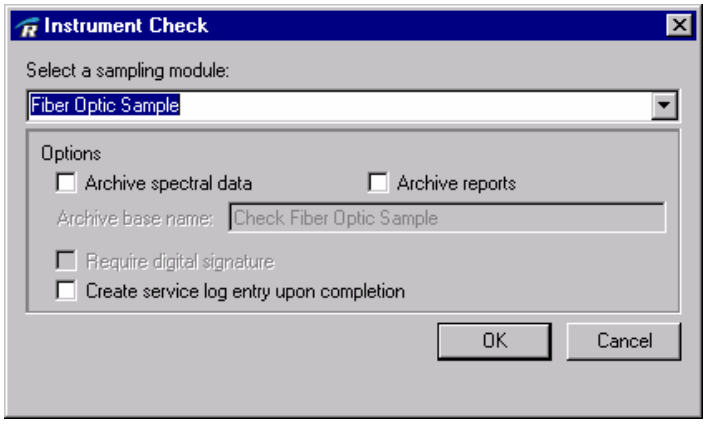
   See "Starting RESULT software" in the "Antaris sampling" chapter for instructions to log on to the software.

2. **Choose the Maintenance menu from the Result Operation main window menu bar.**

   If the Maintenance menu does not appear in the RESULT Operation main window, then you cannot access the Instrument Check feature. See your RESULT software administrator.

3. **Choose Instrument Check from the Maintenance menu.**

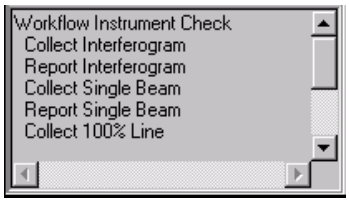
   The software will open the Instrument Check dialog box.



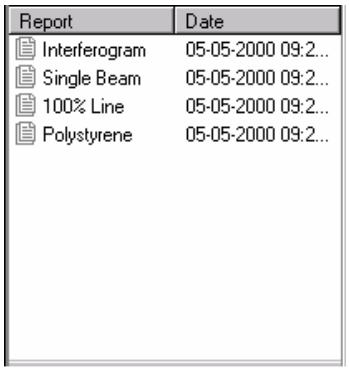
4. **If the Fiber Optic Sample option is not selected, select this option from the Select A Sampling Module drop-down list.**

5. Choose OK to perform the check.

While the test is running, the status indicator on the lower left side of the RESULT Operation main window will indicate the status of the instrument check.



As each spectrum is created, the software will create a report. The title of each report will appear in the report navigation frame.



You can view a report by selecting the report name, and the selected report will open in the display area.

See "Chapter 5 System Maintenance" of "Section 3 RESULT Operation Software" in your *RESULT User's Guide* for information about archiving instrument check results, digitally signing the results, and creating a service log entry related to the check. The "System Maintenance" chapter also contains sample spectra generated from an instrument check and information about each type of spectrum produced.

Using sampling accessories

This section includes information about using the fiber optic sampling module with fiber optic sampling accessories, including connecting the accessories, collecting data, and specifying workflow events. Because the module is compatible with a variety of probes throughout the industry that use various sampling techniques, refer to your accessory documentation for information about sampling techniques, compatible sample types, typical spectra, and maintaining your accessory.

Note If you will be using the module with the Thermo Scientific SabIR probe, "Using the SabIR Probe" in this chapter for specific instructions about connecting the probe, compatible sample types, collecting backgrounds and sample data, developing workflows, and maintaining the probe. ▲

Connecting fiber optic accessories

The fiber optic module is compatible with fiber optic accessories that have standard SMA connectors. Fiber optic accessories can be connected to the module using the fiber optic ports on the right front of the module.

Note The electrical connector on the module is for use with the Thermo Scientific SabIR probe only. Other sampling accessories with SMA connectors can still be used with the sampling module.

If the instrument is powered off while you install a fiber optic accessory and has been powered off for more than 20 minutes, after you power on the instrument, allow the instrument to stabilize for approximately one hour before collecting any data. Each time you power the instrument on and off, be sure to log off and then log back into RESULT software.

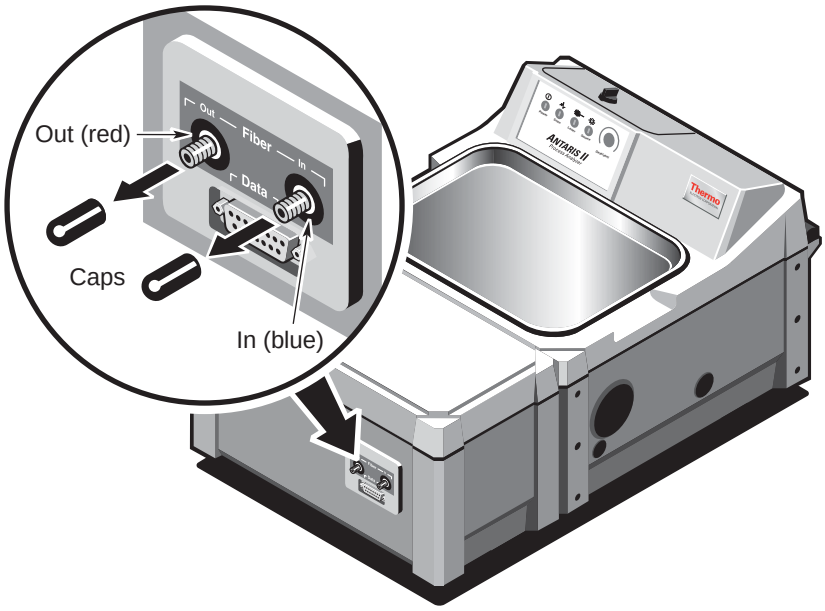
Do not discard the protective caps from any fiber optic accessories or the fiber optic sampling module. The caps should be put back on to the fiber optic connectors when the accessory and/or module are not in use. ▲

To connect a sampling accessory to the fiber optic module:

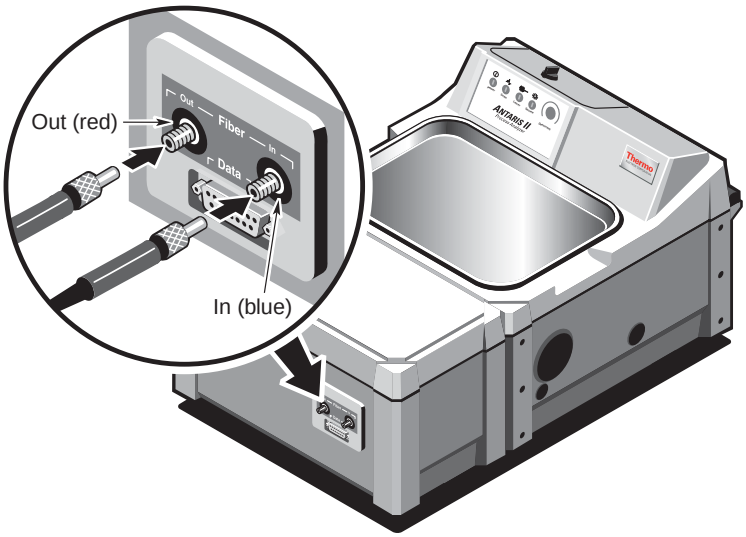
1. **Remove any protective caps from the sampling accessory connectors.**

   Do not discard the protective caps. Save the caps so they can be put back on to the accessory for storage when it is not being used.

2. **Remove the protective caps from the In and Out *fiber optic ports*.**



3. **Connect one SMA connector to each fiber optic port.**



The light travels out the red “out” port and into the fiber optic accessory. The light leaves the accessory and travels back into the module through the blue “in” port. The connectors are color-coded for compatibility with the SabIR diffuse-reflection probe. However, you can use the color coding to assist you in consistently connecting the cables on your sampling accessory to the same ports on the module.

Note It is important to consistently attach the fiber optic cables to the same ports when connecting sampling accessories. If there are differences between the fiber optic cables, and they are not always attached to the same ports, your data may be affected. ▲

Notice Do not over tighten the connectors or use tools to tighten the connectors. Over tightening or using tools may damage the connectors on the probe or the instrument. ▲

4. **Hand-tighten the connectors until you begin to feel a small amount of resistance, i.e., until they are finger tight.**

5. **Power on the analyzer and log into the software.**

   If the analyzer has been powered off for more than 20 minutes, allow the analyzer to stabilize for approximately one hour before collecting data.

Your first experiment

This section goes through a simple experiment using RESULT, the fiber optic module, and the Quick Collect feature in RESULT Operation or RESULT Integration software.

The Quick Collect feature in RESULT software allows you to collect a background and/or sample spectrum without using a workflow. Using Quick Collect is good practice to help you "get the feel" of sampling with the fiber optic module before using the module in actual production workflows. Quick Collect also allows you to easily produce a spectrum without having to develop a workflow for a single collection event.

Before you begin

Before you begin the experiment:

- Connect the sampling accessory to the fiber optic module, power on the instrument, and allow the instrument to stabilize for at least an hour (if the instrument has been powered off for more than 20 minutes).

- Select a background material and sample that is compatible with your fiber optic accessory. See your fiber optic accessory's documentation for information about compatible samples.

Setting up the experiment

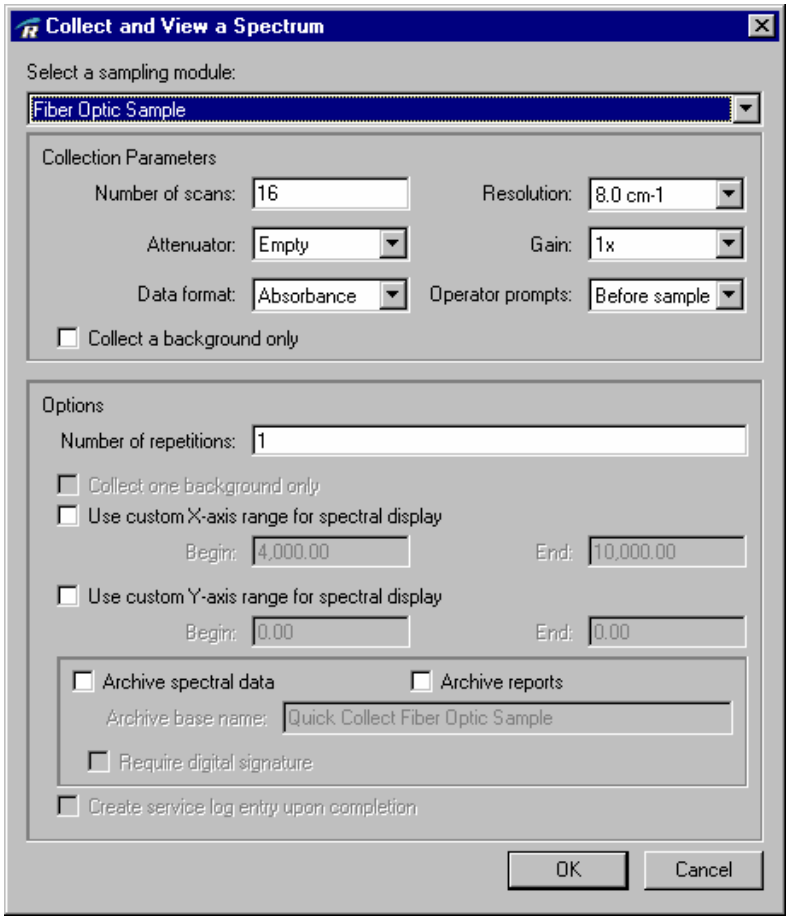
To begin the experiment:

1. **Start RESULT Integration or RESULT Operation software.**

   See "Starting RESULT software" in the "Antaris sampling" chapter for instructions to log on to the software.

2. **Open the Quick Collect dialog box.**

   Quick Collect can be opened from the Tools menu in RESULT Integration or from the Maintenance menu in RESULT Operation. The Quick Collect dialog box should appear. (If you are using RESULT Operation and the Maintenance menu does not appear in the menu bar of the main window, then you cannot access the Quick Collect feature. See your RESULT software administrator.)



3. **If it is not already selected, select Fiber Optic Sample from the Select a Sampling Module drop-down list.**

4. **Set the appropriate number of scans, resolution, attenuator, gain, and data format settings in the Collection Parameters.**

   These collection parameters are highly dependent on the sampling accessory you have connected. See "Tips for developing workflows" in this chapter and the documentation for your sampling accessory for the appropriate collection parameters.

5. **Select the Before Both option from the Operator Prompts drop-down list.**

   This means that the software will prompt you before collecting the background and the sample spectrum.

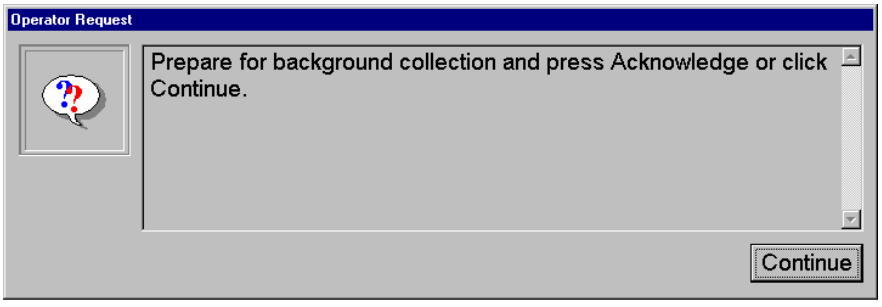
6. **For purposes of this experiment, do not change any of the settings in the Options group.**

   For more information about setting Options in the Quick Collect dialog box, see "Chapter 5 System Maintenance" of "Section 3 RESULT Operation Software" in your *RESULT User's Guide*.

7. **Choose OK to begin the experiment.**

Collecting the background spectrum

The software will prompt you when the instrument is ready to begin collecting the background spectrum.



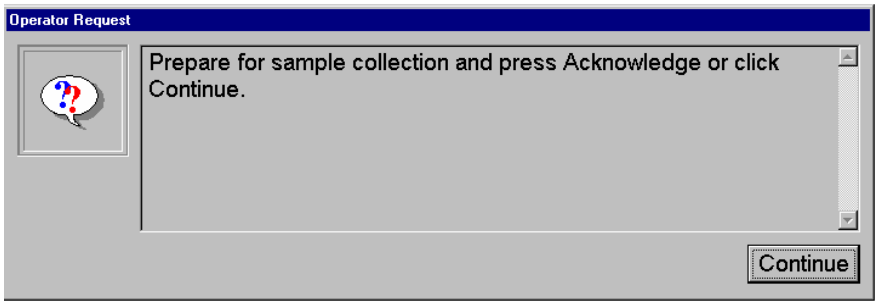
Prepare your sampling accessory and background material for collection. Refer to your sampling accessory documentation for information about how to prepare and collect a background spectrum.

When you are ready for the instrument to begin collecting data, select Continue at the prompt or press the Acknowledge button on the operation panel of the instrument.

The status indicator on the lower left side of the software's main window will display the status of the data collection. Do not move the sampling accessory until the instrument has completed collecting data.

Collecting the sample spectrum

After you have finished collecting the background spectrum, the software will prompt you when it is ready to collect the sample spectrum.



Follow the instructions in your sampling accessory documentation to prepare the sample material and accessory for data collection. When you are ready for the instrument to begin collecting data, select Continue in the software prompt or press the Acknowledge button on the instrument.

The software will begin collecting the sample spectrum. The status indicator on the lower left side of the software's main window will display the status of the data collection. Do not move the sampling accessory until the instrument has completed collecting data.

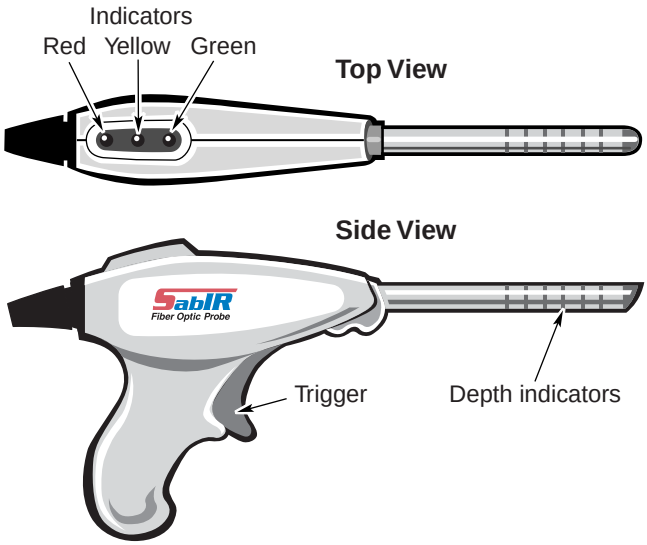
When the instrument has completed collecting data, the spectrum will appear in the display area of the main window.

Using the SabIR probe

The fiber optic module is optimized for use with the Thermo Scientific *SabIR diffuse-reflection probe* to provide easy, remote sampling of solids and powders. This section contains information about SabIR features and provides instructions for attaching, using, specifying workflow settings for, and maintaining the SabIR.

SabIR features

The Thermo Scientific SabIR probe is designed to be used for remote diffuse-reflection sampling of solids and powders in the pharmaceutical, chemical, and polymer industries.



SabIR diffuse-reflection probe

If your module includes the SabIR, the module was fitted with a holster to hold the SabIR. The important features of the SabIR probe and holster include:

- **Probe holster**. The instrument contains a probe holster on the side of the instrument. The probe should rest in the holster at all times when it is not in use but is connected to the module. The holster contains an internal *Spectralon*® reference for collecting background information. The holster also contains a magnet that works in conjunction with a sensor in the probe, which allows the software to determine whether the probe is properly inserted into the holster when collecting background data using the instrument's internal reference.

See "Collecting a background" later in this section for more information about the sensor and magnet features.

- **Probe fiber optic cables.** The *fiber optic cables* are available in two- and three-meter lengths. The cables are color-coded to correlate with the In and Out ports on the instrument. The connectors at the ends of the cables have protective caps to help prevent damage. Keep the protective caps on the cables at all times when the cables are not connected to the module.

- **Probe electrical connector.** The electrical connector attaches to the electrical port on the module, and is the power source to the probe.

Note The system was shipped with a strain release mechanism that attaches to the module. The SabIR fiber optic cables and electrical connector fit inside the mechanism to reduce stress and bending of the fiber optic cables. ▲

- **Probe handle.** The probe handle contains the following items:

  - **LED indicators.** The *LED indicators* on the probe handle have the same function as the indicators on the instrument. The indicators on the handle allow you to tell the status of your collection without being directly in front of the instrument or computer screen.

  - **Trigger.** The trigger on the probe allows you to activate sample collection from a remote location and can be used in place of the Acknowledge button on the instrument.

  - **Sensor.** The top of the probe handle contains a sensor, located near the probe shaft. The sensor works in conjunction with a magnet in the probe holster, which allows the software to determine whether the probe is properly inserted into the holster when collecting background data using the instrument's internal reference. See "Collecting a background" later in this chapter for more information about the sensor and magnet features.

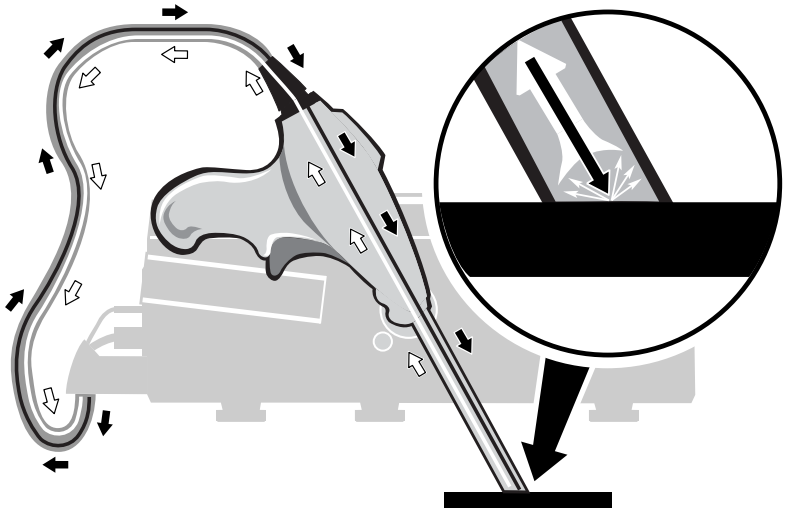
  - **Probe shaft.** The near-infrared (NIR) beam travels through the probe shaft to the probe tip. The probe shaft is 15.8 cm long with a diameter of 1.6 cm, and is made of stainless steel. The probe shaft has graduated rings around it to assist you in inserting the probe into substances at consistent depths.

- **Probe tip.** The probe tip contains an angled sapphire window that can analyze samples directly or indirectly through packaging materials. The probe tip is angled to minimize *specular reflection* (a "mirror-like" reflection without any scattering) from highly reflective surfaces. This means that more light will diffuse, allowing you to obtain more data and produce a more accurate, detailed spectrum. The probe tip comes with a protective cap that should remain on the probe at all times when it is not connected to the module.

Understanding diffuse-reflection sampling

The SabIR probe produces *diffuse-reflection* spectra. Diffuse-reflection spectroscopy is a powerful technique for Fourier transform near infrared (FT-NIR) analysis of rough surface solids and powders, such as pharmaceutical tablets or raw materials in powdered form (e.g., lactose, cellulose, polymers, or talc). Sampling is fast and easy because little or no sample preparation is required.

Diffuse-reflection accessories measure the changes that occur in the light *beam* when it interacts with a sample. When directed onto a sample of finely ground particles, the radiation will interact with the particles by alternately passing through them and reflecting off their surfaces. This causes the light to scatter, or "diffuse," as it makes its way through the sample.



Diffuse-reflection sampling with the SabIR

When using the SabIR probe with the fiber optic module, the light beam leaves the instrument through the fiber optic Out port. The optical fibers carry the light through the probe. When the beam reaches the sample, the scattered (reflected) light is carried back through the optical fibers and into the instrument through the fiber optic In port, and then to the *detector*.

Diffuse-reflection accessories often provide excellent results from powders and crystalline materials, which scatter much of the energy from the beam. Scattering is a benefit for diffuse-reflection spectroscopy because the more scattering that occurs within the sample matrix, the more absorption information you can extract from the sample, and the sensitivity of the measurement is higher.

Connecting the SabIR to the sampling module

The SabIR diffuse-reflection probe was designed to be easy to connect to the fiber optic module.

Notice Because the probe and module have an electrical connection, it is recommended that you power off the instrument before connecting the probe to avoid damaging the instrument's electronics. Each time you power off the instrument, be sure to log off any software applications. ▲

Note The fiber optic module was shipped with a strain relief mechanism that holds the SabIR fiber optic and electrical cables. It is recommended that you first attach the SabIR to the module and then attach the strain relief mechanism to avoid bending the fiber optic cables excessively. Instructions for attaching the strain relief mechanism follow the instructions for connecting the SabIR.

If the strain relief is already connected to the module, remove the strain relief cover, connect the SabIR probe to the module, insert the fiber optic cables into the strain relief mechanism, and then replace the strain relief cover.

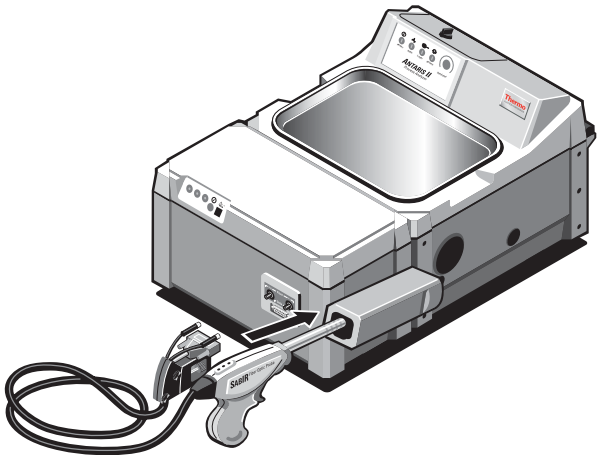
Do not discard protective caps from the SabIR probe cables and tip or from the fiber optic sampling module. Save the caps so they can be put back on the SabIR and fiber optic module when they are not being used. ▲

To connect the SabIR to the fiber optic module:

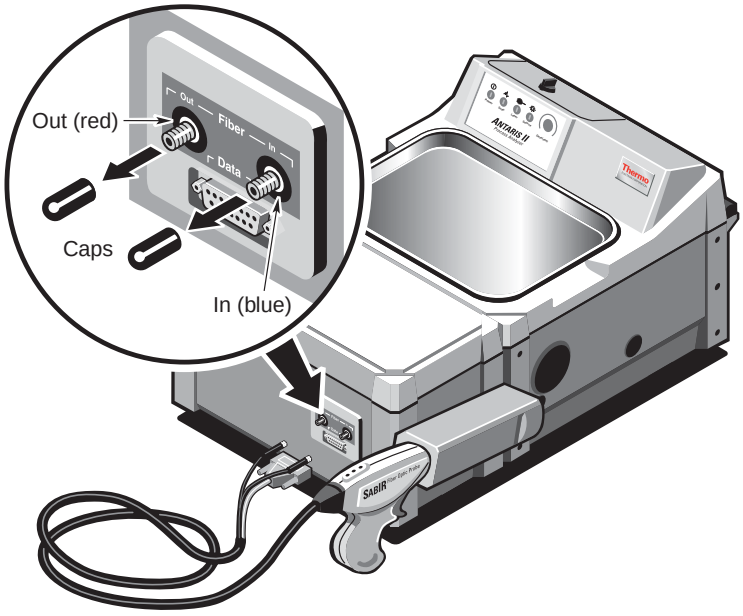
1. **Remove the protective cap from the probe tip.**

2. **Insert the probe into the holster.**

   The probe is in position when you hear it "click" into place.

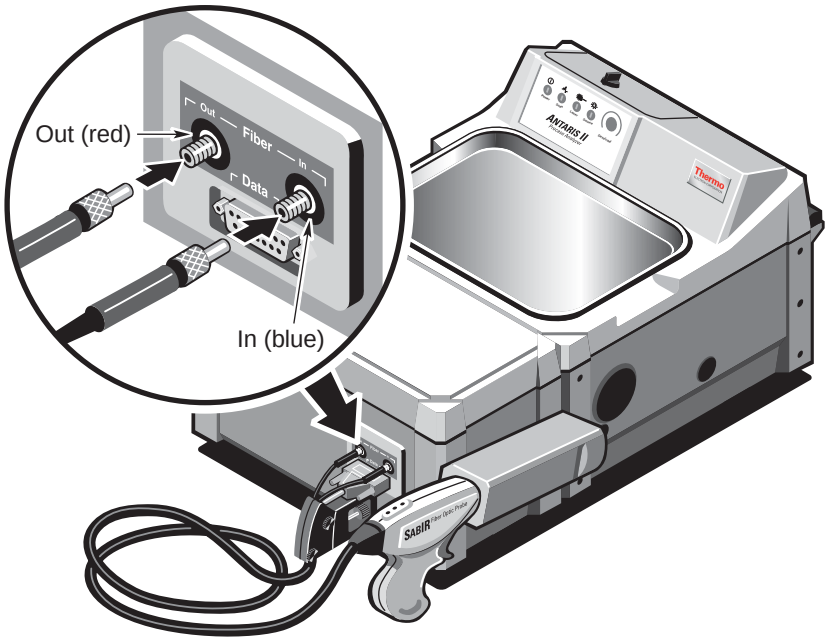


3. **Remove the protective caps from the In and Out fiber optic ports.**



4. **Remove the protective caps from the fiber optic cables.**

5. **Connect the In and Out cables to the In and Out ports.**



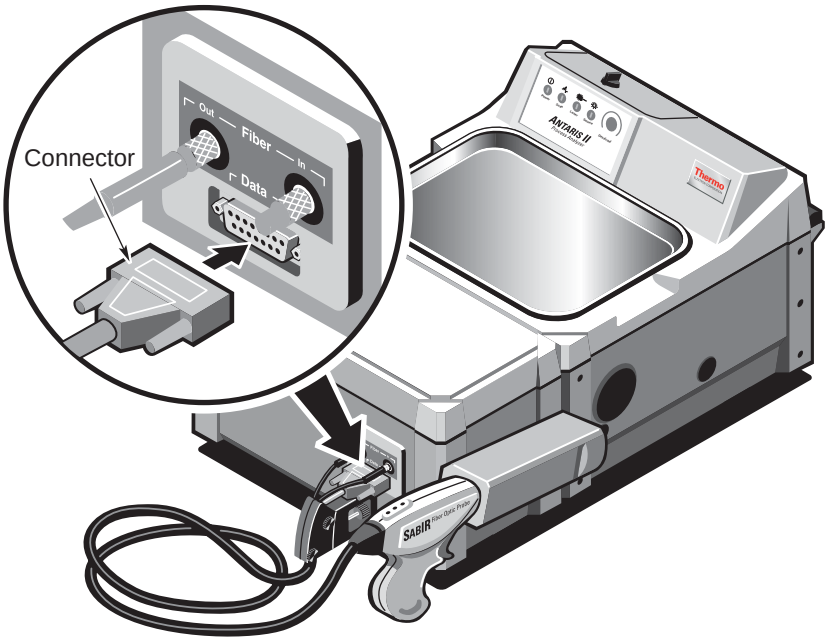
The cables should be attached to the correct ports for proper operation. The ends of the cables and the connectors are color-coded. Attach the red connector to the red Out port and the blue connector to the blue In port.

Note If the cables are attached to the incorrect ports, the SabIR will function, but spectral quality or repeatability may be affected. ▲

Notice Do not over tighten the connectors or use tools to tighten the connectors. Over tightening or using tools may damage the connectors on the probe or the instrument. ▲

6. **Hand-tighten the connectors until you begin to feel a small amount of resistance, i.e., until they are finger tight.**

7. **Connect the electrical connector to the electrical port on the instrument.**



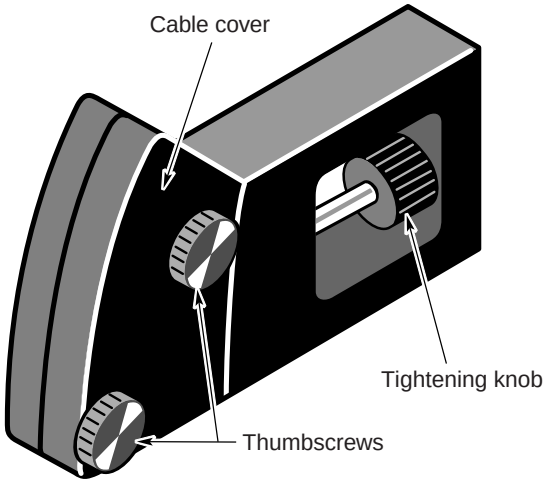
Fit the connector into the port, and then hand-tighten the screws on either side of the connector. As with the fiber optic cable connections, do not over tighten the screws or use tools to tighten the screws.

8. **Power on the instrument.**

Allow the instrument to stabilize for approximately one hour before collecting data, if the instrument has been powered off for more than 20 minutes.

Connecting the strain relief to the sampling module

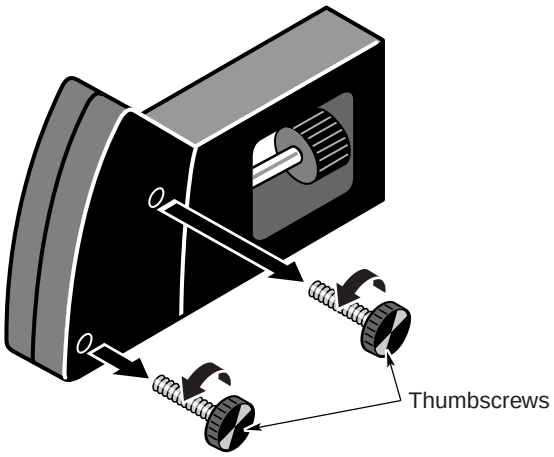
The module was shipped with a strain relief mechanism that holds the SabIR fiber optic and electrical cables. It is recommended that you use the strain relief with the SabIR to help prevent damaging the fiber optic cables.



Note Connect the SabIR probe to the module before you connect the strain relief mechanism. This will help prevent bending the cables excessively and causing damage to the optical fibers. ▲

To attach the strain relief to the sampling module:

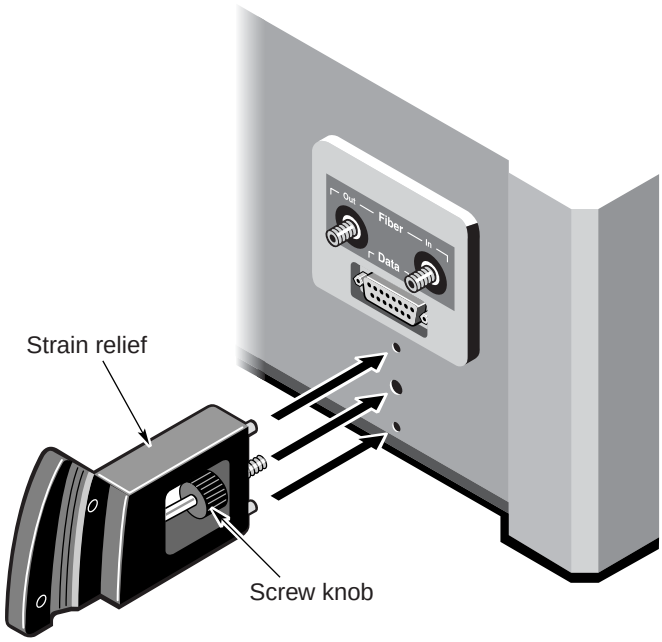
1. **Remove the thumbscrews from the cable cover on the strain relief mechanism.**



Turn the thumbscrews counterclockwise to remove them from the cable cover.

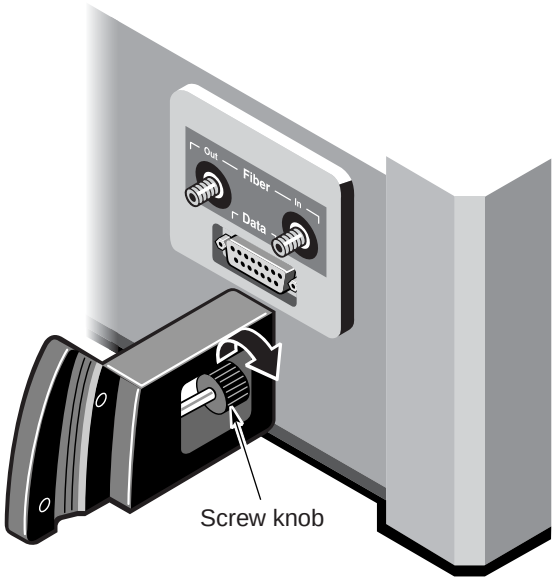
2. **Remove the cable cover from the strain relief base.**

3. Connect the strain relief base to the fiber optic module.



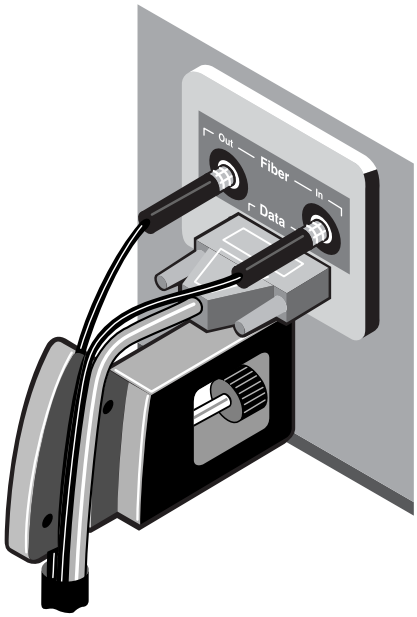
The two pegs fit into the top and bottom holes on the module. The strain relief screw fits into the larger hole in between the peg holes on the module.

4. **Tighten the knob on the strain relief base to affix the base tightly against the module.**



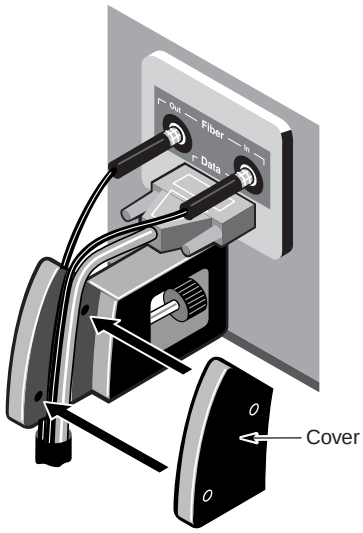
Turn the knob clockwise until the strain relief is pressing tightly against the module and the knob is finger tight.

5. **Gently fit the SabIR cables into the cable grooves.**



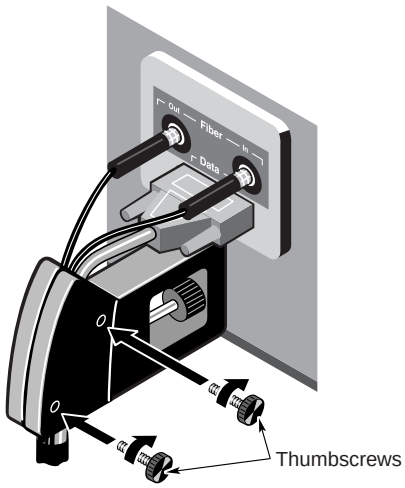
Notice To prevent damaging the cables, do not bend the cables excessively when fitting them into the cable holder. Make sure the cables are resting inside the cable holder and hold them in place with one hand when you proceed to the next step. ▲

6. Gently fit the cable cover back onto the strain relief base.



Notice Make sure the cables are resting in the cable holder and are not being compressed by the cable cover. ▲

7. While holding the cable cover with one hand to secure it in place, insert the thumbscrews into the cable cover.



Turn the thumbscrews clockwise until they are finger tight. The strain relief is now attached to the fiber optic module. It is recommended that the strain relief be attached at all times when the SabIR is attached to the module. The strain relief mechanism can remain attached to the module at all times, even if the SabIR is not connected to the module.

Samples compatible with the SabIR

The SabIR is designed for easy, remote sampling of raw materials in the industrial environments of the pharmaceutical, chemical, and polymer industries. The probe can analyze samples directly or indirectly through clear packaging materials, such as glass and plastic.

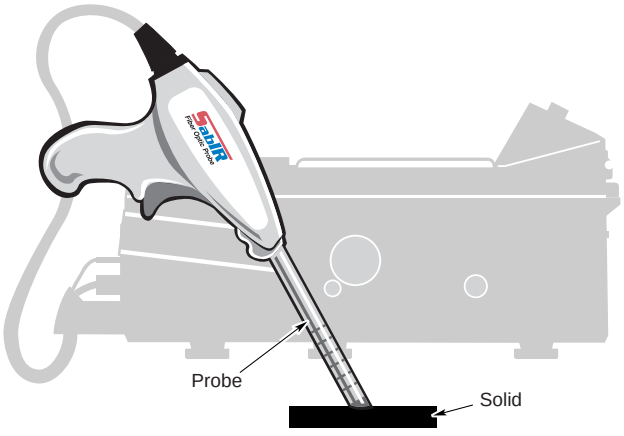
Some examples of sample types include:

- **Solids**. Any solid with a rough or diffuse surface, including paper, wood, plastics (especially plastics with a milky, opaque appearance), coated textiles, polymers, and pharmaceutical tablets.
- **Powders**. The diffuse-reflection probe works well with large quantities of powder samples. The probe can be inserted directly into the sample. If the sample may leave a residue on the probe, the sample can be put into a glass container and sampled indirectly.

Sample thickness or the amount of sample should be taken into consideration when using the SabIR probe. If a solid sample is too thin or if there is not enough of a powder sample, you may have problems with the spectra. See “Common problems” in this chapter for more information.

Sampling solids

When sampling a solid, hold the probe tip flush against the solid surface.



When collecting samples in a workflow, the steady green indicator will alert you when the probe is ready to begin collecting data.

When you are ready to begin collecting data, press the probe trigger. The steady yellow indicator light will be on while the probe is collecting data. Keep the probe in place until the yellow indicator is no longer on and data collection is complete.

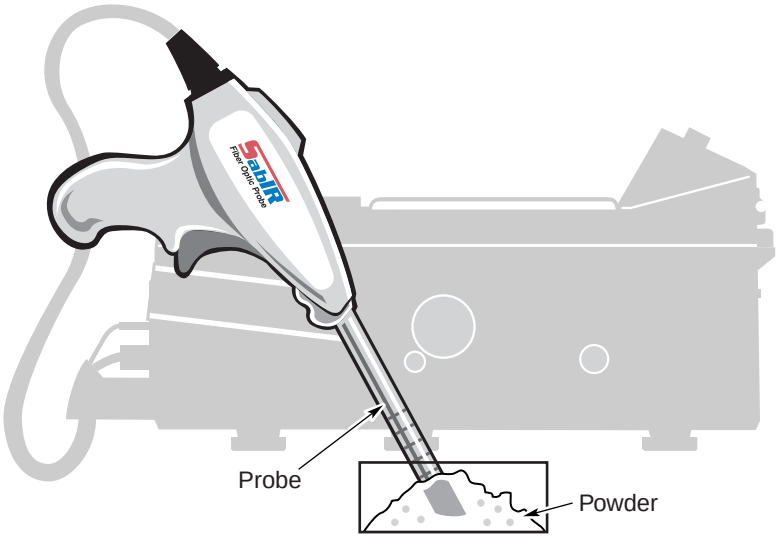
You can also sample solids through clear packaging materials, such as plastic bags, plastic wrap, or glass. Sampling through colored packaging materials may affect spectral data.

Note Polymeric materials, such as plastics, have spectral features which may affect analysis results. ▲

Sampling powders

Like solids, you can sample powders directly or through clear packaging materials such as glass vials or plastics. When sampling a powder through packaging materials, follow the same sampling instructions used for sampling solids.

When sampling powders directly, make sure the sample is thick enough so the probe window is fully covered by the sample material but that enough of the sample material remains underneath the probe window to obtain an accurate reading.



Sampling a powder with the SabIR

The depth indicator rings on the probe shaft can assist you in maintaining a consistent insertion depth when collecting multiple samples.

Note If the sample is likely to leave a residue on the probe, it is recommended that the sample be placed in a clear plastic bag or glass container to prevent residue from accumulating on the probe tip. If residue does get on the probe tip, follow the instructions for cleaning the tip in *Maintaining the SabIR* later in this chapter. ▲

Your first experiment using the SabIR

This section goes through a simple experiment using the SabIR diffuse-reflection probe and the Quick Collect feature in RESULT Operation or RESULT Integration software.

The Quick Collect feature allows you to collect a background and/or sample spectrum without having to create and run a workflow. Using Quick Collect is a good practice to help you "get the feel" of sampling with the SabIR before using the probe in actual production workflows.

Select a sample that is compatible with the SabIR. See "Samples compatible with the SabIR" for assistance in choosing a sample.

Tip If you do not have any samples of items specific to your production environment, you can try a piece of fabric, such as an item of clothing or a cloth, or a piece of paper. ▲

Setting up the experiment

Before you begin the experiment, connect the fiber optic probe and strain relief, and make sure the instrument has been turned on for approximately one hour so it has stabilized. Have your sample material at hand.

To begin your first experiment:

1. **Start RESULT Integration or RESULT Operation software.**

   See "Starting RESULT software" in the "Antaris sampling" chapter for instructions to log on to the software.

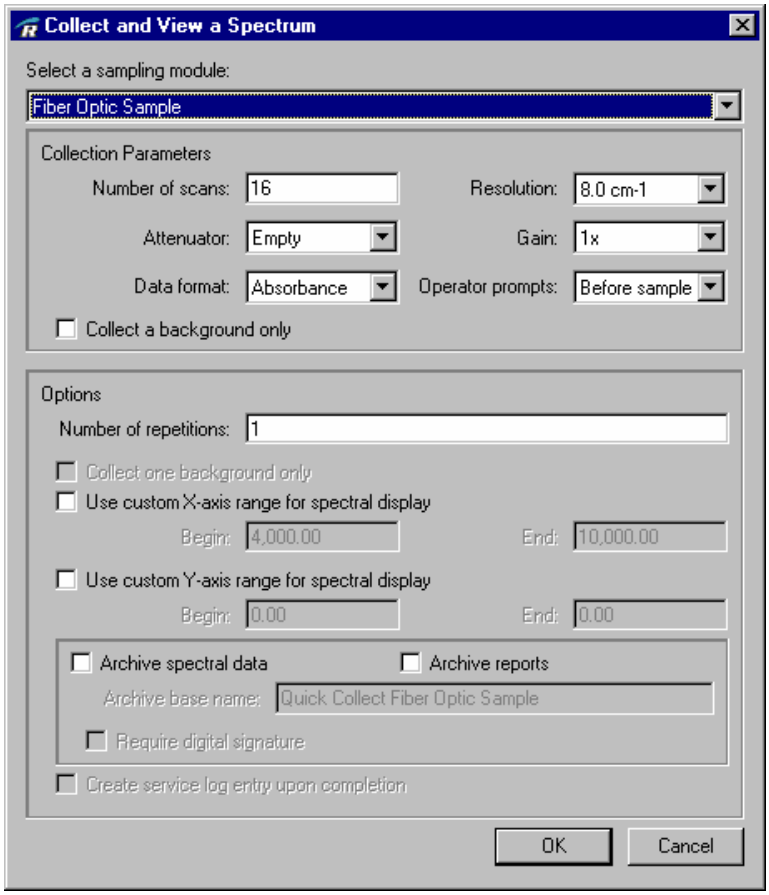
2. **Open the Quick Collect dialog box.**

   If using RESULT Integration software, select the Quick Collect option from the Tools menu in the main window of the software. If using

RESULT Operation software, select the Quick Collect option from the Maintenance menu in the main window of the software.

Note If you are using RESULT Operation and the Maintenance menu does not appear in the menu bar of the main window, then you cannot access the Quick Collect feature. See your RESULT software administrator. ▲

The Quick Collect dialog box should appear.



3. **If it is not already selected, select the Fiber Optic Sample option from the Choose A Sampling Module drop-down list.**

4. **Select Before Both from the Operator Prompts drop-down list.**

   With this option selected, the software will prompt you when it is ready to collect the background information and when it is ready to collect the sample information.

Note When running actual workflows, it is unnecessary to be prompted to begin background collection. However, background and sample prompts are necessary when using the Quick Collect feature with the SabIR. ▲

5. **Enter 3 in the Number of Repetitions text box.**

   This means that you will repeat the collection three times.

Tip When repeating the collection three times, you can approach the experiment from one of two perspectives:

Checking for repeatability. When positioning the SabIR and collecting the sample, try to hold the SabIR in the same position on the sample for each collection. Check the resulting spectra for any major differences.

Viewing the effects of different sampling positions. Position the SabIR on a different portion of the sample during each collection. Note how the different sampling positions affect the resulting spectra. ▲

6. **Select the Collect One Background Only check box.**

   This option becomes enabled if you enter a number other than 1 in the Number of Repetitions text box. When a check mark appears in the Collect One Background Only check box, the software will allow you to take one background collection for the experiment. It will use that same background data for each repetition in the experiment. If you do not select this option, then you will be required to collect a background for each repetition of the experiment.

7. **After you have selected the above options, choose OK to begin the experiment.**

Collecting the background spectrum

The holster on the fiber optic module contains an internal *Spectralon* reference that can be used for collecting backgrounds. The software will prompt you when it is time to collect the background.

To collect the background:

1. **If the probe is not already inserted into the holster, insert the probe into the holster.**

The probe is properly inserted into the holster when you hear it "click" in place.

2. **Press and release the probe trigger, press the Acknowledge button on the instrument, or choose Continue at the operator prompt in the software to begin collecting data.**

   The system will begin collecting the background spectrum. You can view the status of the background scans in the status indicator box in the software. While the SabIR is collecting data, the yellow indicator light will be on. Do not remove the probe from the holster until the yellow indicator light turns off, indicating that data collection is complete.

   After you collect the background, the *background spectrum* remains in memory and will be used to process all sample spectra in this experiment.

Collecting the sample data

After you have finished collecting the background, the software will prompt you when it is time to collect the sample data.

Notice Do not press the trigger while you are removing the probe from the holster. Pressing the trigger will make the probe start collecting data prematurely and may affect your results. If the probe starts collecting data prematurely, you will need to redo the experiment. ▲

1. **Remove the probe from the holster.**

   The steady green indicator on the probe should be on, letting you know that the probe is ready to begin collecting data.

2. **Place the probe against the sample.**

   If sampling a solid material or a powder in a container, make sure the probe window is flush against the sample, as shown in the "Samples compatible with the SabIR" section of this chapter.

   If sampling a powder directly, make sure the probe window is submerged into the sample so the window is completely covered by the

sample material. However, do not submerge the probe too far into the sample. If there is not enough sample material underneath the probe window, you may experience problems with the spectrum.

3. **When the probe is in position, press and release the probe trigger to begin collecting data.**

   You can view the status of data collection in the status indicator of the software's main window. While the probe is collecting data, the yellow indicator light will be on. Do not move the probe until the yellow indicator light has turned off, indicating that the probe has finished collecting data.

4. **When the instrument has finished collecting data, remove the probe from the sample.**

Tip Check the probe tip to make sure there is no residue on it before you repeat the collection. If there is residue on the probe tip, follow the cleaning instructions in the "Maintenance and Service" chapter. ▲

5. **Repeat steps 2, 3, and 4 to repeat the collection.**

   The software will prompt you each time to begin collection. If collecting data from a large sample, you may want to place the probe on a different area of the sample. Continue repeating steps 2, 3, and 4 until the software stops prompting you to begin collection.

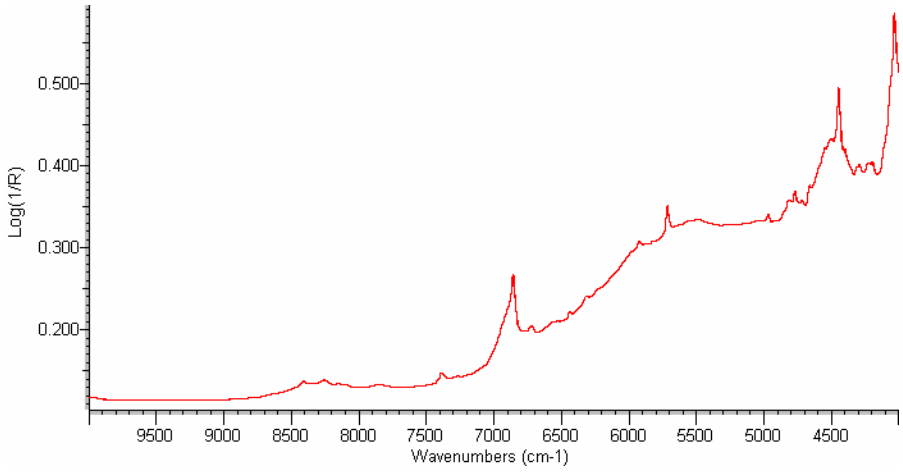
Note If the probe tip became dirty, follow the instructions for cleaning the probe tip in the "Maintenance and Service" chapter before inserting the probe into the holster. ▲

6. **Insert the probe into the holster when you have finished all collections.**

   After you have finished the experiment, each spectrum will be displayed in the report navigation frame. Select one of the items from the report navigation frame to view the spectrum in the display area of the software.

Typical spectrum obtained by using the SabIR

FT-NIR spectra produced by *diffuse-reflection* have unique characteristics. These characteristics were taken into consideration by Thermo Fisher Scientific when making recommendations for collection parameters using the SabIR probe. The following spectrum is representative of a typical near-infrared spectrum taken using the SabIR probe:



Spectrum of ascorbic acid powder

The typical spectral range for a diffuse-reflection sample with the SabIR is 10,000 to 4,200 wavenumbers (cm^{-1}). Solids typically exhibit a broad upward slope in absorbance toward smaller wavenumbers (longer wavelengths). See "Common problems with spectral data" in this chapter for information about some problems you may encounter when collecting sample spectra, along with suggestions for resolving those problems.

Using the SabIR with workflows

This section contains some general information about using the SabIR to collect background and sample data when running workflows developed in RESULT Integration software.

Collecting a background spectrum

A *background* is a reference spectrum that accounts for the unique optics of the sampling accessory and the instrument. Each sample spectrum is ratioed against a background so that the final spectrum is free of these features. You can collect a background with the SabIR using the internal Spectralon reference or an external reference. The workflow you are running should indicate which kind of reference you are using.

The workflow you are running will dictate how often to collect a background spectrum. The most recent background spectrum remains in the system's memory and is compared against sample data until a new background spectrum is collected.

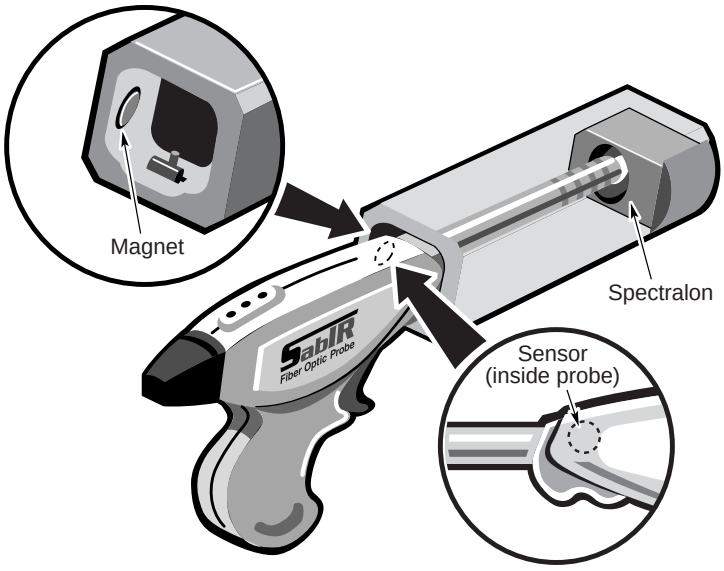
The "Common problems with spectral data" section of this chapter contains suggestions if a background spectrum is atypical from previously-collected background spectra.

Collecting a background using the Spectralon reference

The SabIR probe holster contains an internal *Spectralon* reference that can be used for collecting backgrounds. Spectralon is a very diffuse substance with high reflectance, but it is a soft, porous material that must be handled carefully. It can be cleaned if it becomes dirty. See "Maintaining the Spectralon reference" in this chapter for instructions on how to clean the reference.

Background collection using the module's internal Spectralon reference is a simple procedure. If the probe is inserted into the holster, the instrument can automatically detect this and can collect a background spectrum without any operator prompts.

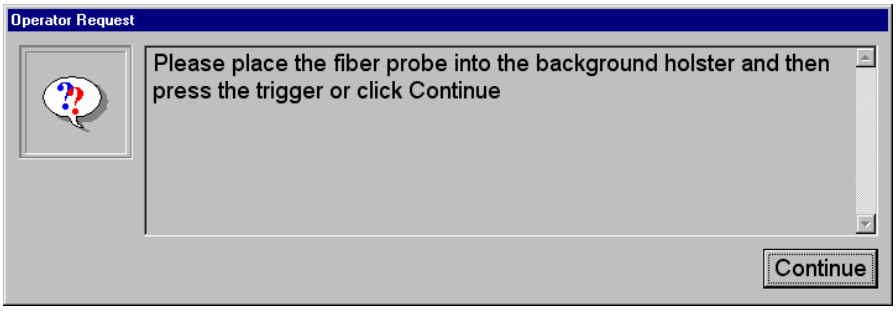
A sensor inside the SabIR probe detects whether the probe is properly inserted into the holster. The holster contains a magnet that is detected by the sensor.



SabIR in the module holster

Note The sensor in the holster is only compatible with the SabIR diffuse-reflection probe. The workflow must also be specifically developed for the SabIR for the sensor to detect when the probe is properly inserted in the holster. See "Tips for developing workflows" in this chapter for more information. ▲

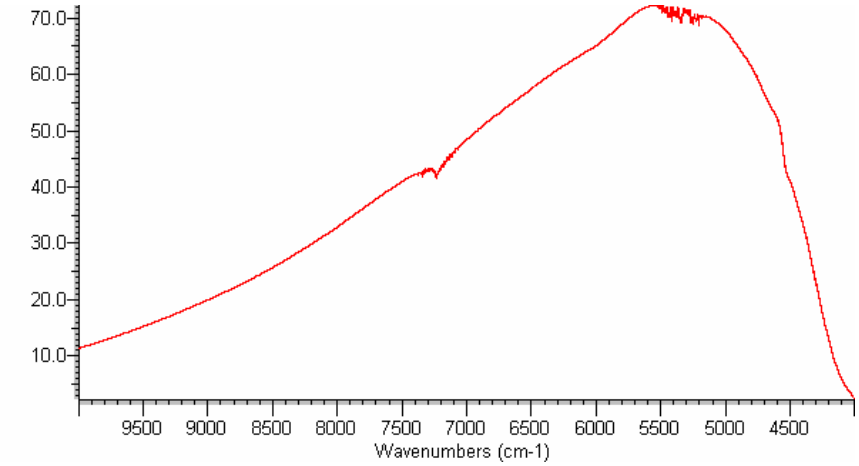
When attempting to collect a background, if the probe is not properly inserted in the holster, the software will display the following message:



If you receive this message, reposition the SabIR and attempt to begin collection again. After three unsuccessful attempts to detect the magnet in the holster, the software will cancel the collection and produce a table of workflow errors noting that the background collection was unsuccessful.

While the instrument is collecting the background spectrum, you can view the status of the collection in the status indicator of the software's main window. The yellow indicator on the SabIR will be on while the instrument is collecting data. Do not remove the probe from the holster until the yellow indicator turns off, indicating that data collection is complete.

A typical background spectrum using the Spectralon reference should resemble the following:



Typical Spectralon background spectrum with the SabIR

See “Common problems with spectral data” in this chapter if your background spectrum is not similar to the above or if a background spectrum you collected is atypical from previous background spectra.

Collecting a background using an external reference

If the workflow dictates to collect an external background reference, then the workflow or any attached instructions should indicate how to prepare and collect the background reference.

The software should prompt you to begin background collection. The green indicators on the probe and the instrument will be on when the instrument is ready to begin collecting the background. To collect the background, hold the probe to the reference material (see “Compatible Samples with the SabIR” in this chapter for instructions on how to position the probe if sampling solids or powders) and start collection.

If the green indicator is steady, then you can start the scan by pressing and releasing the probe trigger, pressing the Acknowledge button on the operation panel of the instrument, or choosing a response to a prompt in the software. If the green indicator is flashing, then you must begin the scan by responding to a software prompt.

The status indicator in the main window will display the status of the collection. While the probe is collecting the background, the yellow indicator light on the probe will be on. Do not move the probe until the yellow indicator light goes off, indicating that data collection is complete.

Collecting sample data

The SabIR and the fiber optic sampling module were designed to make remote sampling easy, requiring little or no sample preparation. However, collecting samples in production is controlled by the workflow you are running. You should pay close attention to the prompts and any instructions that are in the software. The workflow should prompt you to begin sample collection.

The green indicators on the probe and the instrument will be on when the instrument is ready to begin collecting data. To collect the sample, hold the probe to the sample material (see "Compatible Samples with the SabIR" in this chapter for instructions on how to position the probe if sampling solids or powders) and start the collection.

If the green indicator is steady, then you can start data collection by pressing and releasing the probe trigger, pressing the Acknowledge button on the operation panel of the instrument, or choosing the appropriate response in a prompt in the software. If the green indicator is flashing, then you must begin data collection by responding to a software prompt.

The status indicator in the software's main window will display the status of the collection. While the probe is collecting data, the yellow indicator light will be on. Do not move the probe until the yellow indicator light turns off, indicating that data collection is complete.

The "Common problems with spectral data" section in this chapter contains information related to evaluating sample data, along with suggestions for resolving some typical problems you may encounter.

Some materials that can be used as an external reference include:

- Spectralon
- Diffuse gold
- Ceramic or sintered polytef plate (solids)
- Barium sulfate, polytetrafluoroethylene (powders)

Tips for developing workflows for the SabIR

When developing workflows using RESULT Integration software, there are some factors you may want to take into consideration when setting up workflows to make remote sampling with the SabIR as efficient as possible. Sample parameters and specifications are highly dependent on the sample type, the amount of time available to collect data, and the level of interest in different spectral characteristics. This section contains recommendations for starting points when specifying collect event parameters, sample specifications, and background specifications.

See "Chapter 5 Workflow Events and Specifications" in your *RESULT User's Guide* for more information about the items mentioned in this section.

Collection event parameters

A collection event in RESULT Integration software instructs the instrument to collect a spectrum of a sample. The following table contains the recommended starting points for sample collection parameters for the SabIR probe:

Parameter	SabIR Setting
Number Of Sample Scans	30
Data Format	Log (1/R)
Background Frequency	Every Hour

- **Number Of Sample Scans.** To start, try using 30 scans. You can then decrease the number of scans to the smallest number that can still produce tolerable signal-to-noise (determined by error of prediction or pre-defined limit) if sampling time is at a premium. If using a higher resolution, the spectra will contain more spectral noise, so you may need to increase the number of scans to better distinguish sample features from noise.

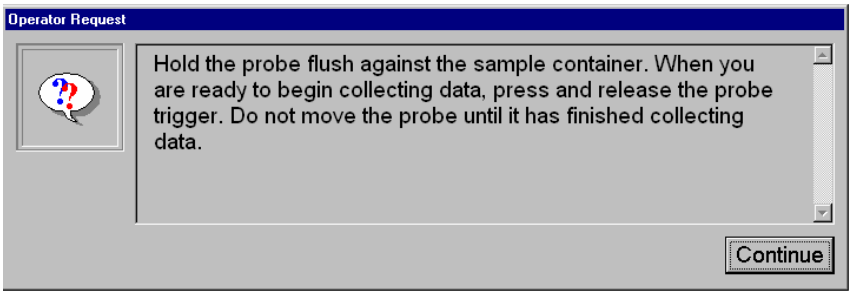
  If sampling time is scarce, you may want to take into consideration the ratio between the number of scans and resolution. See the table in the "Sample Specifications" section of "Chapter 5 Workflow Events and Specifications" in your *RESULT User's Guide* for estimates of collection times based on the number of sample scans and resolution settings.

- **Background Frequency.** If collecting samples only periodically, then collecting a background before every sample is recommended. If collecting many samples at a time, then collecting a background every hour should be sufficient.

Operator prompts

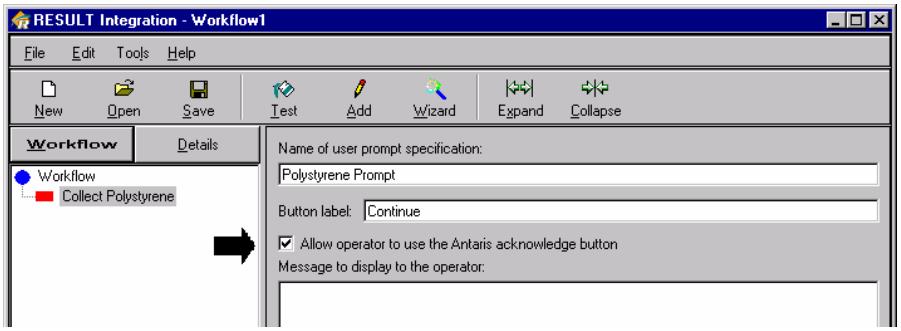
When developing a workflow in RESULT Integration software, the collection event allows you to include operator prompts for both sample and background collection.

When adding a collection event to a workflow, you may want to consider including detailed prompts to assist the operator in properly collecting the data. An example prompt is shown below.



Make sure your prompts include specific information about the application. If the operator is required to reposition the sample, for example, if you've created a repeat loop in a workflow to collect multiple samples of a large quantity of a substance, it is recommended that you prompt the operator each time the SabIR needs to be repositioned.

If the operator will be performing true remote sampling and sampling time is at a premium, you may want to make sure the operator can respond to prompts by pressing the probe trigger. You can do this by leaving the Allow Operator To Use Antaris Acknowledge Button check box enabled in each User Prompt Specification in the software.



If you are using the instrument's internal Spectralon reference, you should include a background prompt. The sensor inside the probe holster will detect whether the SabIR is inserted. If the SabIR is not inserted into the holster properly, then the software will prompt the operator to insert the probe into the holster.

However, if using an external reference for background collection, it is recommended that you include a detailed operator prompt to ensure that the background data is collected properly.

Sample specifications

In RESULT Integration software, a Sample Specification is used to specify advanced collection parameters to optimize the workflow based on a sampling technique. Sample specifications are attached to collection events in workflows. The following table contains the recommended starting points for sample specifications:

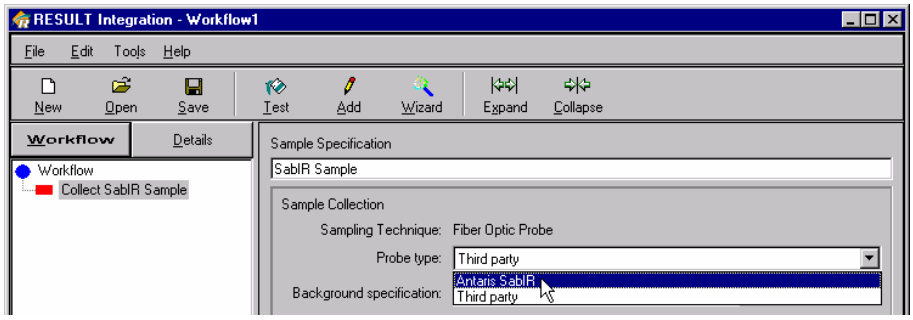
Specification	SabIR Setting
Attenuator	Empty
Resolution	8 cm^{-1}
Gain	1x
Spectral Range	10,000-4,000 cm^{-1}

- **Gain and Attenuator.** You may want to begin with a Gain setting of 1x and an Attenuator setting of Empty. If these settings do not produce the results you are looking for, you may want to use RESULT Integration's Optimize Gain feature to determine the appropriate gain and attenuator settings for your sample. If you use the Optimize Gain feature, the software will scan the sample material using each possible combination of gain and attenuator parameters to find the settings that produce the best results.

  For more information about using the Optimize Gain feature, see the Sample Specification information in "Chapter 5 Workflow Events and Specifications" in your *RESULT User's Guide*.

- **Resolution.** Try 8 cm^{-1} as a starting point. You can increase the resolution (e.g., from 8 cm^{-1} to 4 cm^{-1}) if required by your sample and then increase the number of scans to provide tolerable signal-to-noise. You can try a lower resolution to trade off resolution for signal-to-noise.

- If using an internal reference for background collection, make sure you have selected Antaris SabIR as the Probe Type in the Sample Specification.

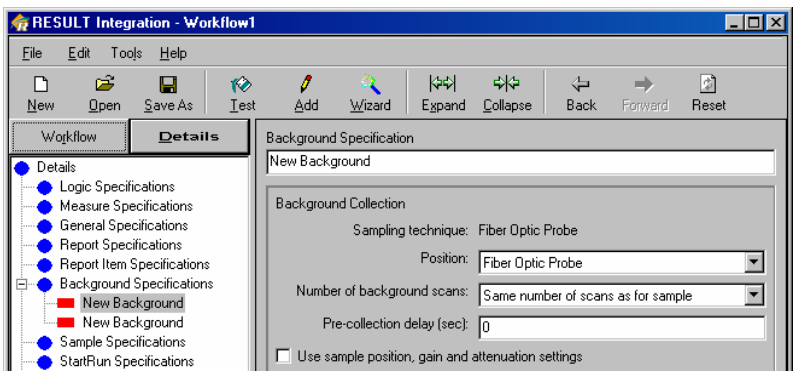


Selecting this option will enable the software to detect when the probe is properly inserted into the holster on the instrument and the software will automatically collect background spectra at the frequency you specify.

If the operator will be sampling very large items, for example, raw material powders that arrive in large barrels, you may want to add repeat events to your workflow so the operator can insert the accessory into different areas of the sample. The spectra produced can be measured to check *homogeneity*, and/or averaged to produce a representative spectrum of a non-homogenous sample. See "Structural workflow events" in "Chapter 5 Workflow Events and Specifications" in your *RESULT User's Guide* for more information about using repeat loops in workflows.

Background specifications

The settings in the Background Specification are affected by whether you will be using an external or internal reference for background collection. If you plan to use an external reference for a diffuse-reflection background, chooe the gain setting based on the most reflective material.



The following table shows the different default gain and attenuator settings that are used with the fiber optic module (with and without the SabIR probe) when the Use Sample Position, Gain, And Attenuation Settings check box is not selected.

Sampling Technique	Background Position	Default Gain Setting	Default Attenuator Setting
Fiber Optic Module using third party probe	Fiber optic module measured with third party probe using external reference	1x	Uses sample Attenuator setting
Fiber Optic Module using SabIR probe	Fiber optic module measured with SabIR probe using internal Spectralon reference	1x	Empty
Fiber Optic Module	Transmission module measured from center position of sample holder (no background material)	1x	C screen
Fiber Optic Module	Transmission module using external reference in rear position of sample holder	1x	C screen
Fiber Optic Module	Integrating sphere using the internal gold reference (reference flag in closed position)	1x	C screen
Fiber Optic Module	Integrating sphere using external reference (reference flag in open position)	1x	C screen

*These settings are applied when Use Sample Position, Gain And Attenuation Settings check box is cleared or unavailable (greyed out) in the software.

Default Attenuator and Gain settings for background collection

If your background spectrum is taken with a channel that is different from that used for taking sample data, you can use a transfer correction. (This situation typically occurs when samples are measured in process applications where the sample is difficult or inconvenient to remove for normal background measurements at the sample location.) The transfer correction requires a transfer spectrum, which is a ratioed spectrum produced from two single-beam background measurements taken at the alternative background location (numerator) and the sample location (denominator). In essence, the transfer spectrum represents the inherent differences between the two beam paths. The ratio of the single-beam

spectra of the sample and background can be multiplied by the transfer spectrum to correct for any artifacts (peaks or peak shapes) in the spectra that are due solely to the change in beam path. See "Sample correction specifications" in "Section 5 Workflow Events and Specifications" in your *RESULT User's Guide* for more detailed information about using transfer corrections.

Disconnecting the SabIR

It is not necessary to disconnect the SabIR after each use. However, if you are not going to be using the probe for a long period of time, or if you need to remove it to attach a different accessory, take the following steps to disconnect the probe:

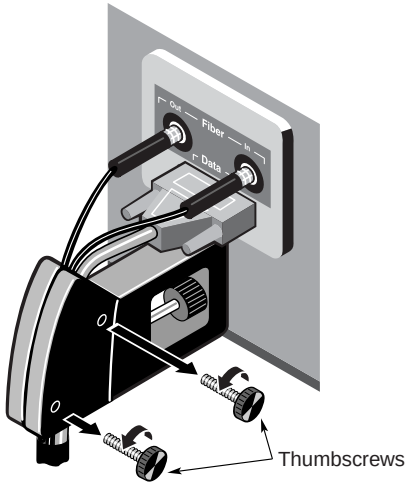
Notice Because the probe and the module have an electrical connection, it is recommended that you power off the instrument before disconnecting the probe to avoid a possible electric charge that may damage the electronics. Each time you power off the instrument, be sure to log off any software applications. ▲

1. **Insert the probe into the holster.**

   Inserting the probe into the holster before connecting and disconnecting the probe will prevent causing strain on the fiber optic cables from the weight of the SabIR.

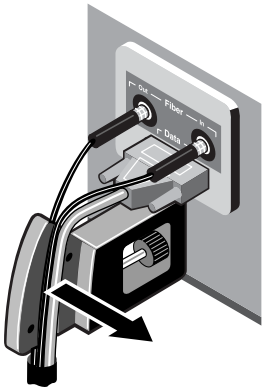
2. **Remove the strain relief cover.**

   Remove the two thumbscrews on the cover by turning them counterclockwise, and then remove the cover.



Notice Do not excessively bend the fiber optic cables. Excessively bending the cables can damage the optical fibers. ▲

3. **Gently remove the cables from the groove in the strain relief base.**



It is not necessary to remove the strain relief base.

Notice Do not use tools to loosen the thumbscrews. ▲

4. **Disconnect the SabIR fiber optic cable connectors from the fiber optic ports on the module.**

5. **Unscrew the thumbscrews and disconnect the SabIR electrical connector from the electrical port on the module.**

6. **Replace the protective caps on the probe tip, the ends of the cables, and the fiber optic ports (if another fiber optic accessory is not being installed).**

7. **Replace the strain relief cover and thumbscrews on the strain relief mechanism.**

Note When reconnecting the SabIR probe, you can remove the strain relief cover. After the probe is reconnected, insert the fiber optic cables into the strain relief mechanism and the replace the strain relief cover. ▲

Storing the SabIR

Store the SabIR probe in a dust-free environment such as a cabinet or box. If coiling the cables, make sure the cables are not coiled in a diameter of less than 30 cm to prevent damage to the cables and optical fibers. Keep the protective caps on the ends of the cables and on the probe tip while the probe is in storage.

Common problems with spectral data

Before using any fiber optic accessory for precise quantitative analysis, evaluate the effects of temperature, position of the fiber optic cables, and sample contact on spectral features. Other items that may influence spectra are problems with optical fibers, improper collection of a background, improper collection of a sample, the amount of noise, and sample particle size, homogeneity, and concentration.

If you encounter a problem, before running any other diagnostics or deeming backgrounds or samples as “bad” you may first want to check the following items:

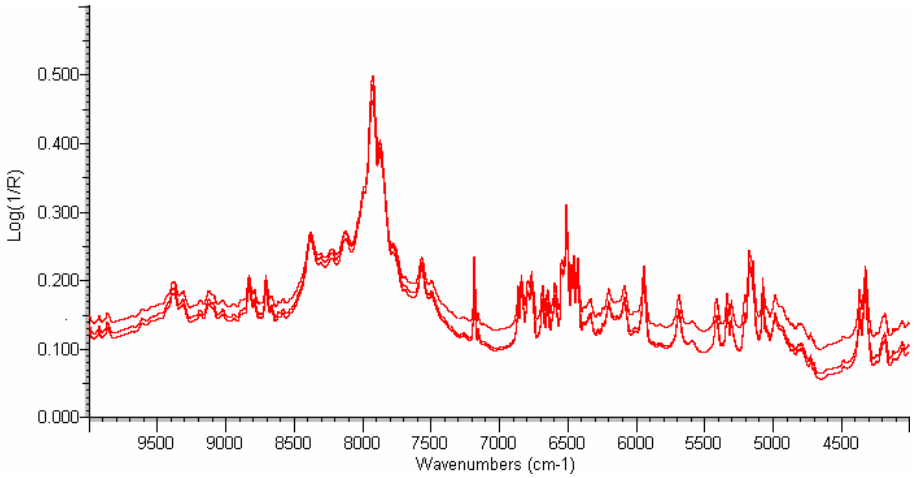
- Make sure the fiber optic accessory is properly attached to the fiber optic ports. Make sure the cables on the accessory have been consistently attached to the same In and Out ports on the module.
- Check the fiber optic accessory connections to the fiber optic ports. The connections should be finger tight. You may want to remove and re-attach the accessory before attempting to recollect the sample.

Notice Do not over tighten the connections or use tools to tighten the connections. Over tightening or using tools may damage the connectors on the accessory or the fiber optic module. ▲

Problems with optical fibers

If the signal-to-noise or predictive ability of your method is failing, you may want to inspect the fibers in the fiber optic cables. Optical fibers are delicate and can be easily damaged, which can create subtle differences in your spectra or measurement results.

Moving or bending fiber optic cables during data collection may also affect your spectral data. The following example shows three spectra collected with the SabIR, with the fiber optic cables in a different position during each collection:



Note that the difference in the cable positions caused subtle changes in the baseline of each spectrum. When sampling, it is recommended that you attempt to collect data with the fiber optic cables in the same position each time, to help ensure data consistency.

Problems with background spectra

If a background spectrum you collected is atypical from previously-collected backgrounds or from the typical spectrum described in the "Collecting the background" section of this chapter, the problem may be one of the following:

- If using the SabIR and the internal Spectralon sample, it is possible that:
  - The Spectralon sample may be dirty or contaminated. Follow the instructions in "Maintaining the Spectralon Background Reference" to clean the sample.
  - The probe window may be dirty. Follow the instructions in "Cleaning the SabIR" to clean the probe window.
  - The SabIR was not properly inserted into the holster. Make sure the SabIR is properly inserted into the holster and retake the background measurement. The SabIR is properly inserted into the holster when you hear it "click" in place.
- If you were not using the internal Spectralon sample as the background material, it is possible that:

- The sample material could have been run as the background.
- The fiber optic accessory was not held flush against the background sample.
- The fiber optic accessory was moved while it was collecting data.

For all problems above, it is recommended that you take test backgrounds using either the Quick Collect (not associated with a workflow) or Test Background (following the steps for background collection in a workflow) features in RESULT Operation software before running the workflow in production mode.

If you are using a sampling accessory other than the SabIR probe, see your accessory documentation for other suggestions related to problems with background spectra.

Problems with sample spectra

Several factors may affect a sample spectrum. Before deeming the sample as "bad," rescan the sample in a diagnostic mode, either by running the workflow offline, using the Test Sample feature, or using the Quick Collect feature in RESULT Operation software.

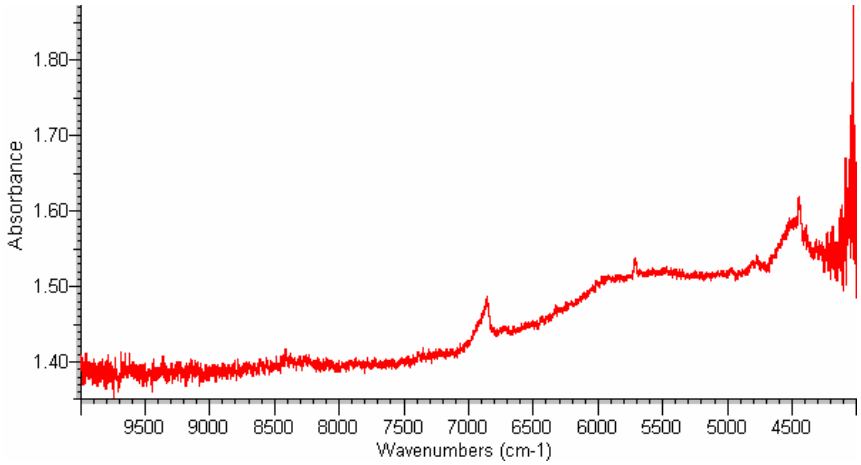
While you are using the diagnostic features, make sure none of the following occur:

- If using the SabIR, do not press the trigger prematurely. Keep your fingers alongside the probe and away from the trigger on the SabIR until you are ready to start collecting data.
- Do not move the sampling accessory while it is collecting data. Hold the accessory in a comfortable position, and do not collect more scans than necessary. Do not remove the accessory from its sampling position until data collection is complete.

The following sections contain information about specific problems with spectra and some suggestions for possible causes and resolutions. If you are using a sampling accessory other than the SabIR probe, also refer to your accessory documentation for other suggestions related to problems with sample spectra.

Spectrum with high noise

A spectrum that contains a high amount of *noise* can resemble the following:



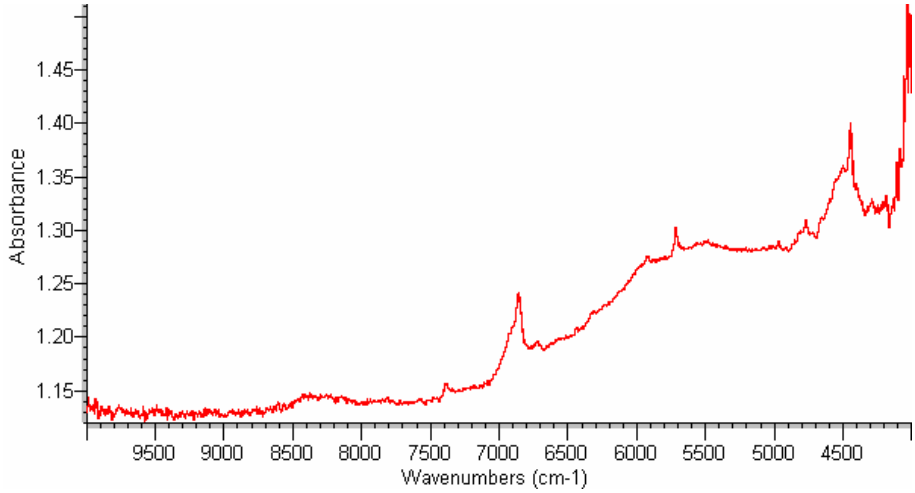
Ascorbic acid spectrum with high noise using the SabIR

As shown above, the high level of noise is represented as very sharp peaks in a spectrum that go above and below the baseline.

If you experience this problem, the accessory may not have been held close enough to the sample. If, after repeating the experiment and holding the accessory closer, the problem is not solved, you may want to increase the number of scans or lower the resolution to decrease the amount of noise in the sample. You can also try increasing the detector gain. Finally, check to make sure any attenuation screens that are in place are needed. If they are not needed, remove them.

Shifted baseline

A spectrum with a shifted baseline may resemble the following:



Ascorbic acid with SabIR probe held too far from sample

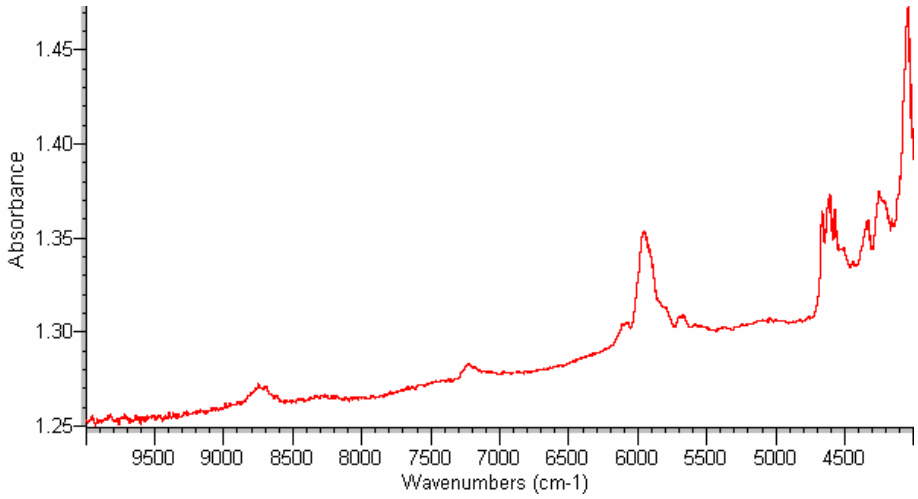
The best baseline would begin at 0.0 absorbance units. However, as shown above, the baseline shifted up from 0.0 absorbance units and the relative intensities of the peaks are smaller. If you experience this problem, one of the following may have occurred:

- The accessory was held too far away from the sample or the tip of the accessory was not held flush against the sample.
- If sampling a solid, the sample material may be too thin.
- If sampling a powder, you may not have enough of the sample or the accessory may have been inserted too far into the powder, so not enough of the powder was underneath the probe tip.

Attempt the scan again in a diagnostic mode. Make sure the accessory tip is against the sample and at the proper angle (flush with the sample if using the SabIR). Do not move the accessory until it has finished collecting data.

Samples not appropriate for the SabIR

If you are using the SabIR with the fiber optic module, be aware that some solid samples may not be diffuse enough to use with the SabIR diffuse-reflection probe. Samples that are diffuse typically have a rough surface. An example spectrum of a smooth sample may resemble the following:



Spectrum of a thin polystrene film using the SabIR

As shown above, the baseline is high because very little light diffused and reflected back into the probe. The spectral features are small. The wavelike pattern in the spectrum was caused by optical interference with the front and back surfaces of the thin film of polystyrene. For this type of sample, you may want to try another sampling technique, such as transmission.

Sample particle size, homogeneity, and concentration

Particle size, *homogeneity*, and concentration all affect the quality of spectra. Changes in particle size can affect scattering and may have ramifications on the effective pathlength. This can cause differences in *band* intensity.

The quality of your spectrum will be most affected if there are extreme differences in particle size throughout the sample (for example, a sample containing particles smaller than 3 microns and above 500 microns).

Homogeneity can affect reproducibility. The degree of heterogeneity in a sample should be taken into consideration when determining the number of collection event repetitions to include when creating a workflow, so you can achieve a representative spectrum of the sample. The spectral data will probably be of good quality, but each individual spectrum may not be representative of the sample as a whole.

Concentration does not affect *signal-to-noise* in a spectrum. Signal-to-noise can, however, become more of a factor when working with lower concentrations of a sample.

To keep these types of problems at a minimum, consider adding repeat loops in workflows so that data can be collected from different areas of the sample. The spectra produced can be measured to check homogeneity and/or averaged to produce a representative spectrum. See "Chapter 5 Workflow Events and Specifications" in your *RESULT User's Guide* for more information about utilizing these features.

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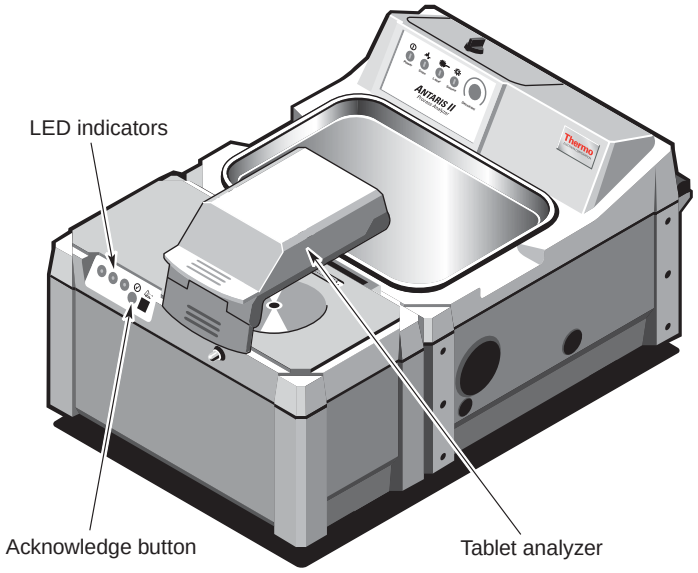
Chapter 6 Tablet Analyzer Module

The Antaris II tablet analyzer sampling module is a powerful, fast, and easy-to-use tool for sample uniformity verification in the industrial environments of the pharmaceutical, chemical, polymer, and food and beverage industries. The module allows you to analyze tablets and other solids using both transmission and diffuse-reflection sampling techniques. You can also use the module in conjunction with the integrating sphere to sample solids and powders.

This chapter discusses how to test and use the tablet analyzer sampling module and optional sampling accessories. It also includes steps to conduct simple transmission and diffuse-reflection experiments, information about typical spectra obtained using both sampling techniques, and some common problems with spectral data and suggestions for resolving them.

Introduction

The Antaris II tablet analyzer sampling module is designed to work with Thermo Scientific RESULT Integration and RESULT Operation software to provide a powerful, fast, and easy-to-use system to analyze tablets and other small solids using transmission sampling techniques. The tablet analyzer can also be used in conjunction with the integrating sphere sampling module to collect diffuse-reflection data from larger solids and powders.



Module features

The important features of the tablet analyzer module include:

- **Tablet analyzers.** The sampling module can use either of the following tablet analyzers to conduct transmission sampling experiments:

  - **Standard tablet analyzer.** This analyzer is recommended for use with dense materials, such as opaque tablets, because it has a narrow band, high-sensitivity InGaAs detector, and covers a spectral range of 12,000-5,880 cm^{-1} (833-1,700 nm).

  - **Softgel tablet analyzer.** This analyzer is recommended for use with samples that are better transmitters, such as softgel capsules, paper, plastics, packaging materials, and polymers. It has a broad-band InGaAs detector and covers a spectral range of 12,000-3,800 cm^{-1} (833-2,630 nm).

  The tablet analyzers are similar to each other in appearance and can accommodate a sample up to 9.8 cm in diameter.

- **Simultaneous diffuse-reflection and transmission data collection.** When a tablet analyzer is used with the integrating sphere, diffuse-reflection and transmission data can be collected simultaneously.

- **Tablet holder kit.** The tablet holder kit contains one universal tablet holder and two custom tablet holders that can be modified to exact tablet dimensions, along with a centering ring for the custom tablet holders.

- **Optional viscous liquid sampler.** The viscous liquid sampler (VLS) can be used to collect transflectance spectra from viscous liquids using the integrating sphere. If the system is equipped with a tablet analyzer, the VLS can also be used for transmission analyses. The apparatus is designed to handle thick, concentrated samples with little mess and quick, easy cleanup. It fits on the sample accessory holder or the tablet analyzer base.

Installing and removing the tablet analyzer

Because the standard tablet analyzer and the softgel tablet analyzer are similar to each other in appearance, you can follow the same procedure for installing and removing either of the tablet analyzers.

Note Because the tablet analyzer has an electrical connection, it is recommended that you power off the instrument while installing and removing the tablet analyzer to avoid possible damage to the electronics. Each time you power off the instrument, be sure to log off any software applications. ▲

Installing a tablet analyzer

To install a tablet analyzer to the sampling module:

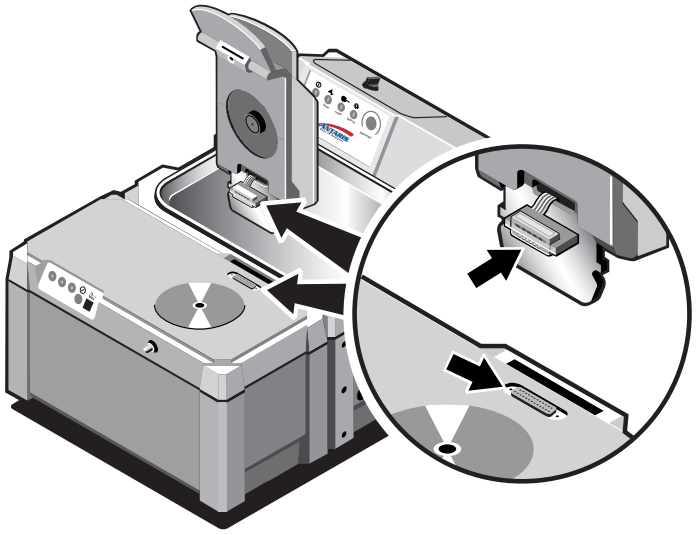
⚠ Caution The lid of the tablet analyzer has a magnetic closure, and closes tightly. Keep your fingers clear of the inside of the tablet analyzer when closing it to avoid getting your fingers pinched. ▲

Notice To avoid damaging the flexible light shield and detector, make sure all sampling accessories (such as the universal tablet holder) are removed from the tablet analyzer before you place the tablet analyzer on the instrument. ▲

1. **Close the lid of the tablet analyzer.**

2. **Inspect the data port on the instrument and the connector on the tablet analyzer.**

   Make sure there is no debris on the male connectors on the tablet analyzer and there is nothing clogging the female connector on the top of the instrument.

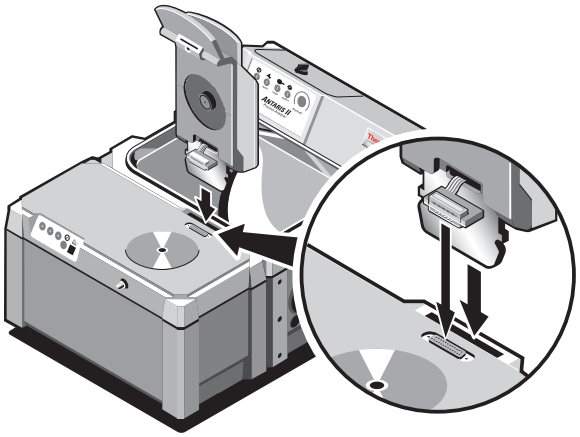


Notice If there is debris clogging the female connectors on the data port, do not unclog the port yourself. Contact Thermo Fisher Scientific Technical support. ▲

3. **With both hands, hold the tablet analyzer upright with the base facing you.**

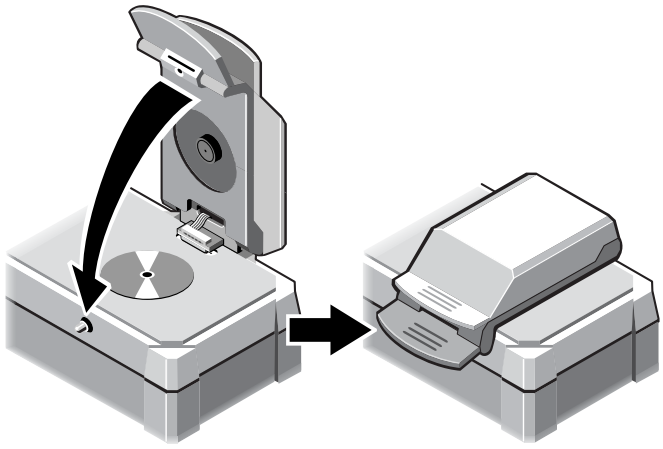
   The silver connector hinge should be facing downward and the connector should be visible.

4. **Insert the connectors into the slot and data port on the instrument.**



   The tablet analyzer is properly connected to the electrical port when you hear it "click" in place and the tablet analyzer is firmly seated.

5. **Gently set the tablet analyzer down on the top of the instrument.**



⚠ Caution The tablet analyzer fits tightly onto the instrument. To avoid pinching your fingers, keep your fingers clear of the tablet analyzer base when pressing on the latch. ▲

6. **Firmly press down on the latch on the tablet analyzer base until it connects into place.**

   If the latch does not close or it will not lie flush against the instrument, or if the tablet analyzer bottom is not resting flatly on top of the instrument, remove the tablet analyzer and attempt to install it again.

Note The tablet analyzer can remain on the instrument at all times unless it is necessary to remove it to sample large items using the integrating sphere, attach a different tablet analyzer or the *sample accessory holder*, or to replace internal parts in the instrument. ▲

Note Because the tablet analyzer has an electrical connection, it is recommended that you power off the instrument while installing and removing the tablet analyzer to avoid possible damage to the electronics. Each time you power off the instrument, be sure to log off any software applications. ▲

Removing a tablet analyzer

To remove a tablet analyzer from the sampling module:

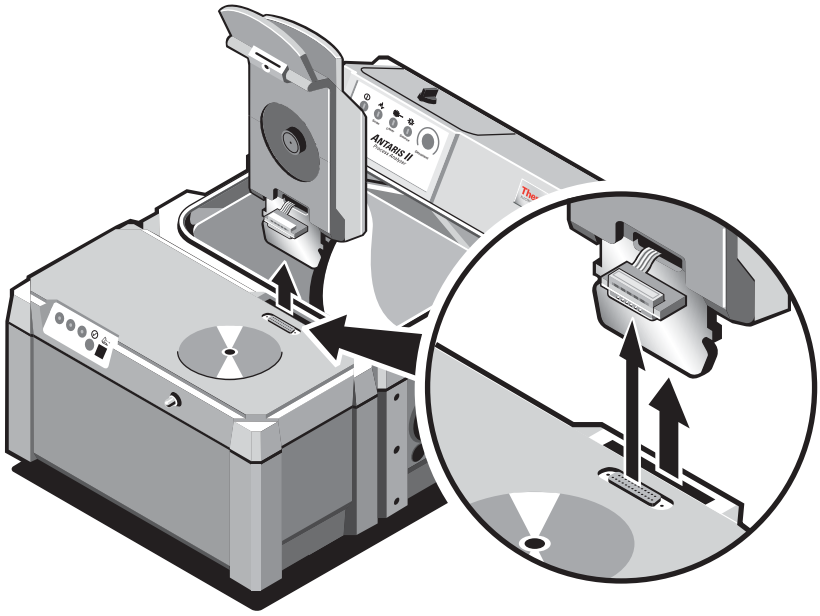
To remove a tablet analyzer:

1. **Remove all sampling materials and accessories from the tablet analyzer and close the tablet analyzer cover.**

2. **Release the latch on the tablet analyzer bottom, and lift the tablet analyzer until it is perpendicular to the instrument.**

   Pull the latch up to release the spring-loaded ball and groove connection.

3. **Carefully pull up on the tablet analyzer to detach the connector from the data port and remove the silver hinge from the sleeve in the instrument.**



Testing the sampling module

RESULT Operation software contains an Instrument Check feature that runs an instrument performance test. Before running the performance test, install the tablet analyzer, power on the instrument and make sure the instrument has remained on for at least an hour to stabilize.

Note If you plan to collect both transmission and diffuse-reflection data from tablet samples, it is recommended that you run an instrument check on both the tablet analyzer and integrating sphere sampling modules. ▲

To run an instrument check:

1. **Log on to RESULT Operation software.**

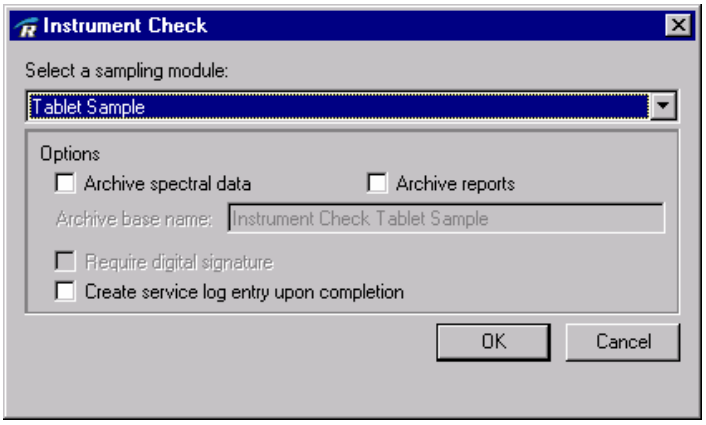
   See "Starting RESULT software" in the "Antaris sampling" chapter for instructions to log on to the software.

2. **Choose the Maintenance menu from the Result Operation main window.**

Note If the Maintenance menu does not appear in the RESULT main window, then you cannot access the Instrument Check feature. See your RESULT software administrator. ▲

3. **Select Instrument Check from the Maintenance menu.**

The software will open the Instrument Check dialog box.



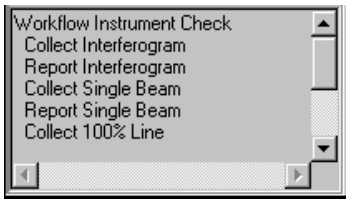
4. **Select the appropriate module from the Select A Sampling Module drop-down list.**

   To test the tablet analyzer, choose either the Tablet Sample (for the standard tablet analyzer) or the SoftGel Sample option, depending on the type of tablet analyzer on your sampling module. To test the integrating sphere, select the Integrating Sphere Sample option.

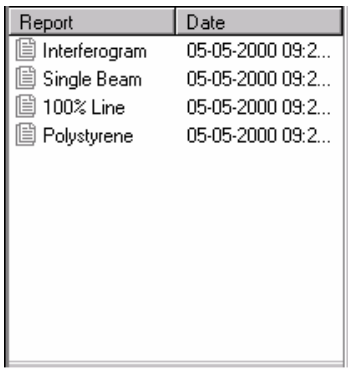
Note When using the Instrument Check feature for a tablet analyzer, be sure to select the appropriate module from the Select A Sampling Module Drop-down List for the tablet analyzer you are using. If you select the incorrect module, the instrument check will still run, but the data produced may be affected. ▲

5. **Choose OK to start the instrument check.**

   While the instrument check is running, the status indicator on the lower left side of the RESULT Operation main window will indicate the status of the instrument check.



   As each spectrum is collected, the software will create a report. The title of each report will appear in the report navigation frame.



You can view a report by selecting the report name, and the selected report will open in the display area.

See "Chapter 5 System Maintenance" of "Section 3 RESULT Operation Software" in your *RESULT User's Guide* for information about archiving the instrument check data, requiring digital signatures for the data, and creating a service log entry of the check. The System Maintenance chapter also contains example spectra with a description of each.

Sampling techniques

The instrument contains one detector for transmission sampling through the tablet analyzer. Your system may have the standard tablet analyzer, the softgel tablet analyzer, or both. (See "Transmission sampling techniques" in the "Transmission Module" chapter for more information about transmission sampling.)

Using both diffuse-reflection and transmission

Diffuse-reflection and transmission can give complementary information in an experiment. The Antaris II standard tablet analyzer sampling module along with the integrating sphere sampling module and RESULT software allow you to use one workflow to perform transmission and diffuse-reflection sampling simultaneously, without needing to reposition your sample. (Simultaneous diffuse-reflection and transmission collection is supported in RESULT workflows but not by the Quick Collect feature.)

Transmission and diffuse-reflection sampling techniques work especially well with layered samples, like coated tablets. The diffuse-reflection experiment can provide you with a spectrum of the outer coating, and the transmission experiment can provide you with spectral information about the tablet's internal composition. For more information, see "Tips for developing workflows" in this chapter.

Note The maximum sampling speed of the tablet analyzer is slower than that of the integrating sphere. So, when performing simultaneous diffuse-reflection and transmission sampling, the integrating sphere operates at the slower mirror velocity of the tablet analyzer. This is because the instrument cannot collect data at two different speeds simultaneously. ▲

Compatible sample types

The Antaris II tablet analyzer sampling module is designed for fast and easy sampling in the industrial environments of the pharmaceutical, chemical and polymer industries. Depending on the type of sampling technique, the module can be used with tablets, solids, and powders.

The tablet analyzer was specifically developed for transmission experiments of tablets. However, it can also be used with small solids that will fit inside the tablet analyzer, such as packaging materials, polymers, and paper. Compatible sample types vary depending on whether you are using the standard tablet analyzer or the softgel tablet analyzer:

- **Standard tablet analyzer.** The standard tablet analyzer has a high-sensitivity detector, but a narrower spectral range. It works well for strongly absorbing or thick materials, such as opaque tablets or heavy bond paper.

- **Softgel tablet analyzer.** The softgel tablet analyzer has a wider spectral range. It works well for thinner or less absorbing materials, such as softgel capsules, paper, plastics, packaging materials, and polymers.

The items compatible with the softgel tablet analyzer can also be used in the standard tablet analyzer, but the spectral range will be limited to approximately 12,000-5,880 cm-1 when using the standard tablet analyzer.

Note For information about samples that are compatible with the integrating sphere, see “Compatible sample types” in the “Integrating Sphere Module” chapter. ▲

Your first experiment

This section goes through two simple experiments using the integrating sphere and tablet analyzer along with the Quick Collect feature in RESULT Operation or RESULT Integration software to produce both a diffuse-reflection and transmission spectrum of a tablet.

The Quick Collect feature in RESULT software allows you to collect a background and/or sample spectrum for investigation and sample setup without developing and running a workflow. Using Quick Collect is good practice to help you "get the feel" of sampling with the tablet analyzer module before using the module in actual production workflows. Quick Collect also allows you to easily produce a spectrum without having to develop a workflow for a single collection event.

These experiments are designed to give you a basic understanding of using both the tablet analyzer and integrating sphere, and how the two types of experiments can easily be conducted simultaneously.

Before you begin

Before you begin the experiment:

- Install the tablet analyzer on the instrument. See "Installing and removing the tablet analyzer" earlier in this chapter for instructions.
- The collection parameters in the experiment should produce a readable spectrum if you use one of the following samples:
  - If using the standard tablet analyzer, a round, non-coated 325 mg aspirin tablet.
  - If using the softgel tablet analyzer, a blank piece of white paper or a Post-It® note large enough to cover the integrating sphere window on the module.

  If you select a different type of tablet, your results may differ greatly, depending on how the sample material works with the recommended collection parameters in this experiment.
- Have the sample material and the universal tablet holder at hand, if using the standard tablet analyzer.

Transmission experiment

The first experiment involves producing a transmission spectrum using the tablet analyzer. This experiment covers collecting a background, preparing a typical tablet sample, and collecting sample data to produce a spectrum.

Setting up the experiment

To begin your first experiment:

1. **Start RESULT Integration or RESULT Operation software.**

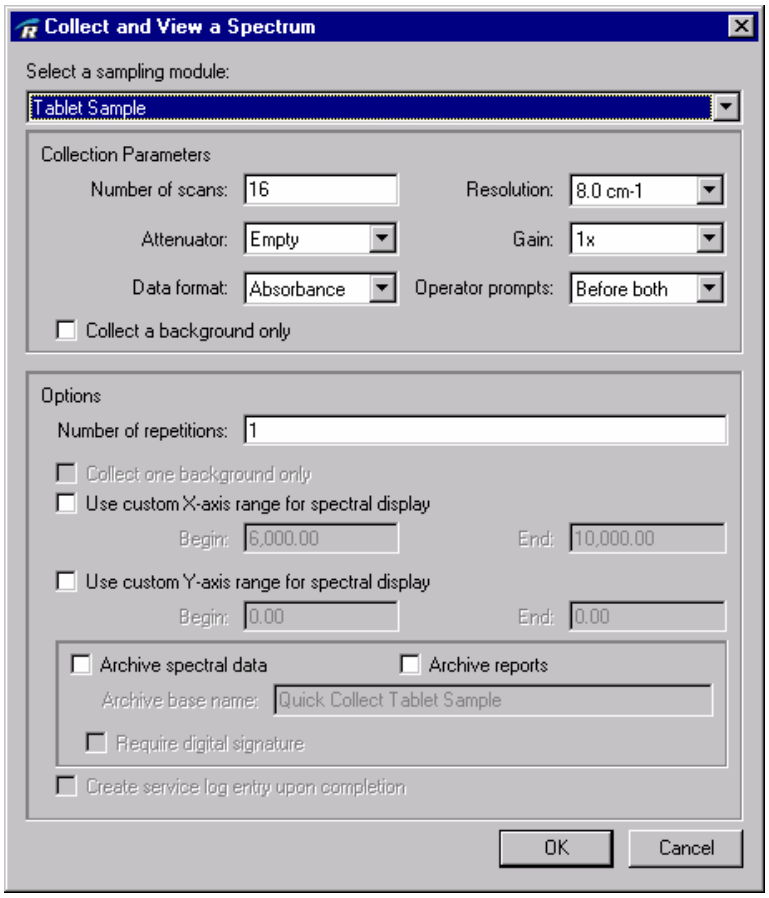
   See "Starting RESULT software" in the "Antaris sampling" chapter for instructions to log on to the software.

2. **Open the Quick Collect dialog box.**

   Quick Collect can be opened from the Tools menu in Result Integration or from the Maintenance menu in Result Operation.

Note If you are using RESULT Operation and the Maintenance menu does not appear in the menu bar of the main window, then you cannot access the Quick Collect feature. See your RESULT software administrator. ▲

The Quick Collect dialog box should appear.



3. **Select the Tablet Sample or SoftGel Sample (depending on the type of tablet analyzer you have) option from the Choose A Sampling Module drop-down list.**

4. **For purposes of this experiment, confirm that the following Collection Parameters are set:**

Parameter	Setting
Number Of Scans	50
Resolution	16 cm^{-1}
Gain	1x
Attenuator	Empty
Data Format	Absorbance
Operator Prompts	Before Both Background And Sample

Note Selecting the Before Both Background And Sample parameter from the Operator Prompts drop-down list means that the software will prompt you when to start collecting the background data and when to start collecting the sample data. ▲

5. **Choose OK to begin the experiment.**

   Do not change any other options for this experiment. For more information about the other options in the Quick Collect dialog box, see "Chapter 5 System Maintenance" of "Section 3 RESULT Operation Software" in your *RESULT User's Guide*.

Collecting the background

The background collection is conducted by simply collecting data through the tablet analyzer without having the sample in place. The software will prompt you when it is time to collect the background.

To collect the background:

1. **If the cover of the tablet analyzer is not already closed, close the cover of the tablet analyzer.**

   The tablet analyzer can be empty, or it can have the universal tablet holder in it, so long as the iris of the tablet holder is completely open

and no sample is in place. Open the black iris adjustment by turning it clockwise.

2. **Choose OK from the prompt in the software or press the Acknowledge button on the instrument's operation panel to begin collecting data.**

   You can view the status of the background collection in the status indicator box in the software.

Notice Do not open the tablet analyzer cover while the instrument is collecting data, as it will affect the quality of your background spectrum. ▲

The background spectrum will remain in memory and will be used to process the sample spectrum.

Preparing and collecting the sample

After you have finished collecting the background data, the software will prompt you to collect sample data.

To prepare and collect the sample:

1. **Open the cover of the tablet analyzer.**

   Make sure the instrument is not collecting data before you open the cover. The status indicator in the software will let you know if the instrument is collecting data.

2. **Insert the sample into the tablet analyzer.**

   If using a sheet of paper with the softgel tablet analyzer, make sure the paper is large enough to cover the entire sample window.

If using an aspirin tablet with the standard tablet analyzer, use the universal tablet holder to position the tablet. To install the universal tablet holder:

- Place the universal tablet holder in the tablet analyzer base. The notch in the universal tablet holder aligns with the pin in the tablet analyzer base to secure it in place.
- Open the black iris adjustment by turning it clockwise.
- Place the tablet you want to analyze in the center of the universal tablet holder.
- Adjust the height of the iris so it is approximately at the center of the tablet's width, by turning the silver height adjustment ring clockwise or counterclockwise to lower or raise it, respectively.
- Slowly turn the black iris adjustment counterclockwise to secure the tablet in place.

Notice Do not over-tighten the iris. Over-tightening the iris may damage the universal tablet holder or the sample. ▲

Note See "Sampling tablets using the universal tablet holder" in the "Integrating Sphere Module" chapter for more information about installing and using the universal tablet holder. ▲

3. **Close the cover of the tablet analyzer.**

   The sample is now ready for data collection.

4. **Choose OK from the prompt in the software or press the Acknowledge button on the instrument's operation panel to begin collecting data.**

   You can view the status of the collection in the status indicator box in the software.

Notice Do not open the tablet analyzer cover while the instrument is collecting data. Opening the cover before the instrument has finished collecting data may affect your spectral data. ▲

When the instrument has finished collecting data, the software will display the spectrum in the display area.

Keep the sample in place and the tablet analyzer installed to perform the next experiment. Do not close RESULT software.

Diffuse-reflection experiment

This second experiment involves producing a diffuse-reflection spectrum using the integrating sphere. The base of the tablet analyzer can act as a sample holder when collecting diffuse-reflection data. This experiment covers collecting a background using the instrument's internal reference and then collecting sample data to produce a spectrum.

Setting up the experiment

To set up the experiment:

1. **Open the Quick Collect dialog box in the software.**

   To open the dialog box, choose the Quick Collect option from the Tools menu in RESULT Integration or from the Maintenance menu in RESULT Operation.

2. **Select the Integrating Sphere Sample option from the Select A Sampling Module drop-down list.**

3. **For purposes of this experiment, confirm that the following Collection Parameters are set:**

Parameter	Setting
Number Of Scans	30
Resolution	8 cm^{-1}
Gain	1x
Attenuator	Empty
Data Format	Log (1/R)

4. **Select the None option from the Operator Prompts drop-down list.**

   Because the sample is already in place and does not need to be removed to collect a background spectrum using the integrating sphere's internal reference, it is not necessary to be prompted to begin collection.

Note If the sample is not in place from the previous experiment, place the sample on the integrating sphere window before choosing OK to begin the experiment. ▲

5. **Choose OK to begin the experiment.**

   Do not change any other options for this experiment. For more information about the other options in the Quick Collect dialog box, see "Chapter 5 System Maintenance" of "Section 3 RESULT Operation Software" in your *RESULT User's Guide*.

Collecting the background

It is not necessary to remove the sample or close the tablet analyzer cover when collecting the background. An internal flag will close beneath the integrating sphere's sapphire window and the instrument will collect background data using the internal reference.

You may hear the flag below the integrating sphere window "click" closed before the instrument begins collecting the background data. You can view

the status of the background collection in the status indicator box in the software.

When the instrument has finished collecting the background, you may hear the flag inside the integrating sphere "click" open.

Collecting the sample

The instrument will automatically begin collecting sample data after it has completed collecting the background data. You can view the status of the data collection in the status indicator box in the software. When the instrument has finished collecting data, the software will display the spectrum in the display area.

When you have finished the experiment, open the tablet analyzer and remove the sample. If using the universal tablet holder, remove the holder from the tablet analyzer.

If the flexible light shield or the universal tablet holder in the tablet analyzer collects residue from the sample, follow the instructions for cleaning these items in the "Maintenance and Service" chapter.

Typical transmission and diffuse-reflection spectra

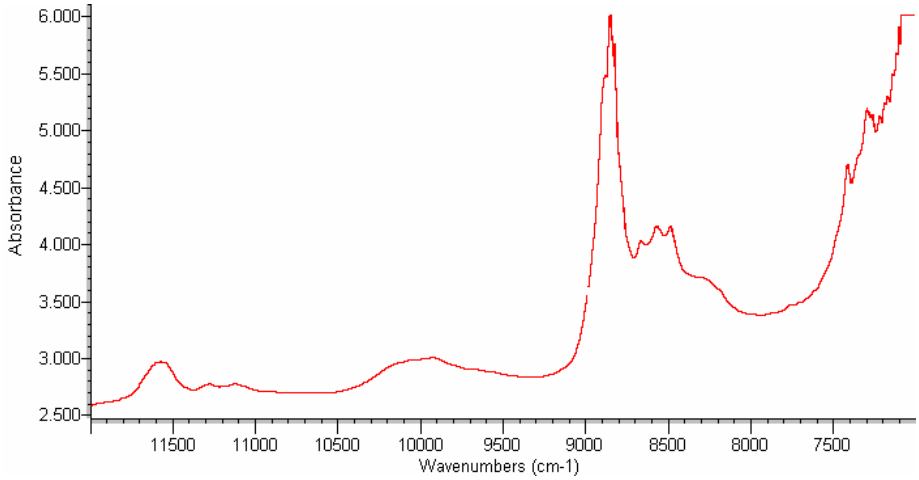
FT-NIR spectra produced by transmission or diffuse-reflection can have unique characteristics. Some problems with these characteristics are discussed in the "Common problems" section of this chapter.

Note

The spectra shown in this section are only examples of the kinds of results you may obtain. The actual spectra produced from your experiments may vary greatly, depending on the sample material and preparation. ▲

Transmission spectra

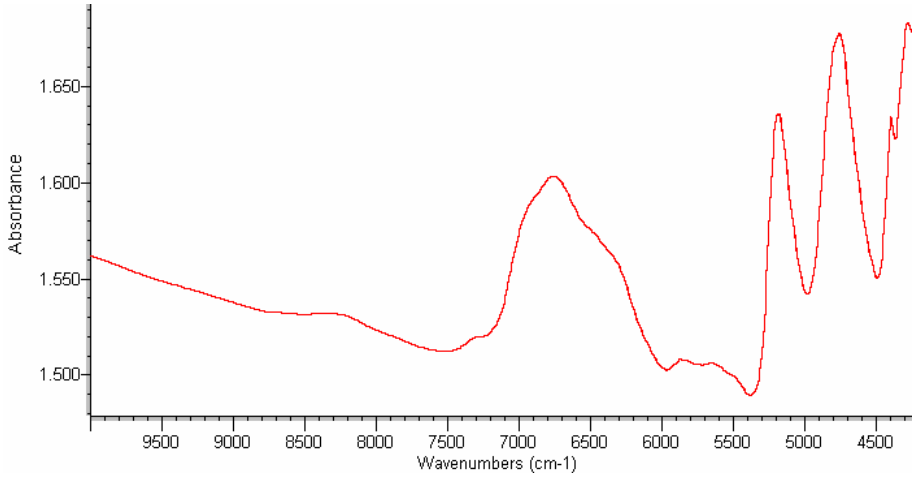
The following is representative of a typical spectrum taken using the standard tablet analyzer:



Transmission spectrum of 325 mg aspirin tablet

The spectral range for the above transmission sample with the standard tablet analyzer is 12,000 to 6,000 wavenumbers (cm^{-1}).

The following is representative of a typical spectrum taken using the softgel tablet analyzer:

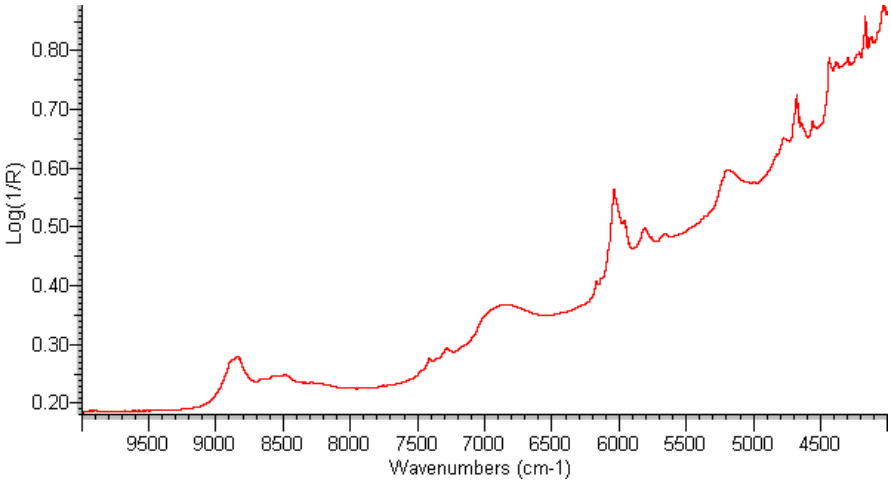


Transmission spectrum of paper

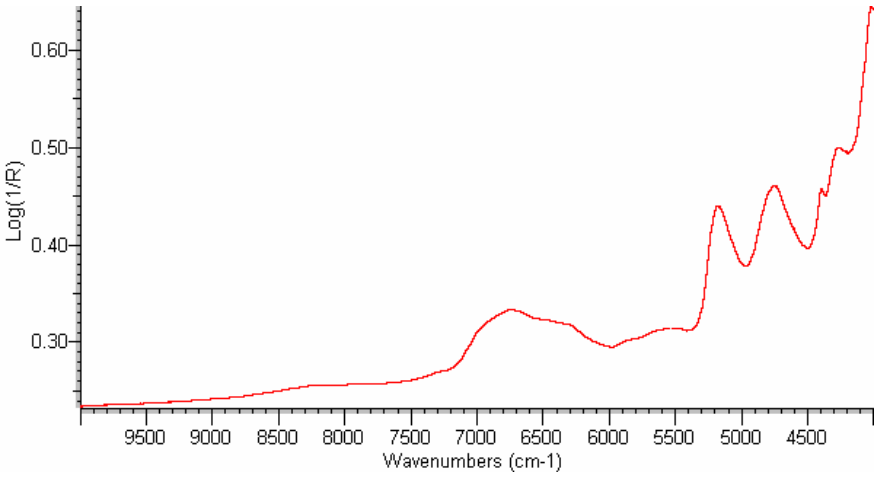
The spectral range for the above transmission sample with the softgel tablet analyzer is 10,000 to 4,000 wavenumbers (cm^{-1}). The baseline is at approximately 1.5 absorbance units, which is normal for paper because it scatters the NIR signal.

Diffuse-reflection spectra

The following spectra are representative of typical spectra taken using the integrating sphere:



Diffuse-reflection spectrum of 325 mg aspirin tablet



Diffuse-reflection spectrum of paper

The typical spectral range for a diffuse-reflection sample with the integrating sphere is 10,000 to 4,000 wavenumbers (cm^{-1}).

Collecting backgrounds

A background is a reference spectrum that accounts for the unique optics of the sampling module and the instrument. Each sample spectrum is ratioed against a background so that the final spectrum is free of these features. You can collect backgrounds using internal or external references, as directed by the workflow you are running.

The workflow you are running will direct how often to collect a background spectrum. The most recent background spectrum remains in memory and is compared against sample data until a new background spectrum is collected.

The "Common problems with spectral data" section of this chapter contains suggestions if a background spectrum is atypical from previously-collected background spectra.

For diagnostic purposes, you can collect a background using RESULT Operation software's Test Background or Quick Collect dialog box. The Test Background feature is helpful if you want to test background collection related to a particular workflow without affecting your production data. The Quick Collect feature is helpful if you want to test background collection independent of a workflow. The Quick Collect feature is also available in RESULT Integration software.

Transmission (tablet analyzer) backgrounds

The tablet analyzer must be connected to the instrument before collecting background data. Background data for a transmission experiment can be collected simply by performing the collection while the tablet analyzer is empty. It is not recommended that you use any background reference material.

When directed by a workflow to collect a background, the instrument is ready to begin collecting data when the green LED indicator is on. If the green indicator is steady, then you can start a background collection by pressing the Acknowledge button on the instrument or choosing the appropriate response in the software. If the green indicator is flashing, then you must begin the background collection by choosing the appropriate response to a prompt in the software.

When collecting the background, be sure to remove any sample materials from the tablet analyzer. You may leave sample holder accessories, such as rings or the universal tablet holder, inside the tablet analyzer when collecting the background data. If you collect the background with the

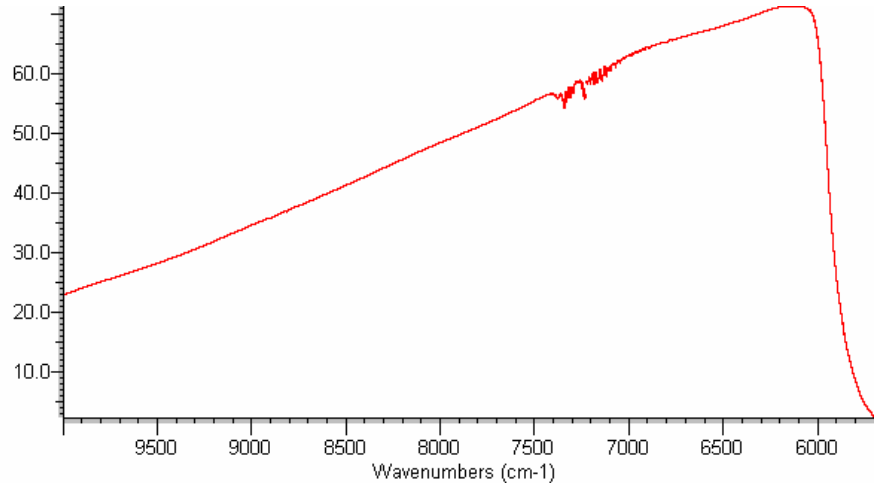
universal tablet holder inside the tablet analyzer, make sure the iris in the tablet holder is completely open.

When prompted by the software to collect the background, close the cover of the tablet analyzer and press either the Acknowledge button on the instrument or choose the appropriate response in the software to begin collecting data.

The status indicator in the software will show you the status of the data collection.

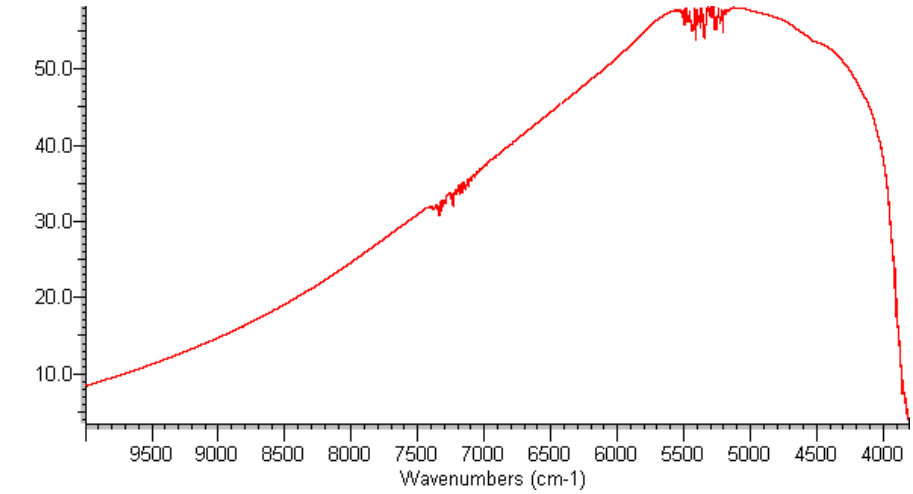
Notice Do not open the cover of the tablet analyzer while the instrument is collecting data. Opening the cover before the instrument has finished collecting data will affect your background spectrum. ▲

A typical background spectrum using the standard tablet analyzer should resemble the following:



Typical background spectrum with the standard tablet analyzer

A typical background spectrum using the softgel tablet analyzer should resemble the following:



Typical background spectrum with the softgel tablet analyzer

See the "Common problems with spectral data" section in this chapter if your background spectrum is not similar to one of the above or if it is atypical from previous background spectra.

Integrating sphere backgrounds

Background measurements for diffuse-reflection experiments can be taken using the internal gold reference, or by using an external reference, such as Spectralon®. For more information about diffuse-reflection backgrounds, see "Collecting backgrounds" in the "Integrating Sphere Module" chapter.

Preparing samples and accessories

This section contains information about how to prepare samples and sampling accessories for use with the tablet analyzer for transmission experiments.

Preparing solid samples

You can conduct transmission experiments on thin, small solids, such as plastics, polymers, packaging materials, and papers, in either of the tablet analyzers. The tablet analyzers can accommodate samples up to 9.8 cm in diameter.

Notice Do not use either of the tablet analyzers to sample solids or powders larger (or in vials larger) than the maximum sampling size dimensions. Attempting to sample a solid too large for the tablet analyzer could damage the tablet analyzer. ▲

Sampling tablets

The Antaris II tablet analyzer sampling module is optimized for collecting data from tablets. The tablet analyzers are shipped with a universal tablet holder that fits most round tablets and custom tablet holders that can be cut to fit the exact dimensions of a tablet. The tablet holder accessories are compatible with both tablet analyzers and the sample accessory holder for the integrating sphere sampling module. (For information about other sampling accessories that are compatible with the tablet analyzer, see "Using sampling accessories" in the "Integrating Sphere Module" chapter.)

Note Because softgel tablets can be compressed easily, when developing methods and workflows that deal with softgel tablets, it is recommended that you carefully test any methods and workflows for softgels. Positioning of softgel tablets during experiments is critical to produce repeatable collection results. ▲

Using the universal tablet holder

The universal tablet holder is meant for round tablets of many sizes and thicknesses, and can be used with either of the available tablet analyzers to conduct diffuse-reflection and transmission experiments using the integrating sphere and/or tablet analyzer. It can also be used with the sample accessory holder to conduct experiments using the integrating sphere. (See the "Integrating Sphere Module" chapter for details.)

Note It is possible to perform diffuse-reflection and transmission sampling simultaneously with the Antaris II tablet analyzer sampling module. For more information, please refer to "Using both diffuse-reflection and transmission" in this chapter. ▲

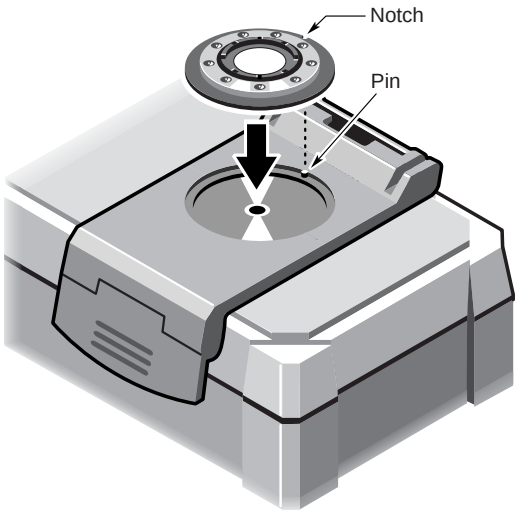
Notice Before installing the universal tablet holder, install the tablet analyzer on the instrument. See "Installing the tablet analyzer" in this chapter or "Installing the sample accessory holder" in the "Integrating Sphere Module" chapter for installation instructions. ▲

To install and use the universal tablet holder:

1. **Open the cover of the tablet analyzer.**

   Make sure the instrument is not collecting data before you open the cover.

2. **Place the universal tablet holder in the sample holder on the tablet analyzer base.**



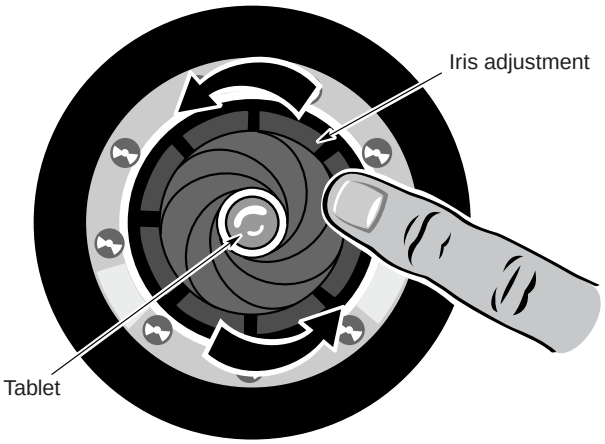
   Align the notch in the universal tablet holder with the pin in the tablet analyzer base to secure it in place.

3. **If the iris in the universal tablet holder is not completely open, gently turn the black iris adjustment clockwise until it is completely open.**

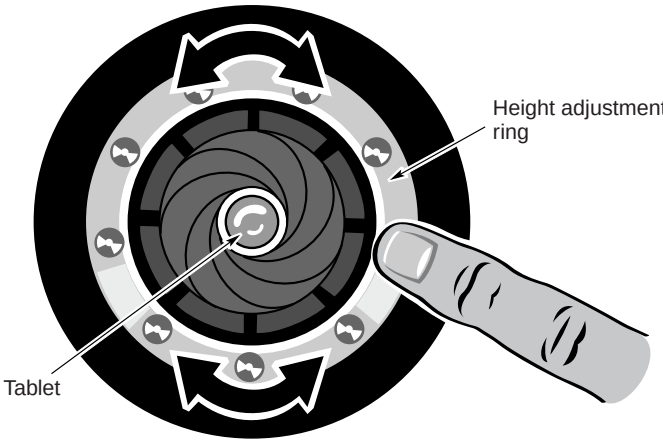
4. **Place the tablet you want to analyze in the center of the universal tablet holder.**

5. **Slowly turn the black iris adjustment counterclockwise until it is almost touching the tablet.**

   The iris should not be closed completely around the tablet. Some room should be remaining so you can see both the tablet and iris sides.

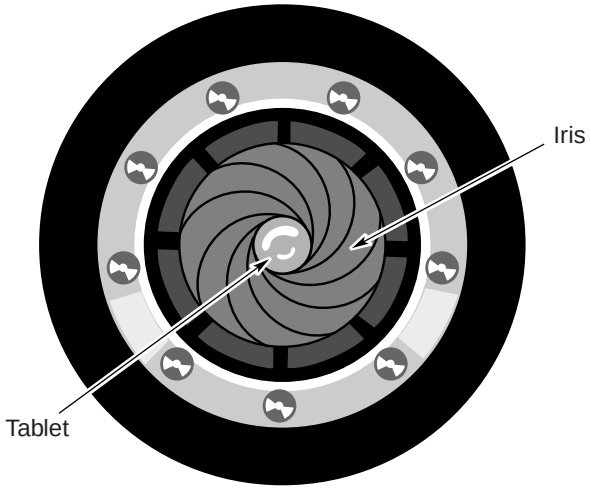


6. **Adjust the height of the iris so it is approximately at the center of the tablet's width.**



   You can adjust the height of the iris by turning the silver iris adjustment clockwise or counterclockwise to raise or lower it. Turning the adjustment clockwise lowers the iris; turning the adjustment counter-clockwise raises the iris.

7. **After the iris has been positioned to the proper height, slowly close the iris.**



Close the iris by turning the black iris adjustment counterclockwise, until the tablet is completely enclosed in the iris.

Notice Do not over-tighten the iris. Over-tightening the iris may damage the universal tablet holder or the sample. ▲

8. **Close the cover of the tablet analyzer.**

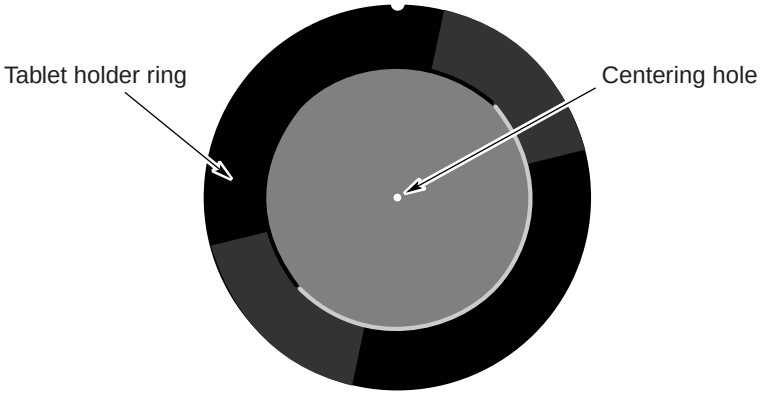
The tablet is now ready for a diffuse-reflection or transmission experiment.

When you have finished collecting sample data, remove the tablet by first turning the black iris adjustment clockwise until it is completely open. You can then remove the sample and remove the universal tablet holder from the tablet analyzer.

Using the custom tablet holders

The tablet analyzer sampling module comes with two custom tablet holders that can be modified to fit the exact dimensions of tablets you want to analyze.

The tablet holders contain a small hole to reference the center of the holder. The hole in the tablet holder aligns with the center of the integrating sphere and tablet analyzer transmission detector when the holder is used with the holder ring.



Custom tablet holder

Depending on the amount of sampling precision and repeatability needed, there are different ways you can customize the tablet holders to fit the tablets you want to analyze:

- If your experiment does not require a lot of precision and/or the tablet holder is not going to be used to ensure tablet placement consistency, the custom tablet holder can be cut to fit a tablet simply by using a utility knife.

- If your experiment requires more precision, or you want to ensure sample placement consistency and repeatability, you may want to consider using a steel-rule die to customize the tablet holder to the precise size of the tablet.

You can use a colored pen or marker to mark an indicator on the tablet holder so it can be aligned with the positioning groove in the tablet holder ring.

Note If your experiments require a great deal of precision, repeatability, and consistency (for mass sampling on the production floor, for example), you may want to consider machining a metal tablet holder that fits the exact dimensions of the tablet analyzer and the tablet. ▲

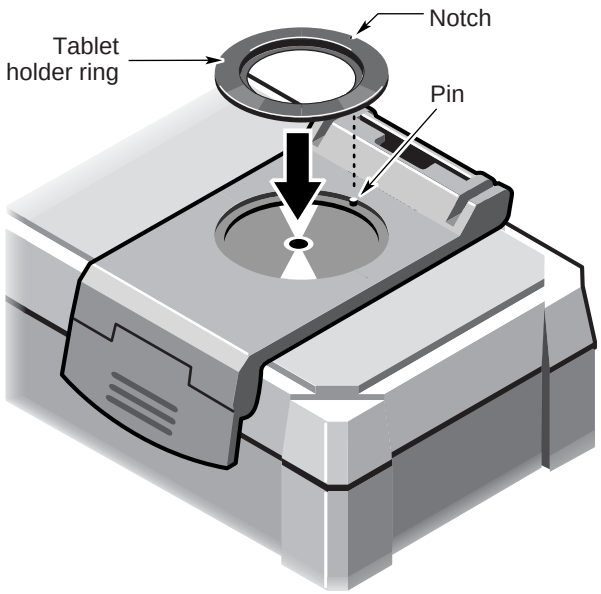
Before installing the tablet holder, install the tablet analyzer on the instrument. See “Installing the tablet analyzer” in this chapter for installation instructions.

To install and use a tablet holder:

1. **If using a tablet analyzer, open the cover of the tablet analyzer.**

   Make sure the instrument is not collecting data before you open the cover of the tablet analyzer.

2. **Place the tablet holder ring in the sample holder or tablet analyzer base.**

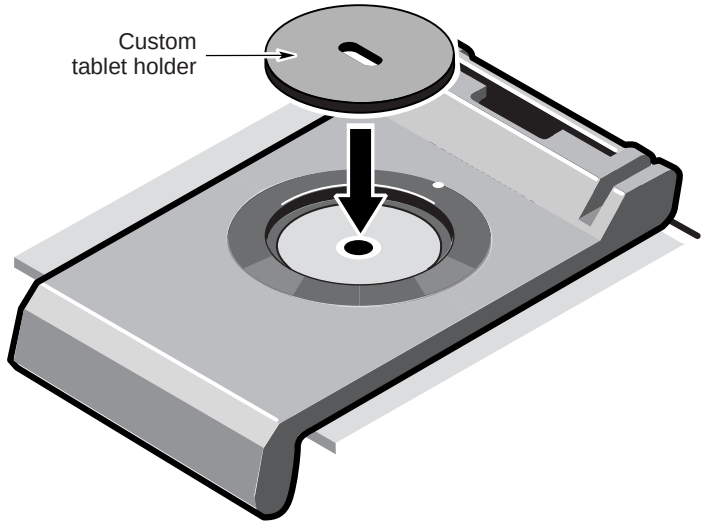


Note The tablet holder ring is similar in appearance to the sample cup rings. To distinguish the tablet holder ring from other sample rings, note the following characteristics of the tablet holder ring: .

- The tablet holder ring has a lip around the inside opening that holds the custom tablet holder.
- The tablet holder ring does not have position indicators around the opening of the ring. ▲

  Align the notch in the ring with the peg in the sample holder or tablet analyzer to secure it in place.

3. **Place the tablet holder in the sample ring.**



If you have made any markings on the tablet holder for alignment purposes, be sure to properly align the tablet holder with the notch in the tablet holder ring.

4. **Gently press around the circumference of the tablet holder with your index finger to ensure the outer edge of the tablet holder is lying flat against the lip in the tablet holder ring.**

5. **Insert the tablet into the tablet holder.**

6. **Close the cover of the tablet analyzer.**

The tablet is now ready for a diffuse-reflection and/or transmission experiment. When you have finished collecting the sample data, be sure to remove all sampling accessories before removing the tablet analyzer.

Other compatible sampling accessories

Thermo Fisher Scientific offers a number of sampling accessories for sampling powders and tablets with the tablet analyzer. This includes the sample accessory holder, along with sample cups and sample cup rings, the universal tablet holder, and custom tablet holders. These accessories can also be used with the integrating sphere. For more information, see “Using sampling accessories” in the Integrating Sphere Module” chapter.

Tips for developing workflows for the tablet analyzers

When developing workflows using RESULT Integration software, there are some factors you want to take into consideration to make sampling with the tablet analyzer sampling module as efficient as possible. Sample parameters and specifications are highly dependent on sample type, the amount of time available to collect data, and the level of interest in different spectral characteristics. This section contains recommendations for starting points when specifying collection event parameters, sample specifications, and background specifications.

Collection event parameters

A collection event in RESULT Integration software instructs the instrument to collect a spectrum of a sample. The following table contains the recommended starting points for sample collection parameters for the integrating sphere and the tablet analyzers:

Parameter	Tablet Analyzer Setting	Integrating Sphere Setting
Number Of Sample Scans	30	30
Data Format	Absorbance	Log (1/R)
Background Frequency	Every Hour	Every Hour

- **Number Of Sample Scans.** To start, try using 30 scans for the integrating sphere and 50 scans for the tablet analyzers. You can then decrease the number of scans to the smallest number that can still produce tolerable signal-to-noise (determined by error of prediction or pre-defined limit) if sampling time is at a premium. If using a higher resolution, the spectra will contain more spectral noise, so you may need to increase the number of scans to better distinguish sample features from noise. See “Collection times” in this chapter for more information about the relationship between the Number Of Sample Scans parameter and the Resolution Specification.

- **Background Frequency.** If collecting samples only periodically, then collecting a background before every sample is recommended. If collecting many samples at a time, then collecting a background every hour should be sufficient.

Note It is possible to perform diffuse-reflection and transmission sampling simultaneously with the tablet analyzer. When doing so, it is recommended that you use the tablet analyzer settings for Number Of Sample Scans and Data Format for both the tablet analyzer and the integrating sphere. This is because the integrating sphere operates at the slower velocity of the tablet analyzer during simultaneous diffuse-reflection and transmission sampling. ▲

See "Collect events" and "Collect dual tablet events" in "Chapter 5 Workflow Events and Specifications" of your *RESULT User's Guide* for more information about sample collection events for the tablet analyzers.

Operator prompts

When developing a workflow in RESULT Integration software, the collection events allow you to include operator prompts for both sample and background collection. It is recommended that you include detailed operator prompts to ensure that background and sample data is collected properly.

Some example prompts for background collection could include:

- **For collecting transmission backgrounds with an empty tablet analyzer:** Make sure no samples are in the tablet analyzer and close the tablet analyzer cover. Press the Acknowledge button on the instrument when you are ready to begin collecting the background data.

- **For collecting diffuse-reflection backgrounds using an external reference:** Place the background reference over the integrating sphere and press the Acknowledge button on the instrument when you are ready to begin collecting the background data.

Because no preparation is necessary to collect a diffuse-reflection background spectrum using the integrating sphere's internal reference, no prompts are necessary before performing this function.

When developing prompts for sample collection, make sure your prompts to the operator include specific information about how to prepare and

position the sample. If the operator is required to reposition the sample, for example, if you've created a repeat loop in a workflow, it is recommended that you prompt the operator each time the sample needs to be repositioned, and include the number of degrees the sample should be rotated.

Sample specifications

In RESULT Integration software, sample specifications are used to specify advanced collection parameters to optimize the workflow based on a specific sampling technique. Sample specifications are attached to collection events in workflows. The following table contains the recommended starting points for sample specifications:

Specification	Tablet Analyzer Setting	Integrating Sphere Setting
Attenuator	Optimize Gain Feature	Empty
Resolution	8 cm^{-1}	8 cm^{-1}
Gain	Optimize Gain Feature	1x
Spectral Range	10,000-7,100 cm^{-1} (standard analyzer) 10,000-4,000 cm^{-1} (softgel analyzer)	10,000-4,000 cm^{-1}

- **Gain and Attenuator.** It is recommended that you use RESULT Integration's Optimize Gain feature to determine the appropriate gain and attenuator settings for your sample. If you use the Optimize Gain feature, the software will collect sample data using each possible combination of gain and attenuator specifications to find the specifications that produce the best results. If you choose not to use this feature, you may want to begin with a Gain setting of 1x for the integrating sphere, 10x for the standard tablet analyzer, or 1x for the softgel tablet analyzer; and an Attenuator setting of Empty for the integrating sphere or C Screen for the tablet analyzers.

  For most analyses, the software automatically uses the selected Attenuator setting to collect both the sample and background spectrum. The tablet analyzer is an exception because, in default mode, it uses the C screen (with a gain setting of "1") to collect background

data with the transmission detector. The Attenuator setting selected in the software is used only for the sample spectrum. Tablet samples are typically collected without a screen (and with a higher gain setting) because they are often highly absorbing. To override the default attenuation and gain settings for transmission backgrounds collected with a tablet analyzer, select Use Sample Position For Background Measurements on the associated background specification. See "Background Specifications" in this chapter for more information.

For more information about using the Optimize Gain feature, see the sample specification information in "Chapter 5 Workflow Events and Specifications" of your *RESULT User's Guide*.

- **Resolution.** Try 8 cm^{-1} as a starting point for the integrating sphere and 16 cm^{-1} for the tablet analyzers. 16 cm^{-1} is recommended for the tablet analyzers because typical samples are strongly absorbing, and therefore, signal-to-noise is at a premium. If your samples are less challenging, you may want to start with 8 cm^{-1} or 4 cm^{-1}. You can increase the resolution (e.g., from 16 cm^{-1} to 8 cm^{-1}) if required by your sample and then increase the number of scans to provide tolerable signal-to-noise. You can try a lower resolution to trade off resolution for signal-to-noise.

Collection times

The settings for Resolution and Number Of Sample Scans can affect the time involved for each data collection. When collecting data from many samples in a production environment, collection time may be a considerable factor when setting up workflows.

The table in the Sample Specification section of "Chapter 5 Workflow Events and Specifications" in your *RESULT User's Guide* has estimates of collection times for most sampling accessories. Because the standard tablet analyzer contains a highly sensitive detector and operates at a slower mirror velocity than other accessories, the collection times for the standard tablet analyzer differ from other sampling accessories.

Use the following table to estimate the sample collection time based on the Resolution and Number of Sample Scans parameters:

Note If you are performing simultaneous diffuse-reflection and transmission sampling, keep in mind that the maximum sampling speed of the tablet analyzer is slower than that of the integrating sphere. So, when performing

simultaneous diffuse-reflection and transmission sampling, the integrating sphere operates at the slower mirror velocity of the tablet analyzer. This is because the instrument cannot collect data at two different speeds simultaneously. ▲

Time (in seconds)	Resolution (cm^{-1})	Number of Scans
15	2	9
	4	10
	8	17
	16	26
	32	35
	64	43
30	2	18
	4	20
	8	34
	16	52
	32	70
	64	86
60	2	36
	4	40
	8	68
	16	104
	32	140
	64	172
120	2	72
	4	80
	8	136
	16	208
	32	280
	64	344

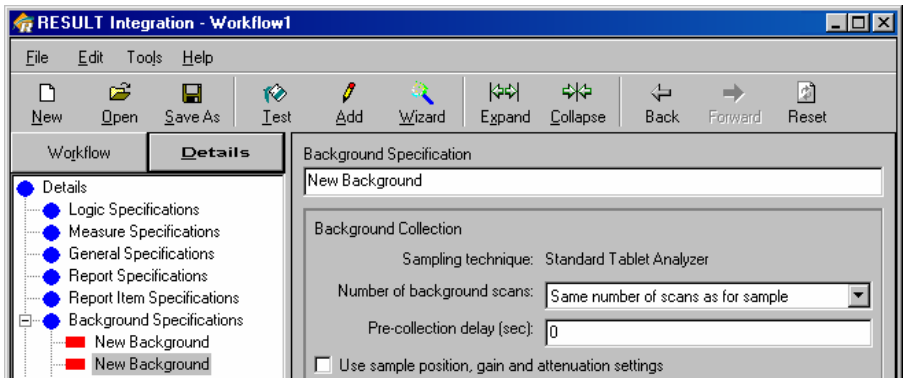
Remember that faster collection times can mean a trade-off of the signal-to-noise level. Be sure your settings for the number of scans and resolution produce spectra that have a tolerable signal-to-noise level.

Background specifications

The settings in the Background Specification are affected by whether you will be using an external or internal reference for background collection.

If you plan to use external references for a diffuse-reflection or transmission background, make sure to select the Use Sample Position, Gain, And Attenuation Settings check box in the Background Specification of your workflow. If this checkbox is not selected, the background will be collected (for either the standard tablet analyzer or the softgel tablet analyzer) with

the transmission detector using no background material. The default gain setting will be 1x, and the default attenuator setting will be C screen.



A good starting point for the Number Of Background Scans parameter is Same Number Of Scans As For Sample, as shown above.

Combining transmission and diffuse-reflection collection

When creating a workflow that will collect both diffuse-reflection and transmission data sequentially, consider setting up the workflow to collect transmission data first, especially if using the instrument's internal referencing for background collections.

Collecting transmission data first saves the operator from having to remove the sample between data collections, because the diffuse-reflection background can be collected while the sample is still in place (if using the integrating sphere's internal reference). Because the sample is not removed, this also ensures that it will be in precisely the same position during both data collection events.

If you conduct the transmission collection prior to the integrating sphere collection, then operator prompts are necessary only for collecting the transmission background and the transmission sample. The instrument can automatically collect the integrating sphere background (if using the internal reference) and sample data.

Note If you are creating a workflow that will collect diffuse-reflection and transmission data simultaneously, see "Collect dual tablet events" in "Section 5 Workflow Events and Specifications" of your *RESULT User's Guide* for more information. ▲

Common problems with spectral data

Before using the instrument for precise quantitative analysis, evaluate the effects of temperature and sample contact on spectral features. Other items that may influence spectra are bad backgrounds; the amount of noise; improper collection of a sample; sample particle size, homogeneity, and concentration.

If you encounter a problem, before running any other diagnostics or deeming backgrounds or samples as "bad," you may first want to check the following items:

- If collecting a transmission sample, make sure the sample material is not in the tablet analyzer when collecting the background spectrum.
- If collecting a transmission sample, make sure the cover of the tablet analyzer is fully closed.
- Make sure the sample is properly positioned over the integrating sphere window (and in the sample holder of the tablet analyzer if collecting a transmission sample) when collecting the sample spectrum.

Problems with background spectra

If a background spectrum you collected is atypical from previously-collected backgrounds or from the typical spectra described in the "Collecting the background" section of this chapter, the problem may be one of the following:

- If collecting a transmission background or diffuse-reflection background using an external reference, the integrating sphere window may be dirty. Follow the instructions in the "Maintenance and Service" chapter to clean the window.
- If collecting a transmission background, the tablet analyzer may not have been completely closed.
- If you were not using an internal reference, it is possible that:
    - The sample material could have been run as the background.
    - The reference was moved while the instrument was collecting data.
    - The reference is dirty. Inspect the reference material and clean it according to proper procedures or replace it, if necessary.

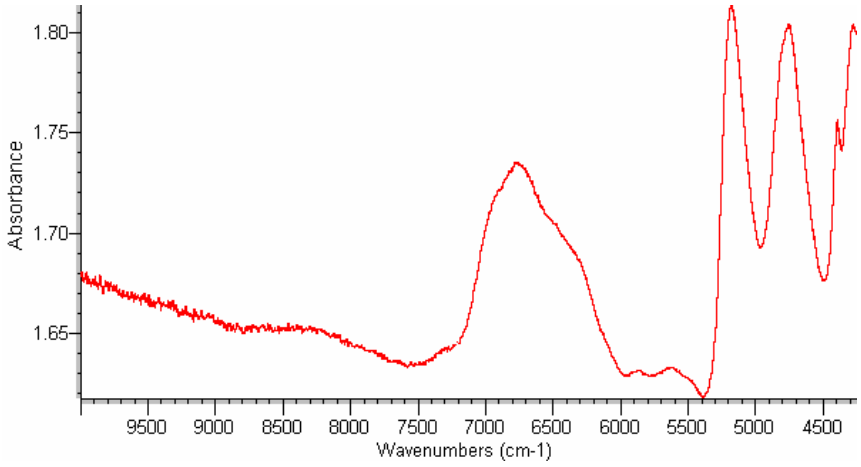
For all problems above, it is recommended that you take test backgrounds using either the Quick Collect (not associated with a workflow) or Test Background (following the steps for background collection in a workflow) features in RESULT Operation software before running the workflow again in production.

Problems with sample spectra

Several factors may affect a sample spectrum. Before deeming the sample as "bad," collect the sample data again either by running the workflow off-line, using the Test Sample feature, or using the Quick Collect feature in RESULT Operation software.

High noise

A spectrum that contains a high amount of noise will resemble the following:

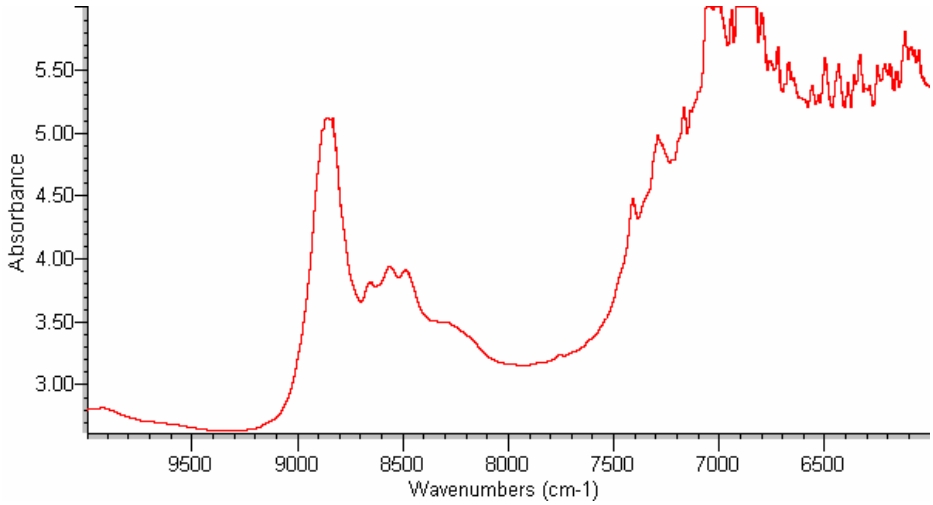


Paper spectrum with high noise using the softgel tablet analyzer

As shown above, the high level of noise is represented as very small peaks in a spectrum. If you experience this problem, you may want to increase the number of scans or lower the resolution to decrease the amount of noise in the sample. If changing these parameters in a transmission experiment does not alleviate the problem, the sample may be too dense to use with the sampling accessory. You can also try increasing the detector gain. Finally, check to make sure any attenuation screens that are in place are needed. If they are not needed, remove them.

Offset baseline

A spectrum with an offset baseline may resemble the following:



Aspirin spectrum with an offset baseline using the standard tablet analyzer

As shown above, the spectrum baseline started at 2.80 absorbance units. Some spectra may normally have a baseline that does not start at zero, depending on your sample material, preparation, and positioning. However, if the baseline of your spectrum is not consistent with previous spectra, one of the following may have occurred:

- In a diffuse-reflection experiment, the sample material may be too thin.
- In a diffuse-reflection experiment, the sample material did not completely cover the integrating sphere window.
- In a transmission experiment, the sample may not have been completely covering the path of the beam, or the sample material may be tilted.

Detector saturation

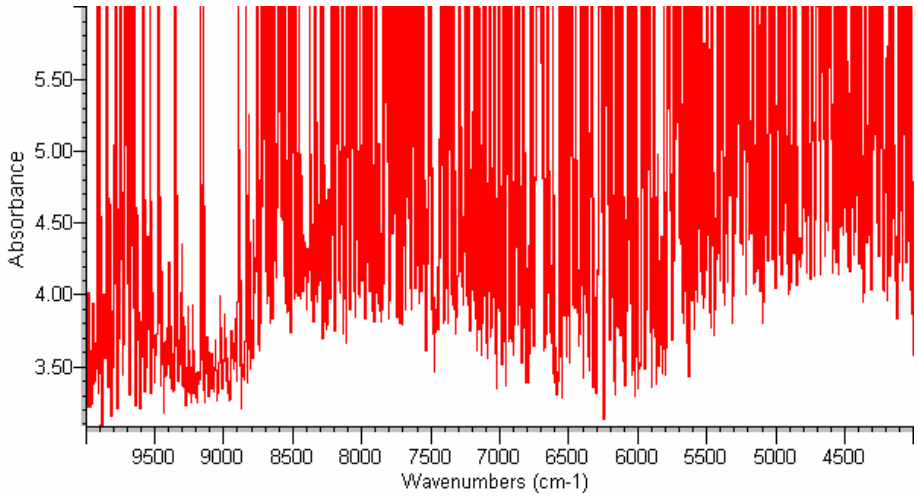
If too much light is getting through your sample material during a transmission experiment, then the detector may have become saturated. When the detector has been saturated, the software will display a message indicating that it was unable to locate the interferogram peak.

If you encounter this problem, you may want to adjust your attenuator setting to allow less light to pass through the sample, or lower your gain setting. If you have not used RESULT Integration's Optimize Gain feature, use this feature to find the best gain and attenuator setting.

If the detector becomes saturated during an experiment, it is recommended that you wait at least ten seconds to allow the detector to clear before attempting to collect data again.

Samples not appropriate for transmission

Some samples may be too dense or thick to use with the tablet analyzer. An example spectrum of a sample that is too dense or thick may resemble the following:

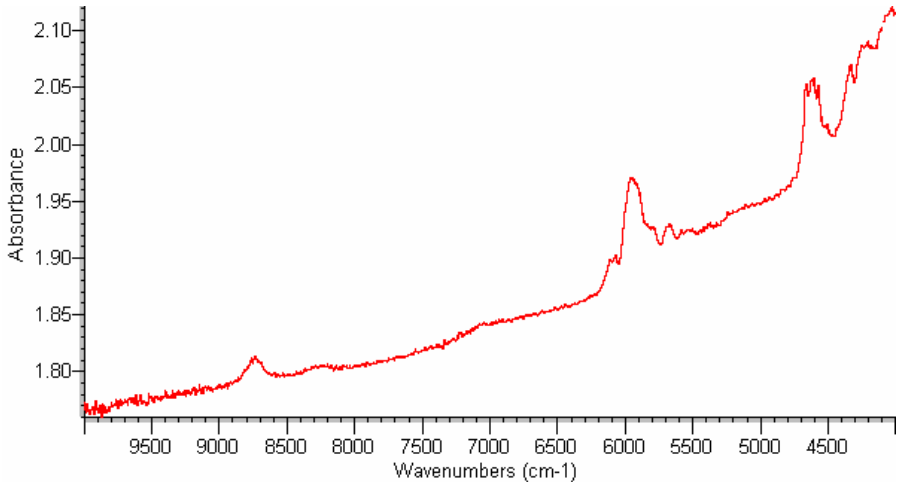


Dense tablet spectrum showing insufficient energy reaching the detector using the softgel tablet analyzer

The spectral features were caused by no light getting through the sample into the detector. For this type of sample, you may want to try another sampling technique, such as diffuse-reflection or using the standard tablet analyzer.

Samples not appropriate for diffuse-reflection

Some samples may not be diffuse enough to use with the integrating sphere. An example spectrum of a smooth sample may resemble the following:



Thin polystyrene film spectrum showing insufficiently diffuse features using the integrating sphere

As shown above, the baseline is high. Very little light was diffused and reflected back into the integrating sphere. The spectral features are relatively small. For this type of sample, you may want to try another sampling technique, such as transmission.

Sample particle size, homogeneity, and concentration

Particle size, homogeneity, and concentration all affect the quality of spectra. Changes in particle size can affect scattering and may have ramifications on the effective pathlength. This can cause differences in band intensity and baseline slope.

The quality of your spectrum will be most affected if there are extreme differences in particle size throughout the sample (for example, a sample containing particles smaller than 3 microns and above 500 microns).

Homogeneity can affect reproducibility. The degree of heterogeneity in a sample should be taken into consideration when determining the number of collection event repetitions to include when creating a workflow, so you can achieve a representative spectrum of the sample. The spectral data will probably be of good quality, but each individual spectrum may not be representative of the sample as a whole.

Concentration can affect signal-to-noise in a spectrum. Signal-to-noise can become more of a factor when working with lower concentrations of a sample.

To keep these types of problems at a minimum, when developing workflows, consider adding repeat trees to your workflows to collect data from samples in different sampling positions.

Chapter 7 Maintenance and Service

This chapter describes general maintenance and service routines that you can perform on the Antaris II analyzer. We define maintenance as an occasional procedure you perform to keep the analyzer running efficiently. Examples include cleaning the analyzer, changing the desiccant and connecting the power supply. Included in this chapter is maintenance information for Antaris II sampling modules.

We define service as a procedure to replace a failing part in the analyzer, such as a power supply, source, or laser. It also describes how to install the optional purge kit.

⚠ Warning Perform only those procedures described in this chapter. If there are other problems with the system, contact Thermo Fisher Scientific technical support. ▲

⚠ Warning If a protective cover on the analyzer or computer appears damaged, turn off the system and secure it against any unintended operation. Always examine the protective cover for transport stresses after shipping. ▲

Tools

Most maintenance procedures can be performed without any special tools. For procedures such as replacing the source or removing the cover, you will need a number 2 Phillips screwdriver. If you are installing a purge system, you will need the following tools and supplies:

- $^{11}/_{16}$ -inch open-ended wrench
- $^{3}/_{4}$ -inch open-ended wrench
- Shutoff valve
- $^{1}/_{4}$ -inch male fitting or a $^{3}/_{8}$ -inch female fitting.

Cleaning the analyzer

If the outside of the analyzer needs cleaning, turn off the analyzer power and disconnect the power cord from the wall outlet or power strip. Then use a damp (not wet), soft cloth and a mild soap to clean the outside of the analyzer.

⚠ Warning Avoid shock hazard. Always move the power switch to the off (O) position and disconnect the power cord from the wall outlet or power strip before cleaning the analyzer. ▲

⚠ Warning Avoid shock hazard. Do not allow liquid to run into the instrument or power supply. ▲

Notice Do not use harsh detergents, solvents, chemicals or abrasives to clean the analyzer; these can damage the finish. ▲

Notice Do not attempt to clean *or even touch* the mirror surfaces. The mirrors in the analyzer are front surfaced and can be easily scratched. Dust will not harm the near-infrared signal, but fingerprints can degrade spectral performance or permanently damage the mirrors. If you wish to remove dust from the mirrors, blow it off with a gentle stream of clean air or nitrogen. ▲

Notice Do not use harsh detergents, solvents, chemicals or abrasives; these can damage the finish. ▲

Notice For further cleaning information, see the "Maintaining your analyzer" book in the on-line spectrometer help system. ▲

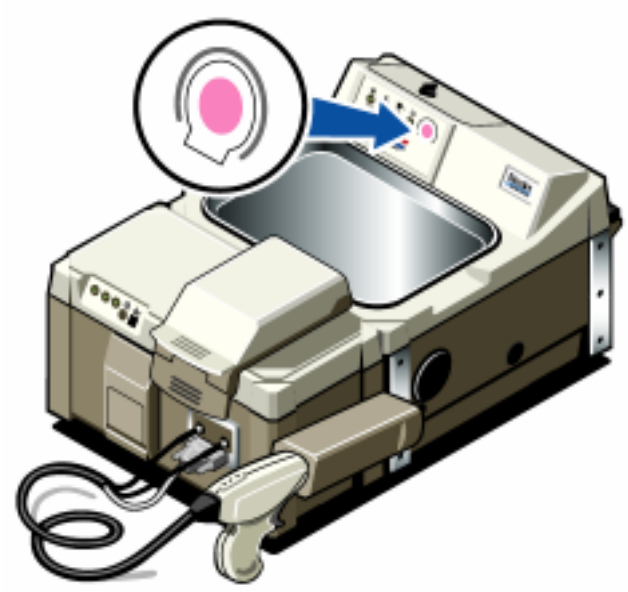
Checking and changing desiccant

Antaris II analyzers are sealed and desiccated. You will occasionally have to check and change the desiccant packets. These packets keep the analyzer optics free of excess moisture. A humidity indicator on the front panel of the analyzer can be used to check the desiccant. You should check the indicator every two months when the analyzer is not in use.

Checking the desiccant

A humidity indicator on the front panel of the analyzer can be used to check the desiccant. Even if the analyzer is not in use, you should check the indicator every two months (more often in excessively humid environments).

To check the desiccant, locate the desiccant indicator. If it is pink, the desiccant needs to be replaced.



Changing the desiccant

The following procedure shows you how to replace the desiccant in your analyzer. This procedure should take 5 minutes, or less, to perform and does not require any tools.

Note Be sure to record the desiccant installation date. Use Update Instrument Information from the Service menu in RESULT Operation software. ▲

1. **Turn the latch and open the desiccant compartment.**

2. **Slide the desiccant packet out of the compartment.**

Warning The desiccant is harmful if swallowed. Be sure that you dispose of packets safely. ▲

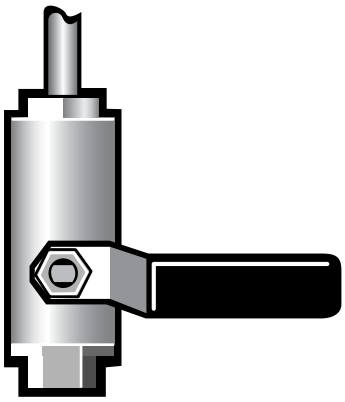
3. **Discard the old packet and put in the new one.**

4. **Close the cover and latch it.**

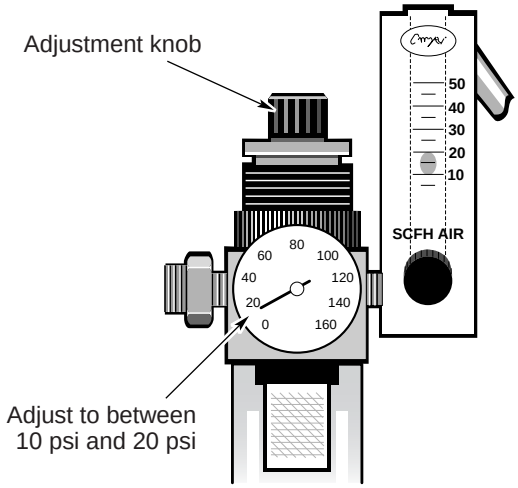
Checking the settings for optional purge gas

If your analyzer is equipped with an optional purge kit, check the regulator and flowmeter settings occasionally to make sure they are correct. To check the purge gas settings:

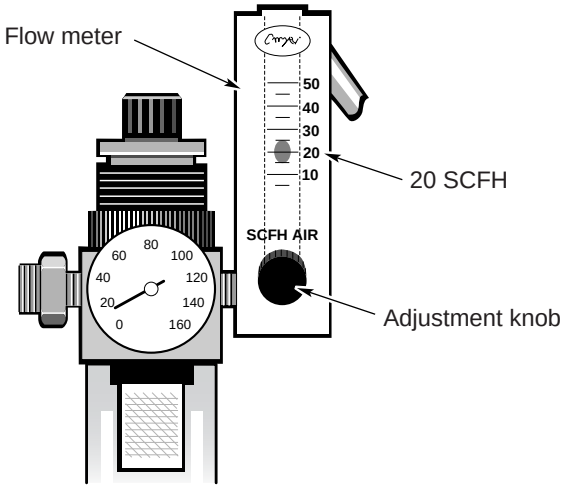
1. **If the shutoff valve is in the off position, turn it to the on position.**



2. **Adjust the pressure regulator until the gauge indicates that the pressure is between 10 psi and 20 psi.**

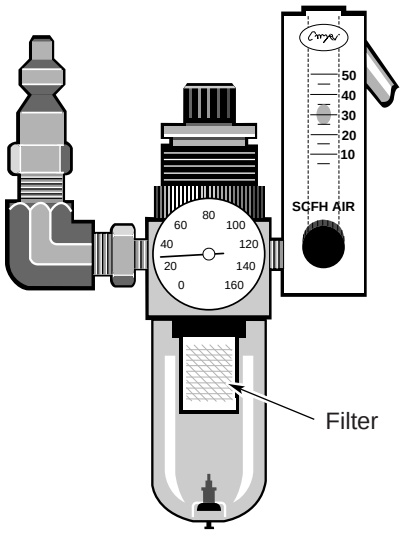


3. **Set the flowmeter to 20 SCFH.**



Checking and changing purge gas filters

If your analyzer is equipped with an optional purge kit, check the purge filter occasionally to make sure it is clean. If the filter appears discolored, replace it.



⚠ Warning Never use a flammable gas to purge the spectrometer. The purge gas must be free of moisture, oil, carbon dioxide and other reactive or infrared-absorbing materials. Use only dried air or nitrogen to purge the spectrometer. Other gasses, even inert gasses such as argon (Ar), can damage the spectrometer. Never use them to purge the spectrometer. ▲

To replace the purge filter:

1. **Turn off the purge gas at the shut off valve.**

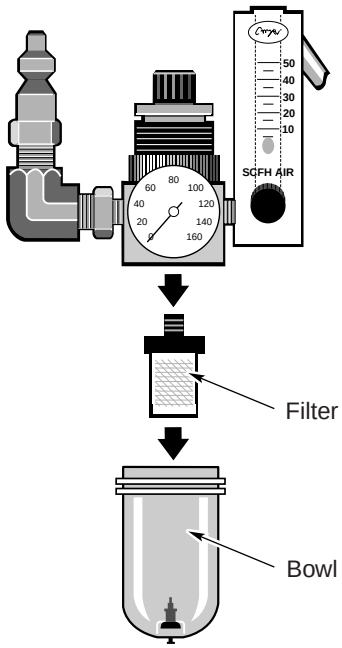
   Do not turn down the flowmeter or the pressure regulator.

2. **Remove the plastic bowl that houses the filter.**

   You can unscrew the bowl by hand.

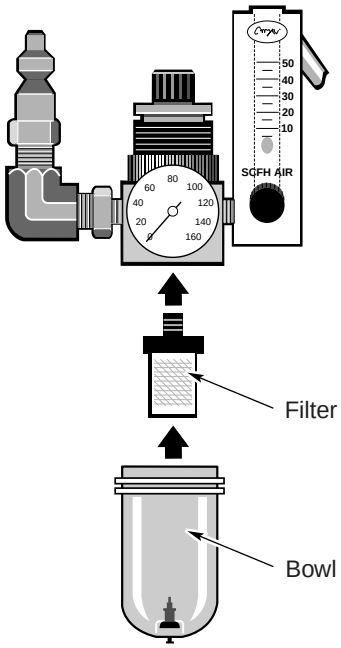
3. **Remove the filter.**

   You can unscrew the filter by hand.



4. **Install the new filter.**

5. **Reinstall the plastic bowl.**



6. **Turn on the purge flow to the analyzer.**

7. **Begin collecting spectra.**

   You may notice increased levels of water and carbon dioxide in spectra collected immediately after you change the purge filter. If this interferes with your data, wait until equilibrium is re-established.

Opening and closing the main cover

Some service procedures require that you open the main cover of the analyzer. Be sure to close and secure the cover upon completion of the service procedure.

⚠ Warning To avoid shock hazard, always turn off the analyzer and disconnect the power supply from the wall outlet or power strip before you open the main cover. ▲

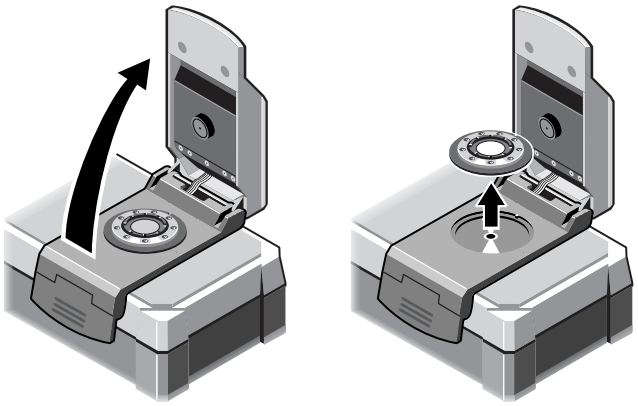
Notice Although the main cover can be opened and closed easily by the system operator, it is recommended that only certified Thermo Fisher Scientific

service engineers or trained Thermo Fisher Scientific on-site maintenance personnel perform this operation. Whenever the main cover is open, there is a potential for damage to sensitive components. Damage to components inside the analyzer will affect the performance of the system. ▲

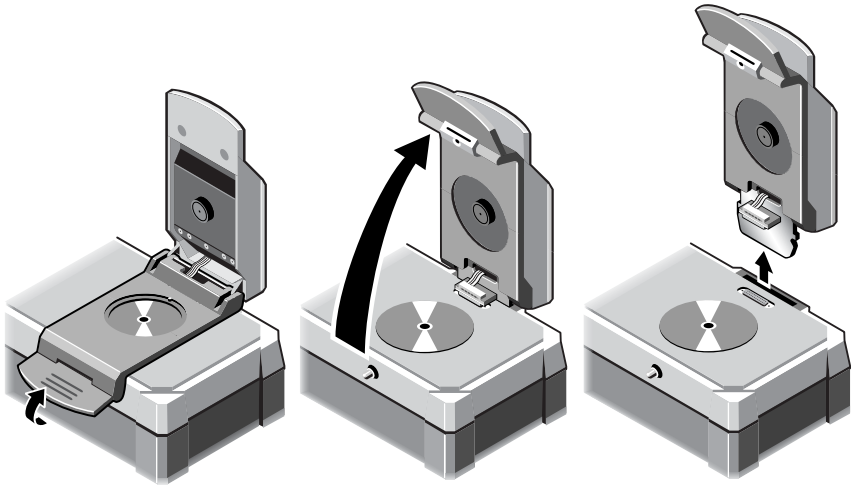
To open the main cover:

1. **Remove any sample materials or other items from the top of the analyzer.**

2. **If the analyzer is equipped with the tablet analyzer module, open the module, remove the tablet holder and set it aside.**



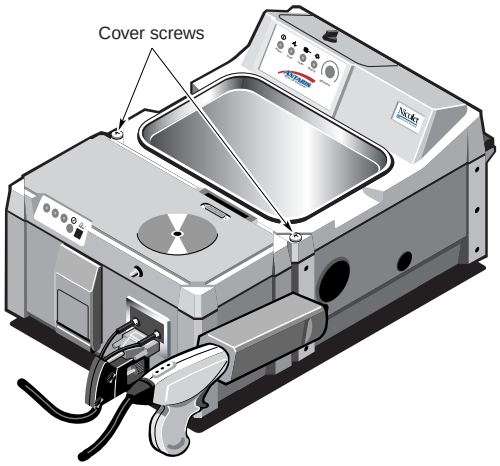
3. **If the analyzer is equipped with an optional tablet analyzer module, remove that module.**



① Lift the latch. ② Expose the connector. ③ Lift the module.

⚠ Warning To avoid shock hazard, always turn off the analyzer and disconnect the power supply from the wall outlet or power strip before you remove the screws for that secure the analyzer cover. ▲

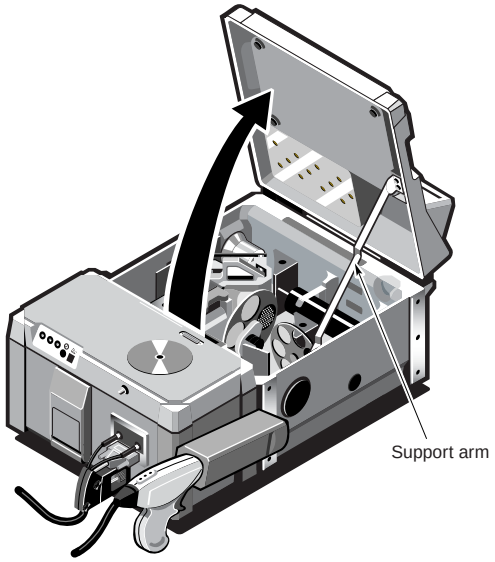
4. **Use a No. 2 Phillips screwdriver to loosen the screws that secure the cover to the analyzer.**



⚠ Caution Even after the analyzer has been turned off, the source bulb remains hot for up to 15 minutes. ▲

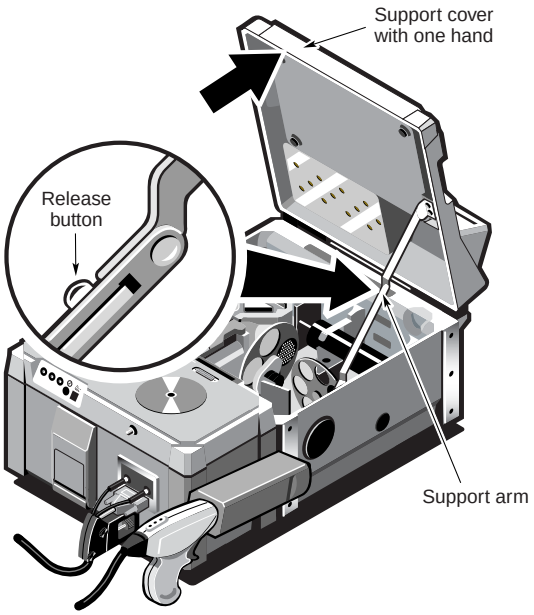
5. **Lift the cover.**

6. **Straighten the support arm until the prop locks into place and supports the cover.**



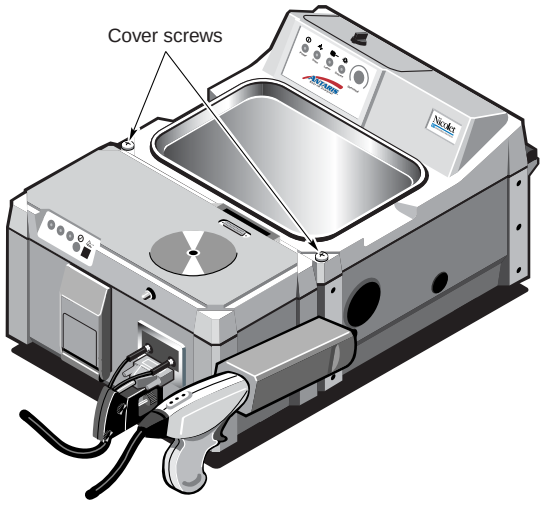
To close the main cover:

1. **Support the cover with one hand, press the release button and fold the support arm back toward the rear of the analyzer.**

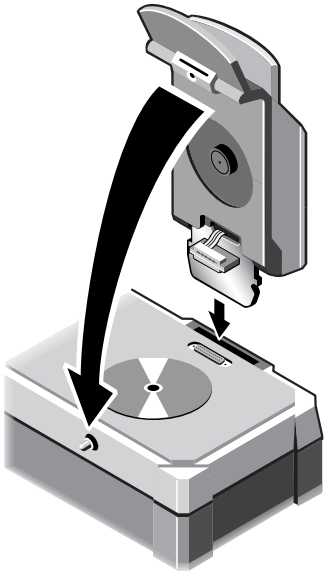


2. **Lower the cover.**

3. **Use a No. 2 Phillips screwdriver and secure the cover with the screws you removed earlier.**



4. **If the analyzer is equipped with the tablet analyzer module, reinstall the module and tablet holder.**



5. **Reconnect power supply to the power strip or wall outlet.**

   See "Replacing the power supply" in this chapter if you need information about reconnecting the power supply.

Replacing fuses

If you need to replace the fuses in the power supply module, refer to the fuse replacement procedure in the site and safety manual that came with your instrument.

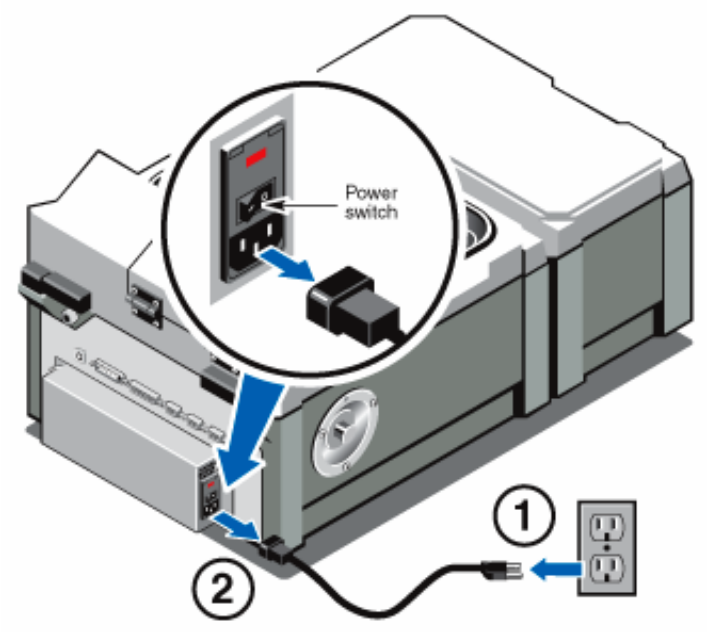
Replacing the power supply

The power supply may need to be replaced if it develops a fault or if the fuses blow. Also, to prevent shock hazard, many procedures require that you turn off the analyzer and disconnect the power supply before you work on the analyzer.

⚠ Warning Avoid shock hazard. Always move the power switch to the off (O) position before disconnecting or reconnecting the power supply. ▲

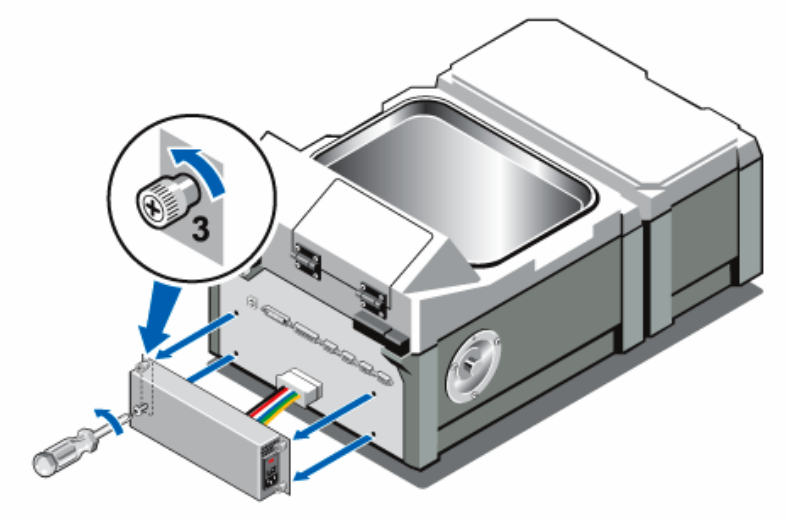
To replace the power supply:

1. **Disconnect the power cord from the power strip or wall outlet, and then disconnect the power cord from the analyzer**



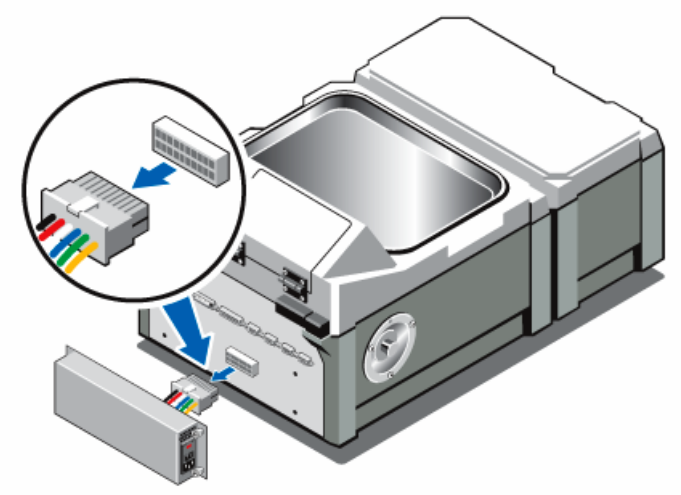
Note Three of the screws on the power supply module are thumbscrews, and the fourth screw is a Phillips screw. All four screws are tightened at the factory, so you will need a No. 2 Phillips screwdriver to loosen them.

2. **Loosen the screws that secure the power supply module to the back of the analyzer, and then remove the power supply from the back of the analyzer.**



3. **Disconnect the power supply cable from the back of the electronics module.**

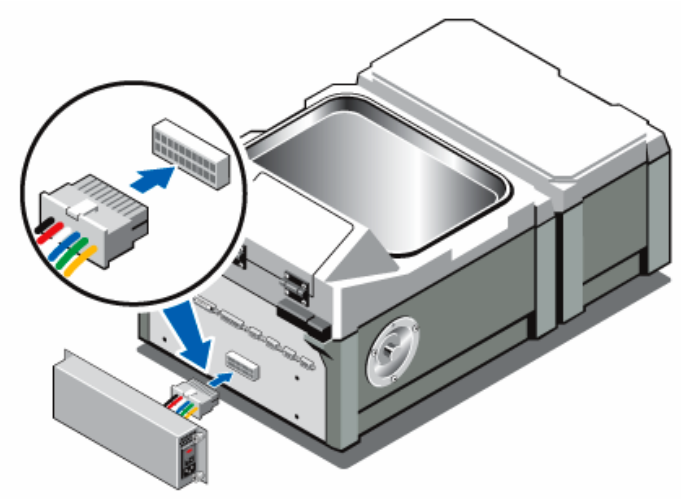
   Press the tab on the top of the connector to release the power supply cable.



Note Be sure to record the installation date and the serial number of the new power supply before you install it. Use Update Instrument Information from the Service menu of RESULT Operation software. ▲

4. **Connect cable from the new power supply module to the electronics module.**

   Make sure the tab on the cable connector snaps into place.

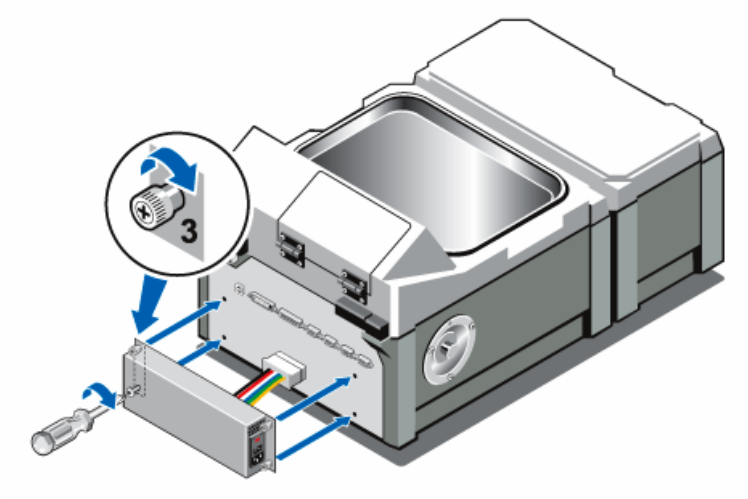


Notice Make sure no cables or wires get pinched under the power supply module when you attach it to the analyzer. ▲

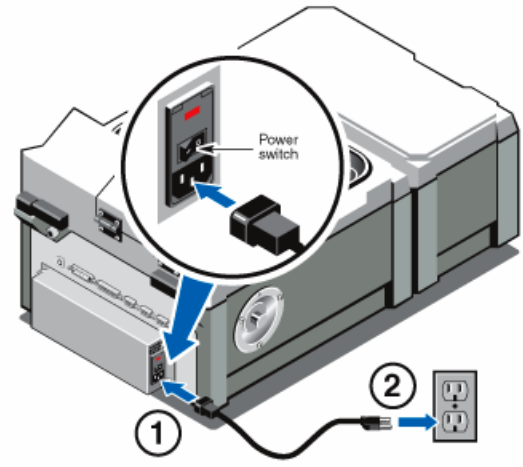
Note Three of the screws on the power supply module are thumbscrews that you can tighten without a screwdriver. The fourth screw is a Philips screw that you will need a No. 2 Phillips screwdriver to tighten. ▲

5. **Attach the new power supply module to the analyzer.**

   Tighten all of the power supply module screws, but do not overtighten them.



6. **Connect the power cord to the analyzer, and then connect the power cord to a wall outlet or power strip.**



7. **Turn on the analyzer.**

   The Power and Scan indicators on the front panel should light and the analyzer should function normally when you turn on the power. If the analyzer does not function normally, turn off the power and check the cable connections between the power supply, the analyzer, and the wall outlet or power strip. If the connectors are seated properly and the analyzer still does not function normally, contact Thermo Fisher Scientific Technical Support.

8. **Begin collecting spectra.**

Replacing the source

As with all light sources, the white light source in the Antaris II analyzer must be replaced occasionally. Use the following procedure if you need to replace the source in your analyzer. This procedure should take ten minutes or less and will require a No. 2 Phillips screwdriver.

⚠ Warning To avoid shock hazard, always turn off the analyzer and disconnect the power supply from the wall outlet or power strip before you replace the source. ▲

⚠ Caution The source bulb becomes extremely hot during normal analyzer operation. Always turn off the analyzer and allow the bulb to cool for at least 15 minutes before removing a source from the analyzer. ▲

Notice Never touch the new source bulb with your bare fingers. Skin oils or other deposits on the bulb will shorten its life. ▲

Notice The Antaris II source is pinned in place and pre-aligned. A system operator can easily replace it. Replacing the source should not affect measurement results. However, an improperly installed or handled source will affect the performance of the system. You may want to have source replacement done by a certified Thermo Fisher Scientific service engineer or trained Thermo Fisher Scientific on-site maintenance personnel. ▲

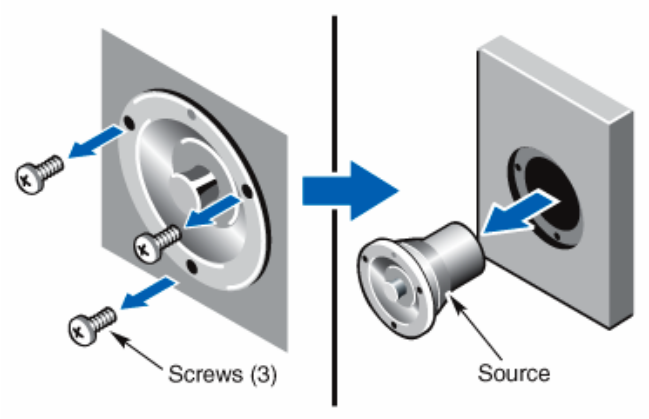
Note Be sure to record the installation date and the serial number of the new source before you install it. Use Update Instrument Information from the Service menu in the RESULT Operation software. ▲

To replace the source:

1. **Turn off the power to the analyzer.**

2. **Remove the screws that secure the source module to the analyzer.**

   Save the screws, you will need them when you install the new source.

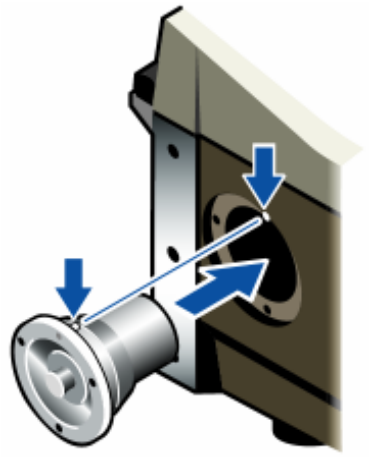


⚠ Caution The source bulb becomes extremely hot during normal analyzer operation. Always turn off the analyzer and allow the bulb to cool for at least 15 minutes before removing a source from the analyzer. ▲

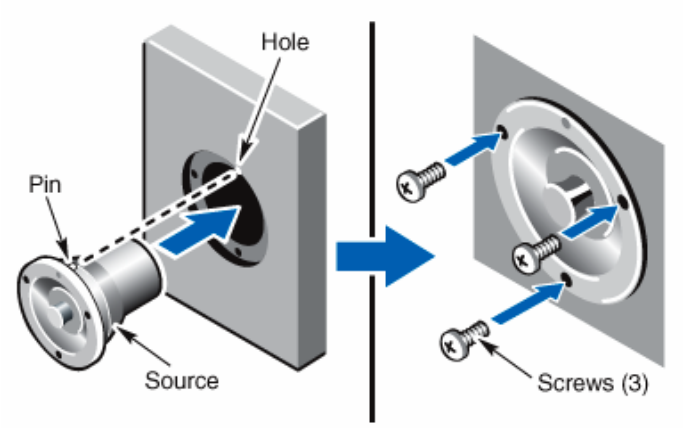
3. **Slide the source module out of the analyzer.**

4. **Slide the new source module into the analyzer.**

   Orient the source module so that the pin is aligned with the hole in analyzer chassis.



5. **Press on the source module until it is flush with the analyzer chassis and then secure it with the screws you removed earlier.**



6. **Turn on the analyzer, start RESULT and verify that the source is working properly.**

   If the new source is working properly, the Source indicator on the front panel remains lit after the power-up diagnostics complete. If the new source is not working properly, check to be sure that the source module is firmly seated and is flush with the analyzer chassis. If the source still does not work, contact Thermo Fisher Scientific Technical Support.

7. **Wait 15 minutes for the new components to stabilize thermally, and then align the analyzer.**

8. **If the analyzer is equipped with optional ValPro software, use it to confirm that the analyzer is performing properly.**

   Use the analyzer qualification procedures and/or run workflows developed for the analyzer, and confirm the results.

Note You may notice increased levels of water and carbon dioxide in spectra collected immediately after you change the source. If this interferes with your data, wait until equilibrium is re-established. ▲

9. **Begin collecting spectra.**

Replacing the laser

The Antaris II analyzer contains a HeNe laser that is used for timing interferometer scans. If the laser burns out or is not functioning properly, the analyzer will not scan. Use the following procedures to remove the old laser and install a new laser. Each of these procedures should take 15 minutes or less to perform. You will need a number 2 Phillips screwdriver, and a pair of needle-nose pliers may be useful as well.

⚠ Warning Before removing the faulty laser, turn off the analyzer power, disconnect the power cord from the wall outlet or power strip. ▲

Notice Although the laser can be replaced easily by the system operator, it is recommended that only certified Thermo Fisher Scientific service engineers or trained Thermo Fisher Scientific on-site maintenance personnel perform this operation. Whenever the main cover is open, there is a potential for damage to sensitive components. Damage to components inside the analyzer will affect the performance of the system. ▲

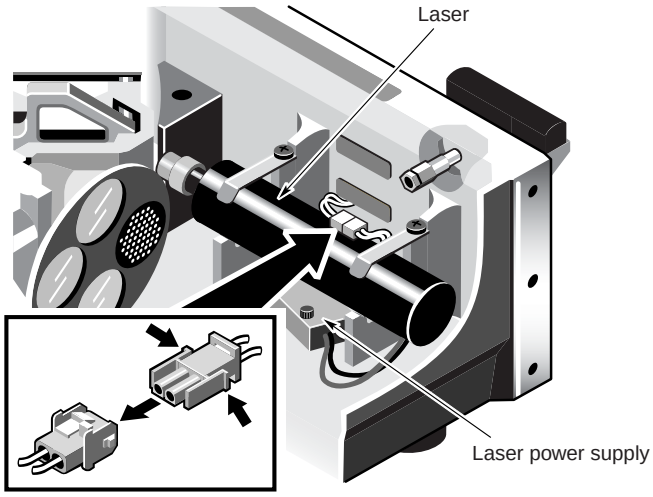
Notice If your system has the ValPro option, you may need to re-qualify your system prior to analyzing production samples. ▲

Note Use Update Instrument Information from the Service menu in RESULT Operation and record the installation date and the serial number of the new laser before you install it. ▲

To remove a laser:

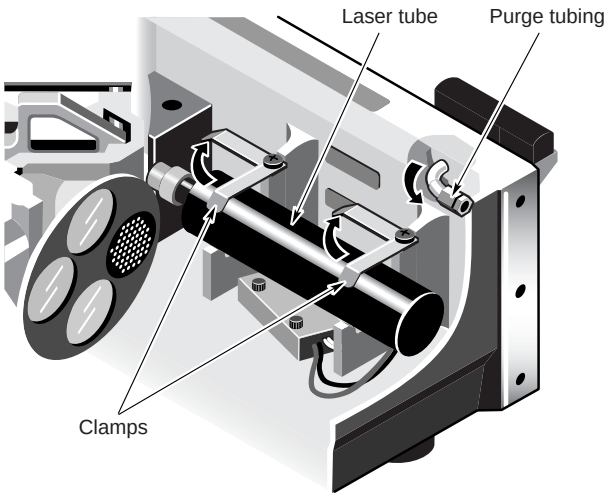
1. **Open the main cover and locate the laser and laser power supply.**

2. **Disconnect the laser power supply cable.**



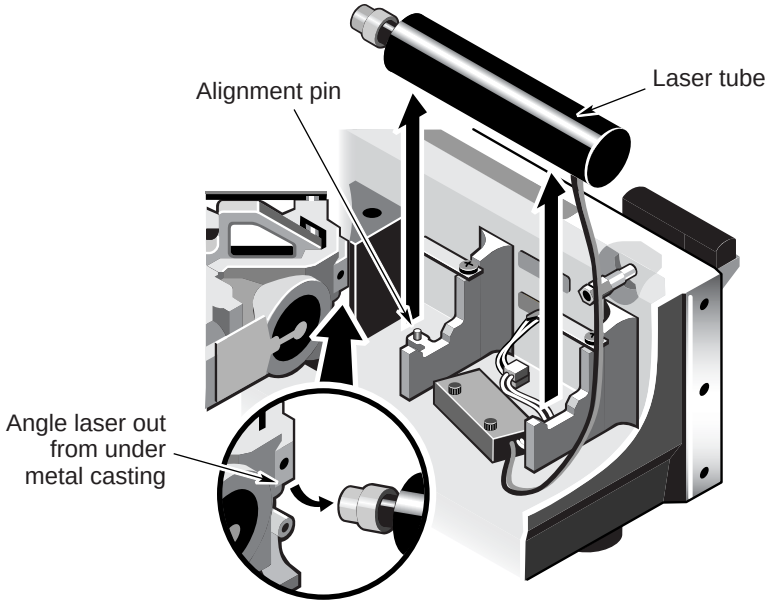
3. **Rotate the clamps that secure the laser tube.**

   The laser tube is held in position with two clamps and an alignment pin. Use a No. 2 Phillips screwdriver to loosen screws and then rotate the clamps off the laser tube. Do not remove the screws. Gently bend the purge tubing out of the way while you loosen the screw that secures the butt of the laser tube.



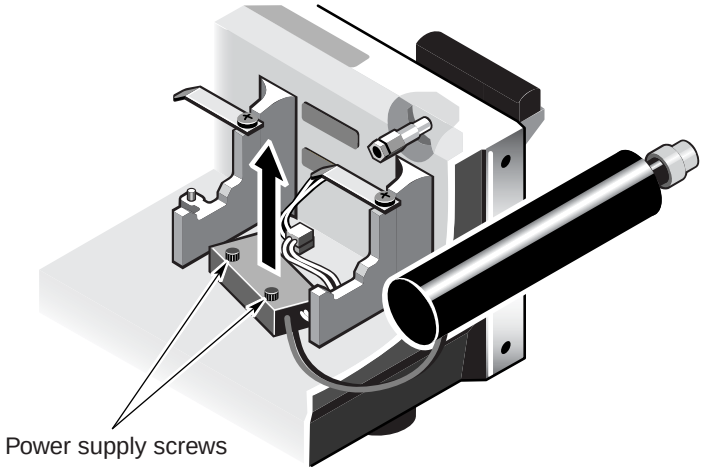
4. **Lift the laser straight up until it clears the alignment pin on the cradle and then angle the laser out from under the metal casting.**

5. **Remove the laser tube from the spectrometer. Hold the laser while you remove the laser power supply.**



6. **Remove the thumbscrews that secure the laser power supply to the analyzer baseplate and then lift the power supply out of the analyzer.**

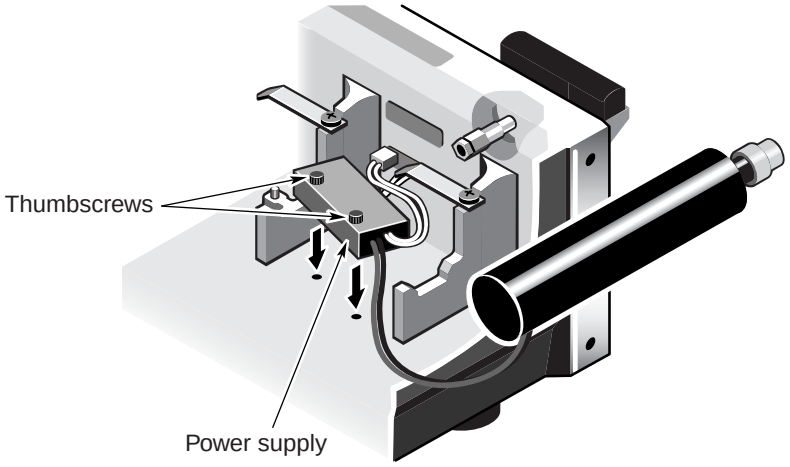
   Save the screws. You will need them to secure the power supply for the new laser.



To install a new laser:

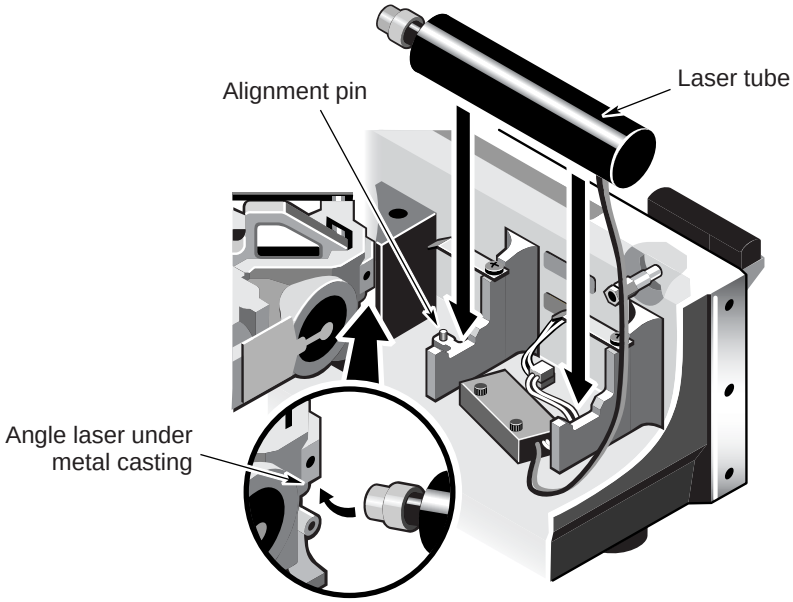
1. **Hold the new laser tube with one hand while you install the laser power supply.**

   Use the thumbscrews you removed from the old laser power supply and secure the new power supply to the analyzer baseplate.



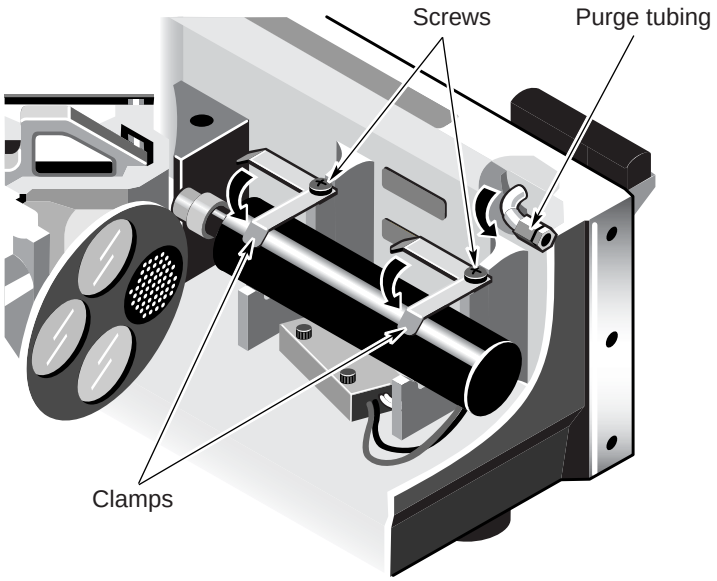
2. **Angle the laser tube under the metal casting and then lower it onto the cradle.**

   Be sure the hole in the laser is aligned with the pin on the cradle.



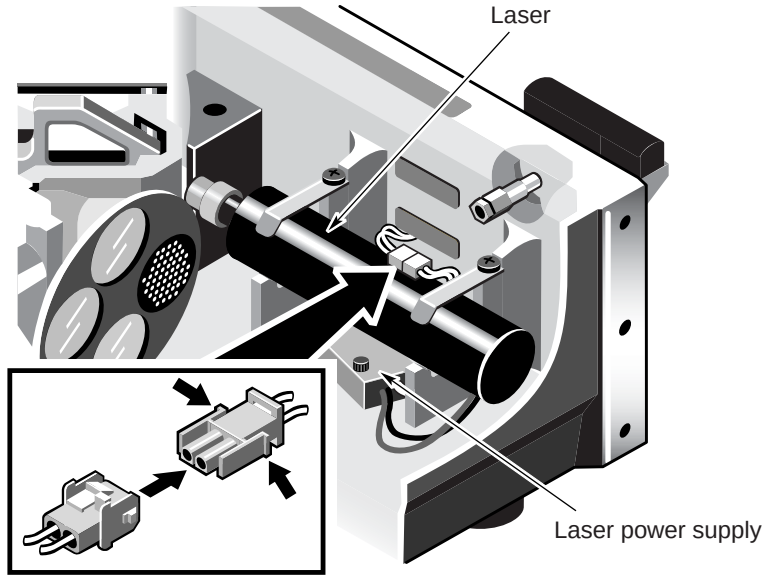
Notice Do not attempt to twist or turn the laser assembly once it engages the alignment pin. If the laser is misaligned the analyzer will not scan. ▲

3. Slide the clips over the laser tube and tighten the screws.



4. Connect the cable to the laser power supply.

The connectors are keyed so that you cannot plug it in backwards.



5. **Close the analyzer cover and secure it with the screws you loosened earlier.**

6. **Reconnect the power supply and turn on the analyzer.**

7. **Verify that the laser is working.**

   If the new laser is working properly, the Laser indicator on the front panel will be lighted. If the new laser is not working properly, check to be sure that the power cable is properly connected to the laser and that the main cover of the analyzer is securely fastened with the screws you loosened earlier. If the laser still does not work, contact Thermo Fisher Scientific Customer Support.

8. **Wait 15 minutes for the new components to stabilize thermally and then align the analyzer.**

9. **Use the analyzer qualification procedures and/or run workflows developed for the analyzer and confirm the results.**

   If the analyzer is equipped with optional ValPro software, run the ValPro Instrument Performance Tests to confirm that the analyzer is performing properly.

Notice You may notice increased levels of water and carbon dioxide in spectra collected immediately after you change the laser. If this interferes with your data, wait until equilibrium is re-established. ▲

Installing an optional purge kit

Antaris II analyzers are sealed and desiccated. Under normal operating conditions, this provides adequate protection against environmental humidity and corrosive elements which can damage the optical components inside the analyzer.

If the analyzer environment is excessively humid (above 95% noncondensing) or contaminated with potentially corrosive solvents or other corrosive agents, you can install an optional purge kit. For best results the purge gas should be dried to a dew point of -70 °C (-94 °F) or below. Use only dried air or nitrogen to purge the analyzer.

⚠ Warning Never use a flammable gas to purge the analyzer. The purge gas must be free of moisture, oil and other reactive materials. Use only dried air or nitrogen to purge the analyzer. Other gasses, even inert gasses such as argon (Ar), can damage the spectrometer. Never use them to purge the spectrometer. ▲

For this procedure you will need the following tools and supplies:

- 3/4-inch open-ended wrench
- 11/16-inch open-ended wrench
- Shutoff valve
- 1/4-inch male fitting or a 3/8-inch female fitting.

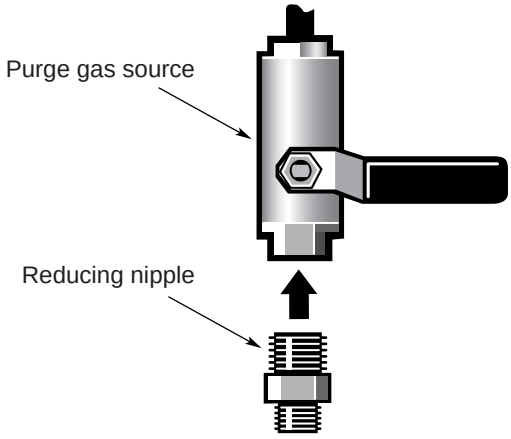
To install a purge kit:

1. **Install a shutoff valve and either a 1/4-inch male fitting or a 3/8-inch female fitting on the purge gas source.**

   Choose a shutoff valve and fittings that are appropriate for the purge gas source.

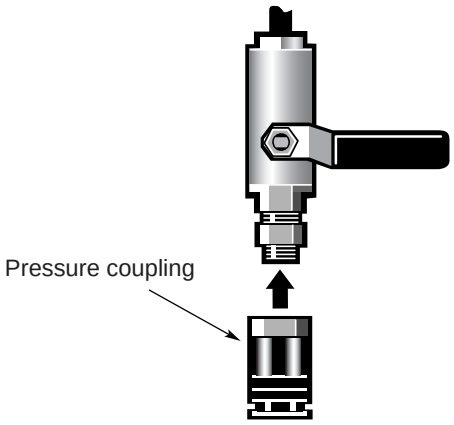
2. **If you used a 1/4-inch male fitting, go on to the next step.**

   If you used a 3/8-inch female fitting on the purge gas source, install the 3/8-inch to 1/4-inch reducing nipple that was included with the pre-installation kit. Use an 11/16-inch open-ended wrench to tighten the connection.



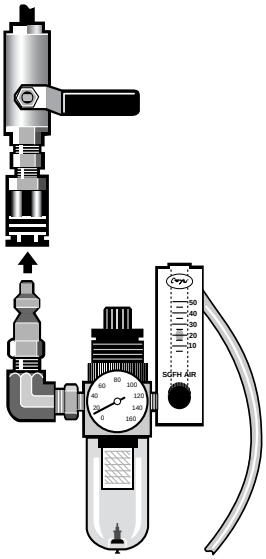
3. Install the pressure coupling.

Use a 3/4-inch open-ended wrench to tighten the connection.



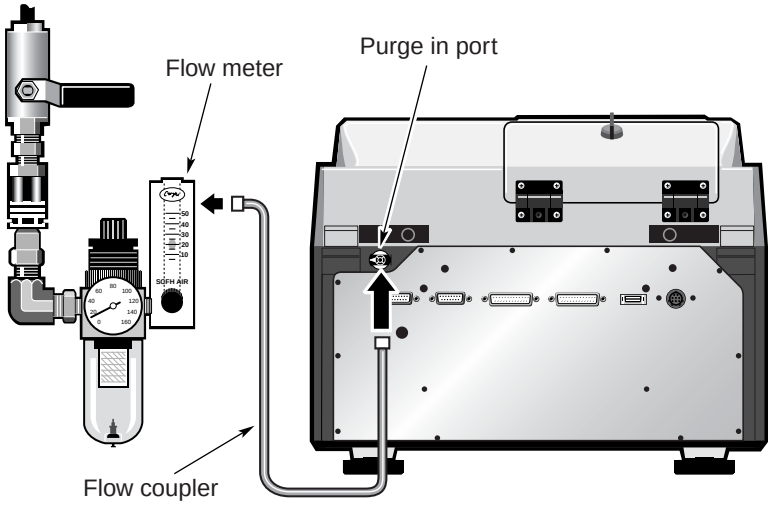
4. Install the purge filter, pressure regulator, and flow meter.

Snap the assembly into the pressure coupling.

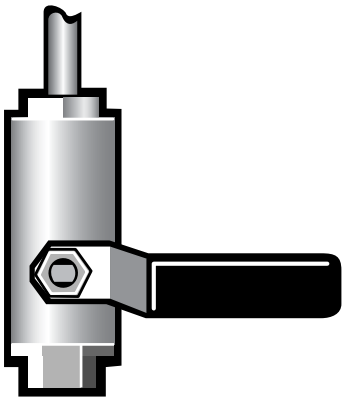


5. Connect the purge controls to the analyzer.

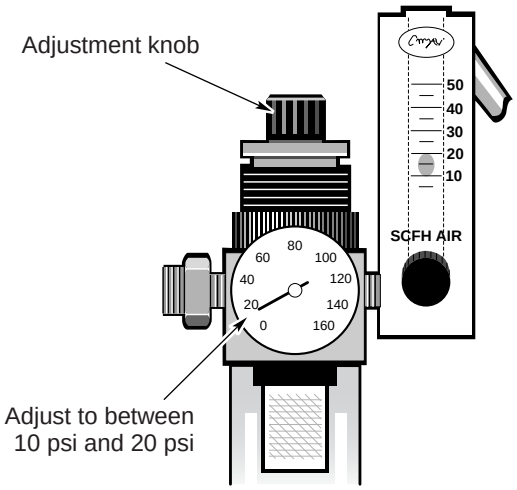
Snap the flow coupler into the Purge in port on the back of the analyzer.



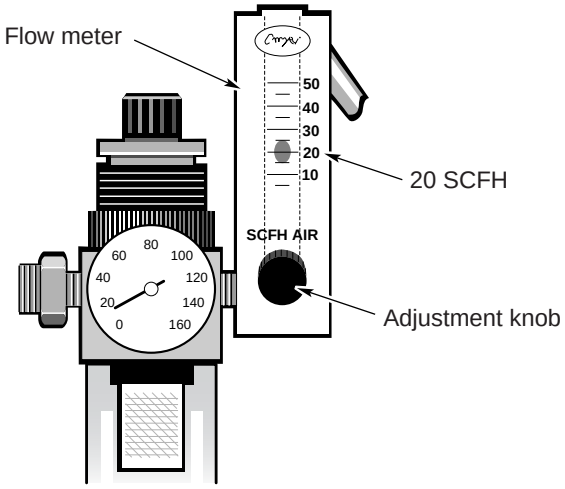
6. Turn on the shutoff valve.



7. **Adjust the pressure regulator until the gauge indicates that the pressure is between 10 psi and 20 psi.**

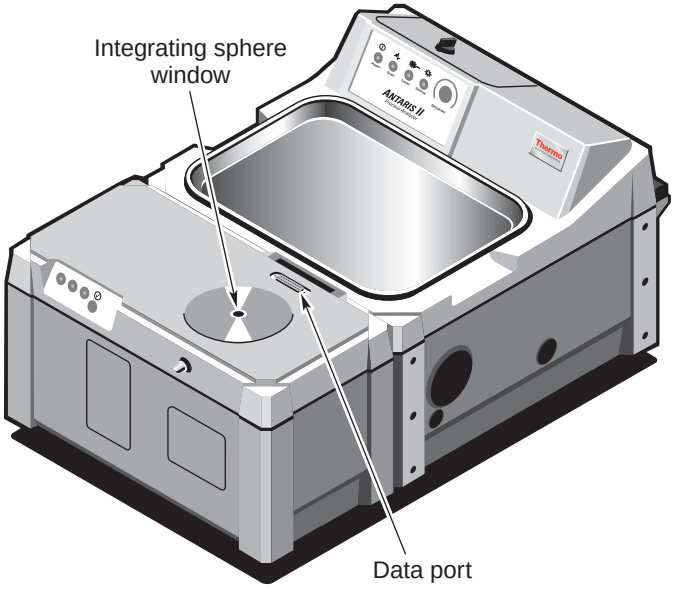


8. **Set the flowmeter to 20 SCFH.**



Maintaining the integrating sphere sampling module

Carefully read and follow the information in this section about storing and cleaning items in order to prevent damage to the sampling module and accessories.



Maintaining the integrating sphere sampling area

If residue accumulates on the integrating sphere sampling area and window, they can be cleaned by using a dry, soft cloth. If this is insufficient to clean the area, you can dampen the cloth with distilled water or isopropyl alcohol. Dry the sampling window with a clean, soft cloth, a jet of air, or allow the window to air dry.

⚠ Warning Do not pour liquids directly onto the sampling area of the instrument. This could pose a shock hazard if the liquid comes into contact with the data port. ▲

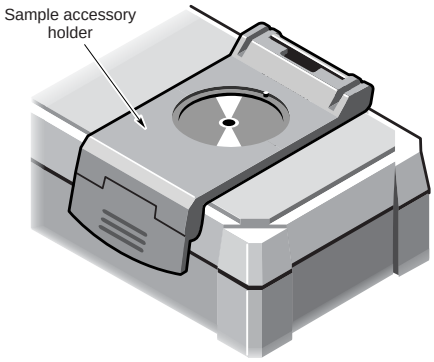
Notice Some chemicals, including, acetone, chlorine, fluorine, and amyl alcohol, can attack the epoxy seal around the integrating sphere window. Do not allows these chemicals to come into contact with the integrating sphere window. ▲

Maintaining sampling accessories

All sampling accessories should be stored in a dust-free enclosure when they are not in use. The following sections contain instructions for cleaning specific sampling accessories.

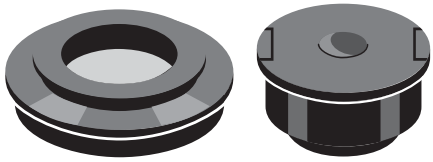
Cleaning the sample accessory holder

If residue accumulates on the sample accessory holder, it can be cleaned by using a dry or damp cloth and a mild soap solution, if necessary. Be sure to remove any residue left by the soap solution with a dry or damp, soft cloth. Dry the holder with a dry, soft cloth.



Cleaning the sample cups

Clean the Thermo Scientific sample cups with a mild soap solution and then rinse the cups in distilled water. Dry the cups with a jet of clean air or a non-abrasive cloth. Make sure the sample cups are dried thoroughly before storing them or using them for data collection.



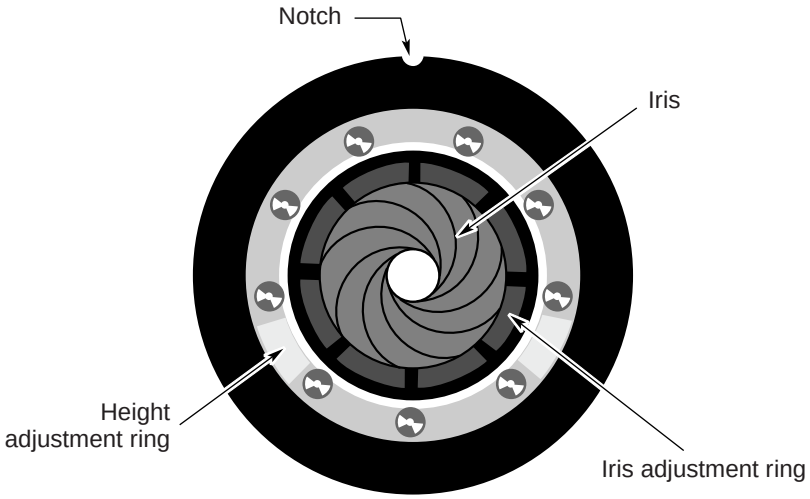
Sample cups

Cleaning the universal tablet holder

If the universal tablet holder accumulates residue, first attempt to clean it with a jet of clean air. If this is not sufficient, then gently rub it with a cloth dampened with isopropyl alcohol. Allow the universal tablet holder to air dry.

Notice Do not use water to clean the universal tablet holder. Water may cause parts of the tablet holder to rust. ▲

Notice The iris of the tablet holder is fragile. Handle the iris of the tablet holder gently when cleaning. ▲

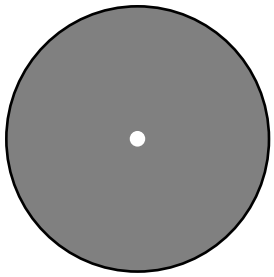


Universal tablet holder

Cleaning the custom tablet holders

If a custom tablet holder accumulates residue, it can be cleaned with a mild soap solution and rinsed with distilled water. The tablet holders can be allowed to air dry, or dried with a jet of clean air.

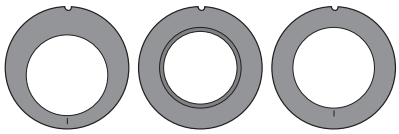
Notice Do not use harsh solvents to clean the custom tablet holders. Chemicals in solvents may damage the tablet holders. ▲



Custom tablet holder

Cleaning the sample rings

If the sample rings accumulate residue, they can be cleaned using a dry or damp, soft cloth. The cloth can be dampened using isopropyl alcohol, distilled water, or a mild soap solution. The sample rings can be dried with a cloth, or left to air dry.



Sample rings

Maintaining the transmission module

To help keep your *transmission module* in good operating condition, the following procedures are recommended:

Cleaning the sample tube holder

If the outside of the sample tube holder (either the heated or unheated version) becomes dirty or contaminated, follow these cleaning instructions:

Notice If the inside of the transmission module or a sample tube holder becomes contaminated, do not attempt to clean it. This could cause permanent damage to the equipment. Call Thermo Fisher Scientific to arrange a service visit. ▲

Notice Do not use any harsh abrasives, cleansers, chemicals, or solvents when cleaning your sample tube holder, and never immerse the sample tube holder. The heated sample tube holder contains electronic circuits that can be permanently damaged by exposure to water. ▲

1. **Prepare a cleaning solution.**

   Mix one part mild detergent with nine parts water in a clean container.

2. **Dampen a soft, clean cloth with cleaning solution.**

   The cloth should be just damp, not wet.

3. **Use the damp cloth to clean the dirty or contaminated areas of the outside of the sample tube holder.**

Notice To avoid permanent damage to your analyzer, always make sure that your sample holders are completely dry before installing them in the transmission module. ▲

4. **Dry the sample tube holder with an air line, or allow the sample tube holder to dry for at least five minutes (until it no longer feels damp) before installing it in the transmission module.**

Cleaning an aperture

If an aperture becomes dirty or contaminated, follow these cleaning instructions:

1. **Remove the contaminated aperture from the sample tube holder.**

   For more information, see "Using apertures with liquid samples" in the "Transmission Module" chapter.

Notice Do not use harsh abrasives, cleansers, chemicals, or solvents when cleaning an aperture. ▲

2. **Prepare a cleaning solution.**

   Mix one part mild detergent with nine parts water in a clean container.

3. **Dampen a soft, clean cloth with cleaning solution.**

   The cloth should be just damp, not wet.

4. **Use the damp cloth to clean the aperture.**

Notice To avoid permanent damage to your analyzer, always make sure that your sample holders are completely dry before installing them in the transmission module. ▲

5. **Allow the aperture to dry for at least five minutes (until it no longer feels damp) before inserting it into a sample tube holder.**

Cleaning the SabIR probe

If the tip or shaft of the SabIR becomes dirty or contaminated with sample or other material:

- **To clean the probe tip**: prepare a cleaning solution of one part isopropyl alcohol with nine parts water in a clean container. Using an eye-dropper, place a small amount of the mixture on a fresh piece of lens paper. Gently rub the lens paper on the optical window for 10 to 20 seconds. Allow the window to air dry for at least two minutes.

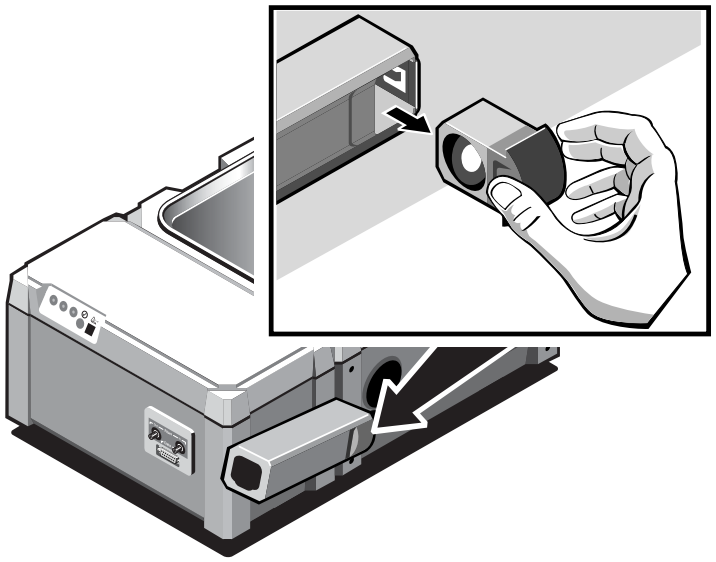
- **To clean the probe shaft**: prepare a cleaning solution of one part isopropyl alcohol with nine parts water in a clean container. Pour a small amount of the mixture onto a soft cloth and gently rub the cloth on the probe shaft for 10 to 20 seconds. Allow the shaft to air dry.

Maintaining the Spectralon reference

Spectralon is an optical standard and should be handled in much the same way as other optical standards. Although the material is quite durable, care should be taken to prevent contaminants such as finger oils from contacting the material's surface. It is a good idea to wear clean gloves when handling the material.

Removing the Spectralon reference from the holster

Keep the Spectralon reference in the holster at all times, unless you need to clean it or replace it. To remove the reference from the holster, firmly grasp both sides of the compartment with your thumb and forefinger and pull it out of the side of the holster.



Notice Avoid touching the surface of the Spectralon reference with your fingers. Dirt and oils from your fingers can leave residue on the sample. ▲

Cleaning the Spectralon reference

To clean the Spectralon reference:

- First, clean it with an air brush, using clean, dry air or nitrogen.
- If this does not sufficiently clean the sample, gently sand it with a 220-240 grit waterproof emery cloth.
- If using high reflectance Spectralon (>90% reflectance) and the sample is still not sufficiently clean, sand the reference under running water with a 220-240 grit waterproof emery cloth until water beads and immediately runs off the surface. Dry the sample with a jet of clean, dry air (i.e., no moisture) or nitrogen, or allow the material to air dry.

If the background quality does not improve after thoroughly cleaning the Spectralon reference, the reference may need to be replaced. See "Servicing the Antaris Analyzer" in the Service menu of RESULT Operation for information on replacing your Spectralon reference.

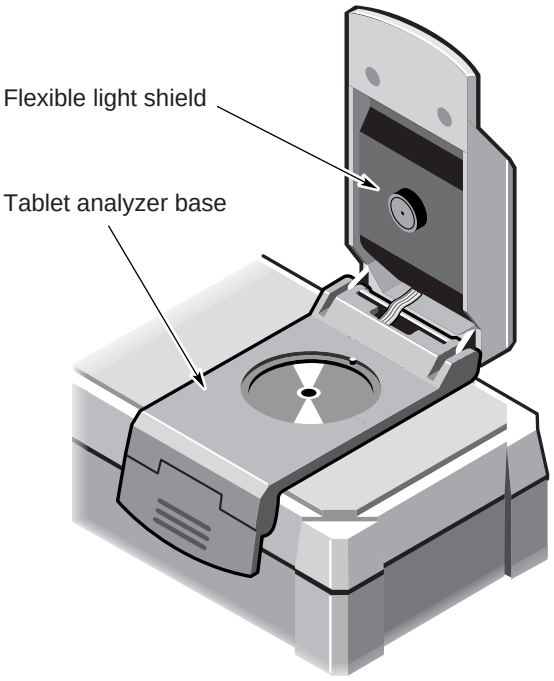
Maintaining the tablet analyzer sampling module

Carefully read and follow the information in this section about storing, removing, and cleaning items in order to prevent damage from occurring to the sampling module and accessories.

Maintaining and storing the tablet analyzer

When the tablet analyzer is not connected to the instrument, store it in a dust-free environment. It is recommended that you store the tablet analyzer in an anti-static bag.

Parts of the tablet analyzer may accumulate debris or become contaminated from sample materials. Follow the recommendations in this section for cleaning and maintaining the tablet analyzer components. Because the tablet analyzer has an electrical connection, if you need to remove the tablet analyzer, it is recommended that you power off the instrument.



Tablet analyzer

Cleaning the flexible light shield

If the flexible light shield accumulates residue or becomes dirty, it can be carefully cleaned using a smooth cloth lightly dampened with distilled water. Do not use solvents, soaps, or any other chemicals to clean the flexible light shield.

Notice Take care not to push any dirt into the hole in the center of the flexible light shield. Do not use sharp objects to clean the flexible light shield or to remove any dirt that may have fallen into the shield hole. The window on the transmission detector could become damaged or contaminated. ▲

Cleaning the tablet analyzer base

If residue accumulates on the tablet analyzer base, it can be cleaned by using a dry or damp cloth and a mild soap solution, if necessary. Be sure to remove any residue left by the soap solution with a dry or damp, soft cloth. Dry the tablet analyzer bottom with a dry, soft cloth.

Notice Because the tablet analyzer has an electrical connection, be sure to power off the instrument and remove the tablet analyzer before cleaning it. ▲

Chapter 8 Accessories and Options

This section may be used to store operating manuals for any component options and sampling accessories for your Antaris II analyzer, whether you purchased those options and accessories with the system or afterwards. For information about the component options and sampling accessories available for the Antaris II analyzers, contact your Thermo Fisher Scientific representative or visit our web site at www.thermo.com/spectroscopy.

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Glossary

A

absorbance A measure of how much of the incident radiation that is directed at a *sample* is absorbed by the sample. Absorbance is defined by the formula $A = \log_{10} (1/T)$, where T is the fractional *transmittance*.

access key A key that corresponds to an underlined letter in a RESULT window. To carry out a command using the keyboard, press ALT plus the appropriate access key.

Acknowledge button A green button to the right of the LED indicators on the *Antaris, Antaris II* and *Antaris MX* analyzers. The Acknowledge button allows an operator to respond to a software prompt from the instrument instead of at the computer. You can enable or disable the Acknowledge feature when developing a *workflow* in *RESULT Integration software*.

administrator A user who has special *rights* to an operating system and/or specific application. Administrators usually have the ability to set up user accounts and modify system settings. See also *RESULT administrator*.

algorithm A procedure for solving a problem.

ambient temperature The temperature of the immediate surroundings of an object. When referring to an object inside the *analyzer*, the ambient temperature is the temperature inside the analyzer. When referring to the analyzer itself, the ambient temperature is the temperature of the location where the analyzer is being used, such as the room temperature or, if the analyzer is installed in a *rack enclosure*, the temperature inside the enclosure.

analyzer An instrument used for chemical analysis. An analyzer is usually dedicated to a specific type of analysis.

Antaris and Antaris II systems An instrument used for *near-infrared transmission*, *diffuse-reflection*, or *fiber optic transflection* analysis of liquids, powders, and solids, including pharmaceutical tablets. The analyzer can accommodate up to four different *sampling modules*, including a *transmission module*, *tablet analyzer module*, *fiber optic module*, and *integrating sphere*.

Antaris EX system A *near-infrared* fiber optic analyzer designed for in-line quality testing in industrial environments. The analyzer is available in multiple configurations. Several configurations are certified for use in environments rated for specific hazards. The system features simultaneous data collection from up to four fiber optic accessories and an internal reference for automatic background measurements.

Antaris IGS An instrument dedicated to *mid-infrared transmission* analysis of gas samples.

Antaris Method Develop Sampling (MDS) system An *Antaris* or *Antaris II* near-infrared analyzer that includes the *integrating sphere* for diffuse-reflection sampling of solids and powders; the *transmission module* for transmission analysis of liquids, transparent solids, and films; and the *fiber optic module* with SabIR™ probe for collecting diffuse-reflection spectra from powders and solids. Optional *tablet analyzer modules* are also available for collecting transmission and diffuse-reflection data from tablet samples.

Antaris Multiplexer system An instrument dedicated to *near-infrared* analysis of samples in remote locations using up to twelve different *fiber optic accessories*. The analyzer is available in two configurations, one with six *channels* for connecting fiber optic accessories, and one with twelve channels for connecting accessories.

Antaris MX system A compact *near-infrared* analyzer for fiber optic measurements. The analyzer is capable of collecting data from up to four *fiber optic accessories* at the same time with automatic background measurements using an internal background reference. The analyzer is available in two configurations, one with two *channels* for connecting fiber optic accessories, and one with four channels for connecting accessories. Each channel has a dedicated *detector*.

Antaris Target Blend system A compact, *near-infrared* analyzer dedicated to real-time monitoring of pharmaceutical powder blending. Features include battery power, wireless communication and *MEMS*-based spectrometer. When used as a *production system*, the instrument can be quickly moved from one blender bin to another. A *bench top sampling kit* and AC power adapter support bench top use for analysis, method development and testing.

aperture An opening that controls the amount of light that reaches a sample. The *Antaris* and *Antaris II analyzers* have a standard fixed aperture or an optional two-position aperture. The two-position aperture is required for the highest *resolution* settings. The *Antaris IGS* includes a variable aperture. The software sets the aperture automatically. The *three-position cuvette/culture tube holder*, or *sample card holder*, for the *transmission module* comes with a removable aperture that is primarily used with culture tubes and vials. The *Antaris MX and the Antaris Target Blend analyzers* do not have an aperture.

Apodization A feature available in some sample specifications in *RESULT Integration*, such as the gas cell sample specification for the *Antaris IGS*. Apodization mathematically removes peak side lobes that can occur because the *interferogram* is not an infinite set of data. Apodization is performed automatically before the *Fourier transform*. Strong apodization reduces the *resolution* of the data and broadens *peaks*.

Archive event A *workflow event* in *RESULT Integration* for archiving spectra and reports. The spectra and reports are automatically saved in the software's specified location for archiving spectra and reports. Each archived spectrum or report is saved with a unique file name.

archiving The process of storing *files* on a computer disk. In *RESULT software*, *workflows*, *reports*, *spectra*, *method files*, and *standards* can be archived in a specific *directory*.

attenuator 1) A component inside the instrument that filters the amount of energy sent to a *sample*. 2) A parameter in some *sample specifications* of *RESULT Integration* that specifies a position or setting for the *attenuator*.

audit log database A database used to track and log items in *RESULT Integration*. The audit log tracks changes made to software settings; pass/fail results, results of instrument qualification runs and *verification workflow* runs; values of items stored from workflow runs; and entries made into the software's on-line service log. Through RESULT Integration, the audit log can be *queried* to produce reports. When an operator performs a query, the audit log can verify the integrity of the data being queried and note any *suspect data*.

autosampler A hardware device for the *Antaris* and *Antaris II* analyzers that allows automated sampling of solids, powders and tablets.

B

background see *background spectrum*

Background Frequency A collect event or collect sequence event parameter in *RESULT Integration* that specifies when to collect a background for ratioing sample spectra produced by the event.

background preview A live background display window that accompanies an operator prompt for background collection from a workflow. Data collection begins when the operator chooses the Continue button in the prompt. Background preview allows the operator to verify the quality of the background data before collection.

background prompt An operator prompt in *RESULT software* that appears before background collection when the workflow is run. Background prompts are generated by *prompt specifications* attached to *collect events* in *workflows*.

background specification A *workflow specification* in *RESULT Integration* that defines data collection for background spectra generated by a workflow, based on the background location or sampling technique.

background spectrum A reference spectrum that accounts for the unique optics of an instrument, sampling module and sample holder, if used. The background spectrum is the result of the output of the source, the response of the beamsplitter optics and detector, and any atmospheric absorptions inside the analyzer. If the background is collected through a sampling module, sample holder or gas cell, then the background spectrum also includes the characteristics of the module, holder or cell. Sample spectra are ratioed against a background spectrum so that the final spectrum is free of those features.

band A spectral region containing a peak.

base name The prefix used to name a group of files, workflow events, or specifications in *RESULT software*.

baseline The portion of an absorbance spectrum that is not part of the peaks. The baseline represents those regions where the sample absorbs little or no energy.

beam In an instrument, the stream of infrared light emitted by the *source* that travels through to a *detector*.

beam path The route followed by the infrared beam as it travels from the *source* to a *detector*. In some Antaris analyzers, the beam path may change depending on the *sampling module* and accessories used and the *sampling technique*.

beamsplitter A device inside the *Michelson interferometer* that splits the infrared beam coming from the *source* into two beams of nearly equal energy. Usually one beam passes through the beamsplitter, is reflected from the interferometer's *moving mirror* and returns to the beamsplitter. The other beam is reflected from the beamsplitter and then is reflected from the interferometer's *fixed mirror* and returns to the beamsplitter. The recombined beam exits the interferometer, passes through or is reflected by the sample and travels to the detector. See also *Fabry-Perot interferometer*.

bench top sampling kit A collar that attaches to the *Antaris Target Blend Analyzer* to permit bench top sampling using powder sample cups, which are placed on top of the collar.

block heater A free-standing unit designed to heat samples held in metal blocks that have openings to accept a variety of different kinds of sample containers.

C

Calculate event A *workflow event* in *RESULT Integration* that instructs the software to calculate statistics using the results from a specified *measure event* and the specified settings for the calculation parameters. Each time a calculation event is performed by a workflow, the workflow produces a set of statistical data, referred to as the calculation result.

calibration 1) The process in which the software analyzes a set of *standards* in order to calculate a *method model* for predicting component concentrations or classes from unknown samples. 2) The process in which an analyzer adjusts the digitizers and amplifiers in the main board of an instrument for optimal performance of the *attenuator* and *detector* gain.

calibration spectrum The spectrum of a *calibration standard*.

calibration standard A *standard* that is used to create the *method model* during *calibration*. In TQ Analyst, calibration standards are also used to calculate a *correction curve*, if one is specified.

channel A sampling location where there is both an output and an input for the infrared beam, such as on a *fiber optic module* or *multiplexer module*.

channeling see *fringing*

check box A selection box in a software dialog box that turns a feature or option on or off. If a check mark (✓) appears in the box, then the feature or option is turned on. If the box is blank, then the feature or option is not turned on.

check event A *workflow event* in *RESULT Integration* for testing the status of a specified item using the indicated settings for the check parameters and a *logical test specification*. When performing a check event in a workflow, the software produces a pass or fail result.

check sample A *sample* for which the sample composition is known.

class A group of *standards* that have a common set of characteristics.

Classical Least Squares (CLS) A *quantitative method* in *TQ Analyst* that looks at many regions of the unknown sample spectrum to find relationships between *absorbance* and *concentration*.

classification analysis To find the *standard* or *class* that most closely matches an unknown *sample spectrum* or verify that the sample spectrum is similar to the spectra in a specified class.

classification method A TQ Analyst *method* that finds the *standard* or *class* that most closely matches an unknown *sample spectrum* or verifies that the sample spectrum is similar to the spectra in a specified class. Classification methods are also known as *qualitative methods*.

classify To find the *standard* or *class* that most closely matches an unknown *sample spectrum* or verify that the sample spectrum is similar to the spectra in a specified class.

class-selection dialog box A *dialog box* developed using a *request event* in *RESULT Integration* that requests the operator to specify the type (class) of material to be analyzed by selecting an option from a list of materials the *workflow* is set up to measure.

clipboard A special memory resource used in *RESULT Integration* that stores a copy of the last information that was *copied* or *cut*. The information on the clipboard can then be *pasted* into another workflow file. *Workflow events* and *specifications* can be cut or copied and pasted into other workflows.

CLS see *Classical Least Squares*

Collect event A *workflow event* in *RESULT Integration* that instructs the workflow to collect an infrared *sample spectrum* based on a *sample specification*.

Collect Dual Tablet event A *workflow event* in *RESULT Integration* that instructs the workflow to collect a *transmission spectrum* and a *reflection spectrum* at the same time with a *tablet analyzer module*.

collection events A group of events in *RESULT Integration* that can be used to collect data from various *sampling modules*. The group includes the *collect event*, which can be used with any sampling module, the *collect dual tablet event*, which works only with the *tablet analyzer modules* (standard and softgel), and the *collect multi-channel event*, which can be used only with the *Antaris MX* and *Antaris EX systems*.

Collect Multi-Channel event A *workflow event* in *RESULT Integration* that instructs the workflow to collect *sample spectra* from selected fiber optic *channels*. Each channel can be linked to a unique *sample specification* optimized for a particular fiber optic accessory, and an optional *background specification* and *sample correction specification*. Sample collection occurs at all defined channels simultaneously.

The collect multi-channel event works with *Antaris MX* and *Process EX* systems only. Collect multi-channel events can also be used to collect spectra with the *validation wheel* if a wheel is installed in the instrument and properly configured in the software.

collection phase see *data collection phase*

Collect Sequence event A *workflow event* available in *RESULT Integration* when the *sequence module* add-in option is installed. A collect sequence event instructs the workflow to collect a series of sample spectra over a specified period of time based on a *sample specification*. Archived spectra are saved in the *Nicolet sequence file* format.

command A word or phrase in a *menu* that you can choose in order to perform an action.

Comma-Separated Values (CSV) A file format for saving spectra as a text delimited file that specifies each data point in the spectrum as a set of X and Y values. The values may be separated by a list separator (defined by the Windows regional settings) or a tab. CSV formatted files can be read by any compatible spreadsheet or other program. CSV files are saved with an extension of .csv.

Compare event A *workflow event* in *RESULT Integration* that instructs the software to measure the spectra from the specified *collect events* using the indicated *measurement specification* and then compare the measurement results (calculated values) using standard statistical techniques.

component A chemical compound contained in a *sample mixture.* In *RESULT software,* a property of a sample mixture may also be referred to as a sample component.

computer name A name assigned to a computer on a Windows network. Each *RESULT User's Guide* computer on a network is assigned a unique computer name.

concentration The amount of a *component* in a given volume or area.

conditional test A test in a *workflow event* that applies a *logical test specification* to an event or group of events and performs an action based on whether the logical test specification is determined to be true or false.

configuration files In *RESULT software*, *files* that contain the settings for how the software works. The configuration files contain software options that are enabled or disabled, such as user settings, workflow settings, and ValPro settings.

Configure Temperature/Pressure event A *workflow event* available in *RESULT Integration* when the software is configured for use with a gas analyzer such as the *Antaris IGS*. A configure temperature/pressure event defines the source for the gas cell temperature and pressure values that will be saved with each collected spectrum (i.e., read from a hardware device or entered manually). Systems that include a temperature controller can also use a configure temperature/pressure event to set up or adjust the controller.

control chart see *trend chart*

Copy A *command* that accesses *RESULT Integration*'s memory features. Information can be copied and stored onto the software's *clipboard* and then *pasted* into another workflow file. The stored information will remain on the *clipboard* until it is replaced by another item of information or until the computer is shut down.

correction curve A zero-order, linear, or higher order polynomial which can be applied to the concentration values calculated by a calibrated *method* to improve the accuracy of the analysis.

correction specification see *Sample Correction Specification*

correction standard A *standard* that is used along with the *calibration standards* to calculate a *correction curve*. Correction standards are not used in *calibration*.

correlation coefficient A measure of the linear relationship between two variables. A value of "one" implies that there is a direct linear relationship between two variables. A value of "zero" implies that there is no correlative relationship between the two variables. Correlation coefficients are produced by a *compare event* in *RESULT Integration*.

CSV see *Comma-Separated Values*

culture tube An inexpensive, cylindrical sample container that is usually made of glass or plastic.

Cut A *command* that accesses *RESULT Integration's* memory features. A cut item is removed from a file and stored on the application's *clipboard* until it is replaced by another item of information, or until the computer is shut down.

cuvette A rectangular sample container that is typically made of quartz. Cuvettes are frequently used when high accuracy is needed such as when performing *quantitative analysis*.

D

dark background correction A correction applied to reflection spectra collected by a workflow to remove contributions from interfering back reflections. Such back reflections can be from the face of a glass vial or other container used for the sample measurement or from unwanted material clinging to the surface of the sample window or, in some cases, the window itself. Requires a *sample correction specification* and a *dark background spectrum*.

dark background spectrum A single beam reflection spectrum that represents the sum of all back reflections that are present in the sample measurement but cannot be attributed to the sample material. The spectrum is used in a *dark background correction*.

data archive The *directories* where data, such as *reports* and *spectra* produced from *workflows*, is stored. In *RESULT Integration*, the *path* for data archives is specified by the *RESULT administrator* in the RESULT Options dialog box. In *RESULT Integration*, the path for data archives is specified in the Options dialog box.

data collection phase A period of continuous data collection in a sequence experiment. The number of data collection phases in a *sequence data set* is determined by the number of *collect sequence events* included in the corresponding *run sequence event* group.

Data Format A collection parameter in *RESULT Integration*. Data Format defines the Y-axis unit that will be used to display or plot the *sample spectrum* in a *sample report*.

data source A vendor-independent link to a database. *RESULT software* uses a data source to access the *RESULT audit log database*.

database A file consisting of a number of records or tables, along with a collection of operations that facilitate *querying*, sorting, and other activities.

date stamp A date/time string generated by the software as a unique identifier for a particular *audit log* record or archived file. The software creates an identifier based on the date and time the record or file was created. The date stamp includes the current month, day, time and year in GMT (Greenwich Mean Time) format plus a three-digit index number.

Delay event A *workflow event* in *RESULT Integration* that instructs the software to pause the *workflow* for a specified interval. A delay event can be used to allow the instrument to stabilize before starting data collection, or to pause the instrument between periodic data collections.

detector A device inside the instrument, sampling module, or accessory that produces an electrical signal in response to the infrared beam striking it. The Antaris near-infrared instruments use *InGaAs* (indium gallium arsenide) detectors. The Antaris mid-infrared *instruments* can use a *TGS (or DTGS)* or *MCT detector*.

device-specific workflow event A *workflow event* in *RESULT Integration* that allows the workflow to control a particular hardware device such as an *autosampler* or *temperature controller*. Some example device-specific workflow events include position autosampler events, position multiplexer events, and *configure temperature/pressure events*.

dialog box A window in a software application that solicits a response from the user. Dialog boxes usually contain groups of related information or options that the user can specify. Most dialog boxes allow the user to close the box by choosing an OK button to save any items that have been specified, or a Cancel button to close the dialog box without saving any settings.

diffuse reflection A spectroscopy technique that measures changes that occur in an infrared *beam* when the beam interacts with a particulate sample. The radiation alternately passes through particles and reflects off their surfaces. This causes the light to scatter, or "diffuse," as it makes its way through the sample. An output mirror collects the diffusely scattered energy and sends it to a *detector* in the analyzer. The detector records the altered beam as an electrical signal, which can be used to generate a spectrum.

digital signature An electronic signature based upon cryptographic methods of originator authentication, computed by using a set of rules and a set of parameters such that the identity of the signer and the integrity of the data can be verified.

directory A way of organizing files on a disk or drive. Directories are usually set up in a tree-like structure and appear as folders in Windows applications. Data can be stored in directory folders.

disabling The process of suspending a feature, workflow, or user account. Disabling makes a feature inactive or suspends a workflow or user account without deleting it. It can then be enabled in the future.

Discriminant Analysis A *qualitative* (*classification*) *method* in *TQ Analyst* that uses multiple standards and multiple *classes* to determine the class or classes of known materials that are most similar to an unknown material. The method reports a list of classes ranked from best match to worst match, and a distance value for each class.

display area In *RESULT Integration*, the region in the main *window* used to display either the general instructions for the selected *workflow event* or the parameter settings for the selected *workflow specification*. In *RESULT Operation*, the region in the main window used to display *spectra* , *trend charts*, and *sample reports*. See also *Spectra tab*, *Trend tab*, and *Report tab*.

display settings file 1) For a given *sequence data set*, a display settings file defines the number of panes in the curve data frame, the order and display mode of the component curves, and the display limits and colors for displayed component curves and spectra. A unique display settings file can be associated with each sequence data set. 2) For the Trend tab display in *RESULT* Operation, a display settings file specifies whether the software will create a graph of trends or display the data in a table, or both of these options. A display settings file can also define styles and labels for the graph and column headings for the table.

Distance Match A *qualitative* (*classification*) *method* in *TQ Analyst* that uses multiple *standards* and multiple *classes* to determine how closely an unknown material matches each class. The method reports a list of classes ranked from best match to worst match, and a match value for each class.

domain A collection of computers that share a common database on a Windows network. Each domain has a unique name on a network.

drop-down list A list inside a box that allows you to select one of a number of options. The list has an arrow button on the right side of the box. Click the arrow button to reveal the list of options.

DTGS detector see *TGS detector*

E

electronic signature A computer data compilation of any symbol or series of symbols executed, adopted, or authorized by an individual to be the legally binding equivalent of the individual's handwritten signature.

event see *workflow event*

expected value The known *concentration* value or spectral measurement for a *spectrum*. Expected values are used by *compare events* in *RESULT Integration*.

F

Fabry-Perot interferometer A device that uses a filtering mechanism to split and then recombine a light beam. The process causes selective interference, allowing one wavelength to pass at a time. This type of interferometer is used in the *Antaris Target Blend* analyzer, which measures the energy at each wavelength over a defined analysis range. The output signal is a *single beam spectrum*.

fiber optic accessory A sampling accessory that uses fiber optic technology to transport a beam of light from an *FT-IR* or *FT-NIR analyzer* through the accessory, where the beam interacts with a sample, and then back to the analyzer. The analyzer can then use the "changed" beam to create a *sample spectrum*.

fiber optic cable A bundle of thin glass or plastic transparent fibers that are enclosed by a less refractive material. The fibers transmit light by internal reflection.

fiber optic port A port on a *fiber optic module* or *multiplexer module* that serves as a connector for a *fiber optic accessory*. Fiber optic ports come in pairs to accommodate the in/out path of a fiber optic accessory.

fiber optic module The module of the *Antaris, Antaris II*, *Antaris MX* and *Antaris EX analyzers* that allows users to collect spectra from remote locations using one or more *fiber optic accessories*. See also *multiplexer module.*

fiber optic shunt A fiber optic cable that directs the infrared beam directly from the input *channel* to the output channel without passing through a sample. A fiber optic shunt minimizes the loss of beam intensity and is typically used as an external reference.

file A collection of *spectral*, *workflow* or *method* information or a report, given a name and stored on a disk.

file name The name that identifies a *file*.

floating point number A numeric format that can be expressed using a decimal point.

flow-through sampling The analysis of a sample gas as it flows through a *gas cell*. This technique operates on the principle that both the *background* gas and *sample* gas are at higher pressures than the gas cell and, therefore, will "flow" from a state of higher pressure to a state of lower pressure through the gas cell. The difference in pressure may be because the background and sample gases are pressurized, or the difference in pressure may be created by using a diaphragm or vacuum pump to draw the sample through the cell.

Fourier transform 1) To convert an *interferogram* (data in the time domain) to a *single-beam spectrum* (data in the frequency domain) to reveal the response to all frequencies within the spectral range. 2) The mathematical operation used to convert an *interferogram* to a *single-beam spectrum*.

frame A portion of a window in a software application that has a set boundary.

frequency The number of light wave cycles that occur per unit of time or space. In *RESULT software*, frequency can be expressed in *wavenumbers* (cm^{-1}) or converted to *wavelength*.

fringing The effect caused by constructive and destructive interference of internally reflected waves from parallel surfaces. Fringes are sinusoidal in appearance, and the number of fringes over a given *wavenumber* range is related to the thickness of the sample.

FT-IR Abbreviation of Fourier transform infrared spectroscopy. An *infrared* spectroscopic technique that uses a *Michelson* or *Fabry-Perot interferometer* for data collection and a digital *Fourier transformation* to process the data.

FT-MIR Abbreviation of Fourier transform mid-infrared spectroscopy. A *Fourier transform* spectroscopic technique that is limited to the *mid-infrared* region of the electromagnetic spectrum.

FT-NIR Abbreviation of Fourier transform near-infrared spectroscopy. A *Fourier transform* spectroscopic technique that is limited to the *near-infrared* region of the electromagnetic spectrum.

G

Gain A *sample specification* parameter in *RESULT Integration* that adjusts an increase in the detector signal amplitude that is due to electronic amplification. Gain also appears in the *Quick Collect* dialog box of *RESULT Integration* and *RESULT Integration*.

Galactic A file format for saving spectra in a binary format that is compatible with other applications and other types of data in the industry, especially spectral and chromatographic data. Galactic files include some file header information and are saved with an extension of .spc.

gas cell 1) A sealed unit used for transmission analysis of gas samples. 2) The *sampling module* of an *Antaris IGS*.

The gas cell is installed in the instrument beam path. Internal mirrors reflect the infrared beam back and forth along the length of the cell, where the energy is selectively absorbed by and transmitted through the sample.

globally unique identifier (GUID) A string of characters generated by the software as a unique identifier for a particular *audit log* record, user ID, or workflow ID. The software creates an identifier based on the date of the record or entry with a number randomly generated by the software. A GUID cannot be used for more than one record.

GUID see *globally unique identifier*

H

Heading Item specification A *workflow specification* in *RESULT Integration* that defines a heading or subheading in a sample report and the text and/or data that will be included in the heading.

heating jacket A kit containing a heating element and insulating sleeve used to heat the *gas cells* for the *Antaris IGS*. Designed to be installed with a *temperature controller*, the heating jacket allows the user to control the temperature of the gas cell. Maintaining a constant temperature with a heating jacket can improve quantitative accuracy and prevent condensation of sample gases.

HeNe laser A helium/neon laser. See also *laser*.

homogeneity When pertaining to a sample, the degree to which the sample is of uniform consistency.

hot key A key that corresponds to an underlined letter in a software window to carry out a command using the keyboard; press the ALT key plus the appropriate hot key.

HTML see *hypertext markup language*

humidity indicator An indicator on the front panel of all Antaris models that can be used to check the status of the *desiccant*. The desiccant protects the analyzer's optical components by reducing the amount of water vapor inside the instrument.

hypertext markup language (HTML) A file format used for the World Wide Web. Web browsers can read HTML documents directly, without using any additional software. HTML documents are commonly saved with the extension of .htm or .html.

I

infrared (IR) A region of the electromagnetic spectrum extending from approximately 12,800 cm^{-1} to 30 cm^{-1}.

infrared beam The infrared light emitted by the *source* in an infrared *spectrometer* or *analyzer*. The beam travels from the source to the *detector*.

InGaAs detector Indium gallium arsenide detector. See also *detector*.

Instrument Check A feature in *RESULT Integration* that produces a series of diagnostic spectra. When compared with previous instrument check spectra, these tests are helpful in determining whether a problem exists with your instrument.

integer A numeric format that must be expressed using whole numbers only (without using a decimal point or fraction).

Integrating Sphere module A device used in *diffuse-reflection* spectroscopy. When an integrating sphere is used, the light beam is angled into the sphere and travels directly through the center of the sphere, through the optical window, and into the sample. Reflected light from the sample re-enters the sphere. An internal detector measures the reflection and sends the information to the *Michelson interferometer*.

Integration Time A *collect sequence event* feature of *RESULT Integration* that estimates the length of time between the start of the collection of successive *spectra* or *interferograms*. The integration time is calculated from the *resolution*, *velocity* and *number of scans per spectrum* or *interferogram*.

intercept The distance from the origin of coordinates along a coordinate axis to the point at which a line or curve intersects the axis.

interferogram The signal produced by the constructive and destructive addition of light when the *infrared beam* in the *interferometer* of a Fourier-transform infrared (FT-IR) *spectrometer* or *analyzer* is recombined.

interferometer See *Michelson interferometer* and *Fabry-Perot interferometer*.

J

JCAMP-DX A file format for saving spectra that is compatible with other applications in the industry and includes only printable ASCII characters and some file header information. JCAMP-DX files are saved with an extension of .jdx.

JDX see *JCAMP-DX*

K

key ID number A sequential number assigned to each record in the RESULT *audit log*. If a record in an audit log contains *suspect data*, then an asterisk (*) will appear before the Key ID number in audit log *query* reports (if the records are verified when you perform the query).

Kubelka-Munk A *data format* option for the Y-axis of diffuse-reflection spectra in *RESULT software*. Converting data to Kubelka-Munk units produces a *spectrum* that is, under certain circumstances, more linear with respect to *concentration* than is a spectrum in *log (1/R)* units.

L

laser 1) For the Antaris FT-NIR analyzers, the laser is an internal calibrator in the instrument that emits light at a known and constant frequency. The laser helps control the position of the moving mirror in the *Michelson interferometer* and signals the capture of data. The laser source in the analyzer is a *helium/neon (HeNe)* laser head.
2) For the *Antaris Target Blend* analyzer, the NIR light source produced by the *MEMS* microelectronic board on the analyzer is a laser.

LED indicator Light Emitting Diode indicator. A semiconductor diode that converts applied voltage to light. LED indicators are used on Antaris instruments to indicate the status of key instrument components, such as the power, scan, laser or source, and on some accessories for the same purpose.

lensing The effect observed when either a sample or a sampling accessory acts as an optical component and has an impact on the beam path and focus.

local group A group of users with a specific set of *rights* and *permissions* for a *workstation*.

Log (1/R) A *data format* option for the Y-axis of spectra in *RESULT software*. Log (1/R) units are derived by taking the logarithm of the inverse of the fractional *reflectance*. Log (1/R) units are analogous to *absorbance* units used in *transmission* experiments.

Logical Test specification A *workflow specification* in *RESULT Integration* that defines a logical test by specifying the workflow results to be tested, a true/false condition for each of those results, and a true/false condition for all of the results combined. The combined true/false result may be used by other workflow events as the basis for a *conditional test*, such as the if-then test for a *Perform-If event*.

logon name A string of characters identifying a user account in *RESULT Integration*. The user's logon name in RESULT must be the same as the user's *user name* in Windows.

M

MCT detector Mercury cadmium telluride detector. See also *detector.*

Measure event A workflow event in *RESULT Integration* that instructs the software to measure the spectrum from a specified *collect event, collect sequence event,* or *collect multi-channel event* using the indicated settings for the measurement parameters and a *measurement specification*. Each measurement event produces a measurement result, such as a spectral peak height, concentration value, or class.

measured value The concentration value or spectral measurement produced by the *calibrated* method for each spectrum. Measured values are produced by a *measure event* or *a compare event* in *RESULT Integration*.

Measurement Only A *spectral measurement method* in *TQ Analyst* that measures attributes of an unknown sample spectrum, such as a peak height or area, and reports the measured value(s).

Measurement specification A workflow *specification* in *RESULT Integration* that contains advanced measurement parameters that are optimized for a given method development software package and measurement type.

Memo Item specification A *workflow specification* in *RESULT Integration* that defines a line or lines of text in a sample report and the specific text that will be included. A memo item specification can be used to add comments, descriptions, or other information to a *sample report*.

MEMS Microelectromechanical Systems (MEMS) is the technology of the very small, with devices measured in micrometers. In the *Antaris Target Blend* analyzer, the heart of the micro-spectrometer is a MEMS microelectronics board. The board houses the *Fabry Perot interferometer* and the *laser* source.

menu A list of *commands* that you can choose to carry out an action or see information.

menu bar The horizontal list of *menu names*, typically near the top of a software application window.

menu name The name of a *menu* that appears in the *menu bar*. You can see the *commands* available in a menu by selecting the menu name.

message-response dialog box A *dialog box* developed using a *request event* in *RESULT Integration* that can contain up to 10 messages requiring responses from an operator when running the *workflow*. The dialog box generates a result containing messages and their corresponding responses.

method A set of parameters and *spectra* that can be used to create a *method model*.

method file A file that specifies the parameter settings and spectra for an analytical *method*.

method model A mathematical relationship that describes how the spectral data for the *calibration standards* correlate with the concentration or classification data.

Michelson interferometer A device that uses a fixed mirror and a moving mirror to split and then recombine the *infrared beam* in a Fourier-transform infrared (FT-IR) or near-infrared (FT-NIR) *spectrometer* or *analyzer*. The process causes constructive and destructive interference across all wavelengths of the infrared light. The output signal is an *interferogram*. A *Fourier transform* is applied to the interferogram to determine the energy at each wavelength. The final output is a *single beam spectrum*.

micrometer The X-axis unit used for *wavelength*. One micrometer equals 1×10^{-6} meter. A micrometer is also known as a micron.

micron see *micrometer*

mid-infrared (mid-IR) The region of *infrared* radiation extending from approximately 4,000 cm^{-1} to 400 cm^{-1}.

model see *method model*

moving mirror The mirror in the *Michelson interferometer* that reflects the infrared *beam* back to the *beamsplitter* while moving toward and away from the beamsplitter in a repeating cycle.

multi-lens optics A system of lenses for efficiently delivering the modulated infrared radiation to the sample.

Multiplexer module The module of the *Antaris Multiplexer system* that allows users to collect *spectra* from remote locations using multiple *fiber optic accessories*. The multiplexer module is available in two configurations, one with six *channels* for connecting fiber optic accessories, and one with twelve channels for connecting accessories. The Antaris Multiplexer offers rapid switching between channels while collecting data from a single detector.

Multiplexer specification A *workflow specification* in *RESULT Integration* that defines the multiplexer module configuration (6 or 12 channels) for the Antaris Multiplexer system and the status of each *channel*. You must specify this information when you set up a workflow to run the *Antaris Multiplexer* system.

N

nanometer An X-axis unit used for *wavelength*. One nanometer equals 1 x 10^{-9} meter.

near infrared (NIR or near-IR) The region of *infrared* radiation extending from approximately 12,000 cm^{-1} to 4,000 cm^{-1}.

Nicolet Antaris see *Antaris*

Nicolet Antaris IGS see *Antaris IGS*

Nicolet Antaris Multiplexer see *Antaris Multiplexer*

Nicolet sequence files A file format for saving the data generated by a *run sequence event* in a *workflow*. Nicolet sequence files are compatible with Thermo Scientific applications such as *RESULT Integration*, *RESULT Operation*, and *TQ Analyst*. Data saved in the Nicolet sequence format contain complete information about the conditions used for data collection. The archived sample *spectra* are saved with an extension of .srs. The archived background and sample *interferograms* are saved with an extension of .sri. The archived measurement results (typically concentration values) are saved with an extension of .cnc. The files are compatible with the *digital signature* features of *RESULT software*.

Nicolet spectral file A file format for saving the spectra generated by a *collect event* or *collect multi-channel event* in a workflow. Nicolet spectral files are compatible with Thermo Scientific applications, such as *RESULT Integration*, *RESULT Operation*, and *TQ Analyst*. Data saved in the Nicolet format contain complete information about the conditions used for data collection, as well as the archived sample and background *interferogram*, and are compatible with the *digital signature* features of *RESULT software*. Nicolet spectral files are saved with an extension of .spa.

noise Random signals produced by electrical or other components in an instrument, which can affect spectral data.

normalization A process that forces conformity to a standard or norm. In *RESULT Integration*, single-beam spectra are normalized to account for natural variations in the *attenuator* and in the *detector* response.

normalize To cause to conform to a standard or norm.

Number Of Sample Scans A *collect event* parameter in *RESULT software* that defines the number of times the analyzer will scan the sample to produce a *spectrum*. Increasing the number of scans reduces the *noise* level of data (increases the *signal-to-noise ratio*).

Number Of Scans A collection parameter in the *Quick Collect* dialog box of *RESULT software* that defines the number of times the analyzer will scan the sample to produce a *spectrum*.

Number Of Scans Per Spectrum A *collect sequence event* feature of *RESULT Integration* that determines the number of *scans* that will be coadded to produce each *spectrum* or *interferogram* in a *phase* of data collection. The setting of this parameter is used to define the *Integration Time*. The greater the number of scans per spectrum, the more time there will be between spectra or interferograms (thus resulting in lower temporal resolution).

0

100% line A spectrum generated by ratioing two single-beam spectra that appears as a generally flat line at 100% transmittance. This spectrum is used as a diagnostic tool to reveal system noise. Although it is called 100% line, it is usually collected and displayed in *absorbance* units.

operational qualification The process of demonstrating that an instrument performs consistently as specified by the instrument vendor, by testing critical areas of the instrument, such as data collection and mathematical algorithms. Thermo Fisher Scientific offers the *ValPro System Qualification* package, which runs a series of workflows that perform operational qualification tests on each *Antaris* system.

Operator Prompt specification A group of parameters that specify what will be displayed in the prompt displayed when the operator runs the open *workflow*. Examples of parameters in the operator prompt specification include the prompt text and the action for the operator's response.

Optimize Gain A feature in *RESULT* software that assists a user in determining the optimal *gain* and *attenuator* (if applicable) parameter settings for a given sample. The optimize gain feature can be found in the *sample specification* in *RESULT Integration* and in the *Quick Collect* dialog box in *RESULT software*.

oxygen clean The state of a gas analysis component that ensures compatibility with oxidizing and corrosive gas samples. *Antaris IGS gas cells* and plumbing fixtures that are oxygen clean are designed and manufactured to comply with ASTM standard G93, which means they are suitable for use in oxygen-enriched environments. The cleaning process involves the use of solvents to remove organic and particulate materials that (when combined with oxidizing or corrosive gases) could cause injury or damage the cell. Thermo Fisher Scientific factory technicians confirm the cleaning with a visual inspection of the component under a polarized light.

P

parameter A property whose value determines the characteristics or behavior of a software application.

Partial Least Squares (PLS) A *quantitative method* in *TQ Analyst* that uses a partial least squares statistical analysis to find relationships between the absorbance spectra and the component concentrations of the corresponding samples.

Paste A *command* that uses *RESULT Integration's* memory features to place information being stored on the application's *clipboard* into another *workflow* file.

path The route followed by an application or operating system to find, *archive*, or retrieve files on a disk.

pathlength The distance a beam of incident energy travels within a *sample*. A longer pathlength increases the absorption of infrared energy by the sample. If the pathlength is too great, totally absorbing bands will result. Since the absorption depends on the pathlength (as well as on concentration), if the pathlengths of the *samples* and the *standards* used to quantify them are not the same, the quantitative method must account for the differences in pathlength. If the pathlength values are known, they can be entered in the quantitative method or specified at run time. A quantitative method can also be configured to predict or calculate the pathlength values if the spectra contain a peak or region that varies with pathlength.

PCR see *Principal Component Regression*

PDF see *portable document format*

peak A region of a *spectrum* where the sample absorbs radiation.

peak area The intensity of a spectral region, determined by finding the sum of the intensity values in the specified X-axis range.

peak height The intensity (Y value) of a spectrum at a given X value.

Perform event A *structural workflow event* in *RESULT Integration* that performs a group of events in sequence. The perform event *parameters* allow you to add comments to the group, check the group for errors, and stop executing the events in the group if errors are found.

performance index A measure of how accurately a *calibrated method* can quantify or classify the *validation standards*.

performance qualification The routine process of verifying that an instrument is performing according to requirements for the instrument's intended use.

Perform-If event A *structural workflow event* in *RESULT Integration* that performs a group of events in sequence. The perform-if event parameters allow you to specify the conditions for when the events in the group should be performed or skipped, based on a *logical test specification* and *conditional test*.

Perform-While event A *structural workflow event* in *RESULT Integration* that performs a group of events in sequence. The perform-while event parameters allow you to specify the conditions for how long the events in the group should be performed, based on a *logical test specification* and *conditional test*.

permissions Rules that govern access to a resource associated with a *workstation* or network, such as a printer or shared folder.

phase see *data collection phase*

Pirouette® A method development software package from InfoMetrix®, Inc. that is compatible with *RESULT software*.

PLS see *Partial Least Squares*

PLSplus/IQ™ A method development software package from Thermo Galactic Corporation that is compatible with *RESULT software*.

Portable Document Format (PDF) A document file format that preserves the exact look and content of documents, including fonts and graphics. PDF files are normally created in Adobe® Acrobat® with an extension of .pdf. The files can be viewed using Adobe Acrobat Reader on various software platforms. PDF files can also be *digitally signed* if they are created in Adobe Acrobat version 4.0 or higher.

pressure gauge An accessory used to monitor the pressure of a gas sample that is captured in a *gas cell* or flowing through a gas handling system.

pressure sensor A device that allows *RESULT software* to read the pressure of a gas sample that is captured in a *gas cell* or flowing through a gas handling system.

Principal Component Regression (PCR) A *quantitative method* in *TQ Analyst* that uses a principal component regression statistical analysis to find relationships between the absorbance spectra and the component concentrations of the corresponding samples.

production system An Antaris analyzer run by *RESULT Operation* and used for routine spectral analysis.

production workflow A *workflow* developed for use on a *production system*.

profile A set of *directory* files that controls a user's Windows environment, such as desktop settings, programs the user can access, and programs that start automatically. Users can modify their profiles to change their Windows environment, or users can be assigned mandatory profiles by a *Windows administrator*.

prompt A software *dialog box* that contains a message and a button for the operator response. The user must acknowledge the prompt before the software can continue.

Prompt specification A *workflow specification* in *RESULT Integration* that defines a dialog box providing information to the operator running the workflow, including message text and a button label. The operator must acknowledge the prompt before the workflow can continue. The prompt can be set up so the operator can respond by pressing the Acknowledge button on the instrument, if one exists, and by pressing the appropriate button in the prompt *dialog box*.

purging Forcing dried air or nitrogen through an *analyzer* to eliminate water vapor and other airborne contaminants. Purging protects the system's internal components from damage due to excessive environmental humidity and corrosive solvents.

Q

QC Compare Search A *qualitative* (*classification*) *method* in *TQ Analyst* that uses multiple standards and multiple classes to determine which standard and class are most similar to an unknown material. The method reports the best matched standard in each class and a match value for each standard. The classes are ranked from best match to worst match.

qualitative analysis A technique used to identify a *sample* material by measuring a characteristic feature or trait.

qualitative method A method that identifies an unknown sample by comparing its spectrum with the spectra of known materials, which represent pre-defined categories, or *classes*. Qualitative methods are also referred to as *classification methods*.

qualitative model A *method model* that can be used to identify the composition of a sample mixture by comparing the sample spectrum with the spectra of known materials, which represent pre-defined categories, or classes. Qualitative models may also be used to determine the degree of similarity between the unknown sample spectrum and a given class.

quantitative analysis A technique used to measure the concentrations of one or more *components* in a *sample mixture*.

quantitative method A *method* that measures the concentrations of one or more *components* in a *sample mixture* by comparing the component's spectrum with the spectra of samples with known concentrations of the individual components.

quantitative model A *method model* that can be used to measure the *concentrations* of one or more *components* in a *sample mixture* by comparing the component's spectrum with the spectra of samples with known concentrations of the individual components.

query The process of retrieving specific data from a database. In *RESULT Operation*, users can perform a query of specific information in the *audit log database* to create reports detailing that information.

Quick Collect A feature in *RESULT Operation* and *RESULT Integration* that allows you to collect a *background spectrum* and/or *sample spectrum* without going through the process of creating and running a workflow.

R

rack enclosure Enclosed housing for instrument components used in industrial settings. *Antaris, Antaris II, Antaris MX,* and *Antaris IGS* systems can be installed as roll-out components in a rack enclosure.

rack mount kit An option that allows the analyzer to be installed as a roll-out component in a *rack enclosure*.

ratioing The process of removing the effects of the instrument and any water or carbon dioxide absorptions (if these gases are not completely purged from the instrument) from a sample spectrum by dividing the spectrum by a *background spectrum*, or a reference background spectrum, at each data point.

read-only A specification when saving files. When files are saved as read-only in *Windows*, they may be opened and changed, but the altered file cannot be resaved with the previous file name. The file must be saved under a different file name.

reference A known *component* of a sample that is measured with the background in order to generate a *reference background spectrum*. See also *reference background spectrum* and *ratioing.*

reference background spectrum A *background spectrum* that includes the absorptions of a *reference*. Reference backgrounds are typically used to remove peaks due to known sample components by dividing the sample spectrum by the reference background spectrum. See also *reference* and *ratioing.*

Reflectance (%) A data format option for the Y-axis of spectra in *RESULT software*. Percent reflectance units are normally used to display a spectrum collected using a *reflection* technique. Percent reflectance shows the amount of *infrared* energy reflected from the sample.

reflection-absorption see *transflection*

Repeat event A *structural workflow event* in *RESULT Integration* that performs a group of events in sequence. The repeat event *parameters* allow you to define the number of times the events in the group should be repeated, or to stop repeating the group if specified conditions are met.

report see *sample report*

Report event A *workflow event* in *RESULT Integration* that instructs the software to create a *sample report* using the indicated settings for the report parameters and a *report specification*.

Report Item specification A *workflow specification* in *RESULT Integration* that defines a particular section in a *sample report*. Examples include *heading item specifications*, *sequence heading item specifications*, *memo item specifications*, *spectrum item specifications*, *table item specifications*, *summary item specifications*, and *sequence summary item specifications*.

report navigation frame A *frame* in *RESULT Operation* that contains a list of reports. You can select a report from the list to display it in the *display area* of the software.

Report specification A *workflow specification* in *RESULT Integration* that defines the sections to be included in a *sample report* and their order when the report is displayed or printed.

Report tab A *display area* in *RESULT Operation* that automatically displays a *sample report* after a *workflow* has finished running if the workflow includes a properly configured *report event*.

Request event A *workflow event* in *RESULT Integration* that instructs the software to create a dialog box requesting information from the operator. Request events can be used to define two kinds of dialog boxes: a *message-response dialog box* and a *class-selection dialog box*. Responses to request events can be set up as either optional or required.

Request specification A *workflow specification* in *RESULT Integration* that defines a dialog box requesting information from the operator of the workflow. The request specification allows you to specify the format of the operator response and whether the response is required or optional.

Resolution A *sample specification* parameter in *RESULT Integration*. Resolution measures how well closely spaced peaks in a spectrum are differentiated. The higher the resolution, the more separated two closely spaced peaks will appear. Increasing the resolution (i.e., using a lower Resolution setting) requires that the distance traveled by the *moving mirror* in the *interferometer* be increased. Resolution also appears in the *Quick Collect* dialog box of *RESULT Integration* and *RESULT Operation*.

RESULT administrator A user who has administrative access to *RESULT Operation*. The RESULT administrator can set up users, perform process setup and maintenance, and perform system setup and maintenance. See also *administrator*.

RESULT Data View An application for viewing *sequence data files* collected from time-based experiments in *RESULT software*. Use RESULT Data View to display the spectra collected from a *run sequence event* as well as the measured concentration values or other analysis results.

RESULT Integration The development portion of the Thermo Scientific *RESULT software* for routine spectral analysis. Use RESULT Integration to create and test *workflows*.

RESULT Operation The production application for *RESULT software*. Use RESULT Operation to configure and run *workflows* on a *production system*.

RESULT software The Thermo Scientific software for routine spectral analysis. RESULT comprises two software applications, *RESULT Operation* and *RESULT Integration*.

right A rule that governs tasks within an operating system that can be assigned to users, such as changing the system date and time, logging on to the system, or shutting down the system.

RMSEP see *root mean square error of prediction*

root mean square error of prediction (RMSEP) The uncertainty of prediction for a component, which is calculated by squaring the error values, calculating the average, and then taking the square root of the result. RMSEP is produced by a *compare event* in *RESULT Integration*.

Run Sequence event A *workflow event* available in *RESULT Integration* when the *sequence module* add-in option is installed. A run sequence event instructs the workflow to begin collecting sequence data by implementing one or more *collect sequence events*. If the run sequence event group contains one or more *measure events*, the software will also process the data. The archived concentration data are saved with an extension of .cnc. The archived sample *spectra* are saved with an extension of .srs. The archived background and sample *interferograms* are saved with an extension of .sri. The files are compatible with the *digital signature* features of *RESULT software*.

Run Time Test window A window in *RESULT Integration* that allows a user to test *workflows* in development in a simulated production environment. The Run Time Test window simulates *RESULT Operation* and is also used for collecting *standards* and using the *Quick Collect* feature in RESULT Integration.

S

SabIR diffuse-reflection probe The Thermo Scientific *diffuse-reflection* probe that can be used with the *fiber optic module* or *multiplexer module*. The SabIR probe allows the remote analysis of solid and powder samples.

sample A compound or mixture being analyzed.

sample accessory holder An accessory for the integrating sphere module that supports other accessories for tablet analyses such as the *universal tablet holder*. The sample accessory holder resembles the base of the tablet analyzer and can be used to run reflection experiments with tablet samples and accessories.

sample beam path compartment The upper compartment of an *Antaris IGS*. The sample beam path compartment houses multiple mirrors that send the *infrared* energy out of the *spectrometer compartment,* through the *gas cell* and back to the *detector*. See also *spectrometer compartment.*

sample card A card into which transparent solids or thin films are placed for sampling.

sample card holder see *three-position sample card holder*

Sample Correction specification A *workflow specification* in *RESULT Integration* that defines a correction for spectra collected with a workflow. Typical corrections include *dark background corrections* and *transfer corrections*. The correction specification is used to select a correction function and identify the spectra used in the correction.

sample mixture A sample that contains two or more *components*.

sample preview A live spectral display window that accompanies an *operator prompt* for sample collection from a *workflow*. Data collection begins when the operator chooses the Continue button in the prompt. Sample preview allows the operator to verify the quality of the sample data before starting the collection.

sample prompt An operator *prompt* in *RESULT software* that will appear before sample collection when the workflow is run.

sample report A compilation of sample data produced by a *report event* in a workflow. A *report specification* defines the sections in the report, and *report item specifications* define the spectra, measurement results, or other results included in each section. A sample report can include any of the following: headings, spectra, workflow results, summarized workflow results, and text. An *archive event* can be used to archive the *sample reports* produced by a workflow.

sample specification A *workflow specification* in *RESULT Integration* that defines how the spectral data will be collected for a particular sample type or material. Examples of parameters in the sample specification include *Gain* and *Resolution*.

sample spectrum The *spectrum* of an unknown material being analyzed.

sample track The platform inside the *transmission module* where sample holders are placed. The sample track moves sample holders into and out of the beam path and shifts the position of sample holders during data collection as required.

sample tube holder see *three position cuvette/culture tube holder*

sampling module A component of the *Antaris analyzers* that allows dedicated sampling using a particular technique. For the *Antaris* and *Antaris II*, four different sampling modules are available: the *transmission module*, *tablet analyzer module*, *fiber optic module*, and *integrating sphere*. The *Antaris Multiplexer system* includes a *multiplexer module* with 6 or 12 fiber optic channels. The Antaris MX and Antaris EX systems include a *fiber optic module* with two or four fiber optic channels. The Antaris IGS system has a *gas cell* module. For *Antaris Target Blend* analyzers, the sampling module refers to the a set of sapphire windows between the analyzer and the blender, where light energy passes into the blender and sample information (in the form of diffusely reflected light) is passed back to the analyzer detector.

saturate In terms of spectroscopy, to send too much light through a sample and into a *detector*. The term is also sometimes used to describe a distorted electronic signal from the detector. Detector saturation can be reduced by adjusting the *attenuator* to allow less light to pass through it, or by reducing the *gain* setting.

scan 1) To collect data with an *interferometer*. 2) For a Michelson interferometer, a scan refers to one movement of the *moving mirror* from the point closest to the *beamsplitter* to the farthest point or vice versa. 3) For a *Fabry-Perot interferometer*, a scan refers to one sweep across the spectrometer's wavelength range (occurs approximately once every 100 milliseconds). 4) A feature available in some *sample specifications* in *RESULT Integration*, such as the gas cell sample specification for the *Antaris IGS*. Scan determines the path of the moving mirror in the interferometer. The Scan setting affects the length of time required to produce a spectrum and, more subtly, the total number of data points each spectrum will contain.

Search Standards A *qualitative* (*classification*) *method* in *TQ Analyst* that uses multiple classes and one standard per class to determine which known material is most similar to an unknown material. The method reports a list of standards ranked from best match to worst match, and a match value for each standard.

sequence concentration file A possible component of archived *sequence data* if the *run sequence event* contains at least one properly configured measure event. The concentration file is saved with an extension of .crc and contains the concentration values or other measured data produced from the run sequence event. The sequence concentration file will have the *base name* specified in the workflow archive event.

sequence data set The files that contain the data generated by a *run sequence event* in a *workflow*. The files are stored or archived in the *Nicolet sequence file* format with the *base name* specified in the workflow archive event.

Sequence Heading Item specification A *workflow specification* available in *RESULT Integration* when the *sequence module* add-in option is installed. A sequence heading item specification defines a sequence heading section in a *sample report*. The report includes the sequence title, the date and time the sequence collection started and ended and the file names of any archived data, followed by details of each *data collection phase* defined in the sequence.

sequence interferogram file A component of archived *sequence data* that contains the *interferogram* data used to process the spectra produced from a *run sequence event*. All the interferograms collected over the time of the sequence data collection are archived in a sequence interferogram file. The sequence interferogram file is saved with an extension of .sri and the *base name* specified in the workflow archive event.

Sequence module An add-in option for *RESULT Integration* that allows sequence data collection with *RESULT software*. With the sequence module installed, RESULT is capable of collecting and processing a series of spectra at regular intervals over a specified period of time using a combination of *run sequence events*, *collect sequence events*, and *measure events*.

sequence spectral file A component of archived *sequence data* that contains the processed spectra produced from a *run sequence event*. All the spectra collected over the time of the sequence data collection are archived in a sequence spectral file. The sequence spectral file is saved with an extension of .srs and the *base name* specified in the workflow archive event.

Sequence Summary Item specification A *workflow specification* available in *RESULT Integration* when the *sequence module* add-in option is installed. A sequence summary item specification defines a sequence summary section in a *sample report*. The sequence summary section provides a summary of the sample component data produced by a *run sequence event*. The summary can include the following for each selected component: count (number of measurements), minimum, maximum and average values, range, number of failures, and total area (of the measured *peak*).

Sequence tab An optional display area that appears in *RESULT Operation* when you are running a *workflow* that contains a properly configured *run sequence event*. The run sequence event configures *RESULT software* to collect and process spectra continuously. Continuous data collection provides information about samples that change composition over time. The data and other information that may appear on the sequence tab are defined by the workflow.

settle time A specified amount of time allowed for the temperature of the *heated sample tube holder* or *gas cell* to stabilize. The amount of time that is appropriate depends on the nature of the *sample* and the temperature to be maintained.

shortcut menu A *menu* that appears in a software application when a user right-clicks in a window.

signal-to-noise ratio (SNR) The ratio of the intensity of a signal to the intensity of the noise that accompanies it.

Similarity Match A *qualitative* (*classification*) *method* in *TQ Analyst* that uses multiple *standards* and one *class* to determine how closely an unknown material matches a known material. The method reports a match value, which indicates the quality of the match.

Simple Beer's Law A *quantitative method* in *TQ Analyst* that uses the classic Beer-Lambert-Bougher law (absorbance increases proportionally with concentration) to create a *method model*.

simple workflow event A *workflow event* in *RESULT Integration* that carries out a single task, such as collecting a spectrum, measuring a spectrum, or using data to create *sample reports*. Simple workflow events are the building blocks that define the overall task the workflow is to perform. Some example simple workflow events include *collect events*, *measure events*, and *report events*. Compare with *structural workflow event*.

Single Beam Raw A data format option for the Y-axis of spectra in *RESULT software*. A single beam raw spectrum has not been processed or *normalized*.

single-beam spectrum A *spectrum* (data in the frequency domain) obtained by Fourier transforming an *interferogram* (data in the time domain). A single-beam spectrum shows the response at all *frequencies* in the *spectral range*. A *sample* single-beam spectrum can be ratioed against a *background* single-beam spectrum to produce a sample spectrum with the background information removed.

slope The rate at which an ordinate of a point of a line on a coordinate plane changes with respect to a change in the abscissa (i.e., the rise divided by the run).

SMA connector An industry standard connector (Sub-Miniature, Type A) used for fiber optic connections. SMA connectors have a cylindrical sleeve and threaded locking unit.

SMLR *see Stepwise Multiple Linear Regression*

SNR see *signal-to-noise ratio*

SoftGel Tablet analyzer The *Antaris tablet analyzer* optimized for use with samples that are good transmitters, such as softgel capsules, paper, plastics, packaging materials, and polymers. The softgel tablet analyzer has a broad-band *InGaAs detector* and covers a spectral range of 12,000 cm^{-1} to 3,800 cm^{-1} (833 nm to 2,630 nm).

SOP see *standard operating procedure*

source A component inside an infrared *spectrometer* or *analyzer* that emits the infrared radiation that travels to the *detector*.

SPA see *Nicolet spectral file*

SPC see *Galactic*

specification see *workflow specification*

specification name The name assigned to a particular *workflow specification*.

specification tree A hierarchical grouping of *workflow specifications*. You can use the specification tree to view the names and associated parameters for any specification in the open *workflow*.

spectral data file A file that contains one *spectrum*.

spectral measurement method A TQ Analyst *method* that measures spectral features. You can set up a spectral measurement method that measures *peak heights* or *peak areas* in a *sample spectrum*, calculates the ratio of two measured *peaks*, measures random *noise* or peak widths, or finds peak locations.

spectral range The range of *frequencies* included in a *spectrum*.

spectral region A portion of a *spectrum* between two *frequencies* or *wavelengths*.

Spectralon® A soft, porous and highly diffuse sample with high reflectance that can be used as a background reference for *diffuse-reflection* sampling.

Spectra tab An optional *display area* in *RESULT Operation* that displays individual spectra as they are collected by a *workflow* if the workflow contains a properly configured *collection event*. The data are updated each time the instrument scans the sample. The Spectra tab must be enabled in the *RESULT* Options dialog box before it will appear in *RESULT Operation.*

spectrometer An instrument for measuring a spectrum. Thermo Fisher Scientific produces *FT*-infrared, FT near-infrared, and Raman spectrometers.

spectrometer compartment The lower compartment of an *Antaris IGS*. The spectrometer compartment houses the instrument optics, including the *source*, *laser*, *beamsplitter*, and *detector*. See also *sample beam path compartment*.

spectrum A graphical representation of the intensity of the radiation reaching the *detector* at each frequency (X-axis value) measured. The intensity at a given X-axis location is determined by the characteristics of the instrument used to collect the spectrum and the *sample*, if one is present.

Spectrum Item specification A *workflow specification* in *RESULT Integration* that defines a spectral plot in a *sample report* and the collection results (spectra) that will be included in the plot.

specular reflection Reflection of light in which the angle of incidence equals the angle of reflection; i.e., "mirror-like" reflection.

standard operating procedure (SOP) A written authorized procedure documenting instructions that should be followed for performing an operation. An SOP can include general instructions for maintenance and cleaning, equipment operation, and sampling.

Standard Tablet analyzer The *Antaris tablet analyzer* optimized for use with dense materials, such as opaque tablets. The standard tablet analyzer has a narrow band, high-sensitivity *InGaAs detector* and covers a *spectral range* of 12,000 cm^{-1} to 5,880 cm^{-1} (833 nm to 1,700 nm).

standards Known samples that model the behavior of the unknown samples that will be analyzed with a *method*. For *quantitative analyses*, standards are samples which have known concentrations of each *component* the method will be used to analyze. For *qualitative analyses*, standards are samples that have the characteristic the method will be used to track.

status indicator 1) A display panel on the analyzer front panel that shows the status of the analyzer power, scan, laser, and source. 2) A display in *RESULT Operation* that reveals the status of workflows, tests, and digital signature information related to archived items.

Stepwise Multiple Linear Regression (SMLR) A *quantitative method* in *TQ Analyst* that expresses concentration as a function of the *absorbance* at specific *frequencies*.

stop-flow sampling The analysis of a sample gas that has been captured in a *gas cell*.

Store event A *workflow event* in *RESULT Integration* that instructs the software to store selected results generated by a workflow in the *RESULT audit log* when the workflow is run in *RESULT Operation*. When results are stored in the audit log, they can be displayed on the *Trend tab* or *queried* to create reports of trends in workflows, events, and values. The store event can be used to store the results of *calculate events*, *compare events*, *measure events*, and *request events* if those results are numeric.

string A data type *option* that allows both text and numeric entries.

structural workflow event A *workflow event* in *RESULT Integration* that operates on a string of events that are placed in a group. The grouped events can be performed or repeated based on the results of a *conditional test*. Structural events can be used to control when and how certain workflow tasks are performed. Some examples of structural workflow events include *perform events*, *repeat events*, *perform-if events*, and *perform-while events*. Compare with *simple workflow event*.

Summary Item specification A *workflow specification* in *RESULT Integration* that defines a table of summarized results in a *sample report* and the workflow results that will be included in the table. Summary item specifications can be used to produce a useful summary of results from a variety of operations, and to serve a variety of needs, ranging from a simple compilation of data produced by multiple iterations of a repeat loop to an elegant presentation of statistical results from a multi-component analysis.

suspect data Data in the RESULT *audit log* that has been marked as possibly being tampered with or incorrect. Suspect data is noted with an asterisk (*) before the Key ID entry in reports created by *RESULT Operation*.

T

Table Item specification A *workflow specification* in *RESULT Integration* that defines a table section in a *sample report* and the workflow results that will be included in the table. Numerical or other results from *workflow events* can be added to a table item specification.

tablet analyzer module A *sampling module* used to collect *transmission* data of tablets. When connected to the *Antaris or Antaris II analyzer*, the light beam is directed into the tablet analyzer and through the *sample*. The amount of light that passes through the tablet is measured by the *detector* in the tablet analyzer cover. These Antaris products work with two types of tablet analyzers: a *standard tablet analyzer* and a *softgel tablet analyzer*.

tamping Packing a powder tightly into a container by gently tapping it against a hard surface.

temperature controller A component or accessory used to monitor or control the temperature of an *Antaris, Antaris II,* or *Antaris IGS* system component. Typically used to monitor or control the sampling temperature of gases and liquids.

temperature sensor A device that allows *RESULT software* to read the temperature of an *analyzer* component, such as a *gas cell* or *block heater*.

template In *RESULT Integration*, a template contains the default information for a certain type of *workflow event* or *specification*.

test fiber A fiber included with the *fiber optic module* or *multiplexer module*. The test fiber can be used to run an instrument test without a *fiber optic accessory*, to validate whether the module is performing correctly.

TGS (or DTGS) detector Tri-glyceryl sulfide (or deuterated tri-glyceryl sulfide) detector. See also *detector*.

The Unscrambler® see *Unscrambler*

three-position cuvette/culture tube holder The sample holder that is used with the *transmission module* to collect data from samples held in cuvettes, culture tubes, or vials. The cuvette/culture tube holder has three locations (front, middle, and rear) through which collections can be taken, but samples can be collected only from the front and rear positions. The middle position is only for collecting backgrounds without a reference. *Also called a sample tube holder.*

three-position sample card holder The sample holder that is used with the *transmission module* to collect data from transparent solids or thin films held in *sample cards*. The sample card holder has three locations (front, middle, and rear) through which collections can be taken, but samples can be collected only from the front and rear positions. The middle position is only for collecting backgrounds without a reference. *Also called a sample card holder.*

throughput The intensity of the infrared energy that reaches the *detector* in an *analyzer*.

thumbscrew A screw attached to a connector that can be tightened by the thumb and forefinger. Tools should not be used to tighten thumbscrews.

title bar A bar that normally appears at the top of the *main window* in a software application. The title bar usually identifies the name of the application you are using and the name of the file you currently have open. In *RESULT Integration*, the title bar contains the name of the software, along with the name of the *workflow file* that is currently open.

toolbar A long narrow strip at the top of a software application *window* that contains action buttons. Toolbars provide a convenient way to initiate frequently used *commands* and other functions in a single step.

Total Collection Time A *collect sequence event* feature of *RESULT Integration* that determines the length in seconds of the *phase* of data collection. The total collection time is used along with the *number of scans per spectrum* to determine the total number of sample *spectra* or *interferograms* taken during the phase. The longer the total collection time, the more spectra or interferograms there will be in the *sequence data set*.

TQ Analyst The Thermo Scientific software package for creating, calibrating, testing and troubleshooting *methods* for measuring spectral data. TQ Analyst provides a wide range of tools for creating *quantitative*, *classification* and *spectral measurement methods* in a user-friendly application.

transfer background spectrum A single beam spectrum of a background reference taken at the same location as the normal background (defined by the associated *collection event*). The spectrum is used to generate a *transfer spectrum* for a *transfer correction*.

transfer correction A correction applied to sample spectra collected by a workflow to account for differences in the beam paths used to measure the sample and background. Requires a *sample correction specification* and a *transfer spectrum*.

transfer sample spectrum A single beam spectrum of a background reference taken at the same location as the sample. The spectrum is used to generate a *transfer spectrum* for a *transfer correction*.

transfer spectrum A ratioed spectrum produced from the single beam *transfer background spectrum* (numerator) and the single beam *transfer sample spectrum* (denominator). The transfer spectrum represents the inherent differences between the two beam paths. The ratio of the single beam spectra of the sample and background can be multiplied by the transfer spectrum to correct for any artifacts (peaks or peak shapes) in the spectra that are due solely to the change in beam path.

transflection Also known as reflection-absorption. A spectroscopy technique in which a beam enters the sample, reflects off a reflective surface, and passes through the sample layer a second time. Under many conditions, particularly when you are studying liquids, the resulting spectrum resembles a *transmittance* spectrum.

transmission A spectroscopy technique that measures the percentage of light transmitted through a *sample*.

Transmission module The module of an *Antaris* or *Antaris II analyzer* that allows users to collect spectra from liquid samples and transparent solids and films using *transmission* spectroscopy.

Transmittance (%) A data format option for the Y-axis of spectra in *RESULT software*. Percent transmittance units are normally used to display a spectrum collected using a *transmission* technique. Percent transmittance shows the fraction of the radiation that remains after a beam of electromagnetic radiation passes through a sample. Percent transmittance is defined by the formula $T = (P/P_0) * 100$, where P is the radiation that passes through the sample and P_0 is the radiation when no sample is present.

trend chart A graph of numerical data such as component concentration values collected over a period of time. In *RESULT software*, the *Sequence tab* can be used to display trend charts of data collected in rapid succession while a workflow is running. The *Trend tab* can be used to create trend charts of data stored in the *audit log*.

Trend tab An optional *display area* in *RESULT Operation* that can be used to display numeric results produced by events in *workflows* over a period of time. Examples of events that can produce numerical values include *measure events*, *request events*, *compare events* and *calculate events*. The Trend tab pulls the data from the *audit log*. Workflows can be configured to store data in the audit log with a *store event*. Trend data can be viewed in tables and graphs or in both formats and can include historical data or data from a workflow that is currently running or a combination of the two. The Trend tab must be enabled in the *RESULT* Options dialog box before it will appear in *RESULT Operation*.

two-zone purge An option for the *Antaris IGS* that includes a set of optional ZnSe (zinc selenide) windows and a second set of ports for *purging* the instrument. The windows isolate the *sample beam path compartment* from the *spectrometer compartment* and allow the two compartments to be purged independently. Two-zone purge prevents potentially corrosive materials from entering the spectrometer compartment if a *gas cell* window seal fails during an experiment.

U

universal tablet holder A tablet holder that can be used in conjunction with a *tablet analyzer* or *sample accessory holder.* The universal tablet holder can be adjusted to hold round tablets of varying thicknesses and circumferences.

Unscrambler® A method development software package from Camo ASA that is compatible with *RESULT software*.

USB port A universal serial bus connector on a computer. A USB port uses standard "A" (toward the computer) and "B" (away from the computer) connectors and a standard format that works with any USB-compatible device such as a printer, disk drive or mouse. The computer operating system will automatically detect a USB device after it is plugged in the first time; these devices can be connected and disconnected at any time.

user name A string of characters identifying a user account in the Windows® operating system. A user keys in his or her user name when logging on to Windows.

V

validation standard A *standard* that is used to evaluate the performance of a calibrated *method*. The results from the validation standards are also used to calculate the *performance index*.

validation wheel An optional component of the all *Antaris analyzer* models except the *Antaris Target Blend* analyzer. The validation wheel is used along with the optional *ValPro System Qualification* package to validate the performance of the instrument. The wheel contains standards that are traceable to standards certified by the National Institute of Standards and Technology (NIST) or National Physical Laboratory (NPL).

ValPro System Qualification An optional software and documentation package that includes a comprehensive set of qualification tests, including Pharmacopoeia-recommended tests, to verify instrument performance. ValPro Qualification software works within *RESULT Operation*.

Velocity A feature available in some *sample specifications* in *RESULT Integration*, such as the gas cell sample specification for the *Antaris IGS*. Velocity defines the linear speed of the *moving mirror* in the *interferometer*. The Velocity setting determines the measurement time for each *scan* and affects the *detector* response.

verification workflow A *workflow* that helps ensure that a particular *production workflow* is working properly for its intended purpose.

vial An inexpensive, cylindrical sample container that is usually made of glass or plastic. Vials are often unsuitable for taking high accuracy measurements such as those involved in *quantitative analysis*.

W

wavelength The distance between corresponding points in consecutive light waves. Wavelength is measured in *micrometers* or *nanometers*.

wavenumber The frequency depicted in the number of waves per centimeter, expressed as cm^{-1}. Wavenumber is the inverse of *wavelength* (measured in centimeters) and is often used as the X-axis unit of an *infrared spectrum*.

window A rectangular area on the screen that contains the main features of a software application or a significant component of an application.

Windows® The Microsoft® operating system that runs with *RESULT software*. Windows can run on a stand-alone computer or on a computer connected to a Windows network.

Windows administrator A user who has special rights to the Windows operating system software. The Windows administrator has the ability to set up user accounts and specify security settings within the operating system. See also *administrator*.

workflow A series of instructions for collecting, measuring, reporting or saving spectral data. Workflow files comprise *workflow events* and *workflow specifications* created using *RESULT Integration*. Functional workflows can be transferred to a *production system* where they can be systematically called up and run using *RESULT Operation*.

workflow event An item in a *workflow* that specifies a task to be carried out when the workflow is run.

workflow file A *file* that contains instructions for collecting, measuring, reporting or archiving spectral data. Workflow files comprise *workflow events* and *workflow specifications*.

workflow navigation frame The region of the *RESULT Integration* main *window* used to create, add to or display the contents of the open *workflow*.

workflow specification A group of related parameters that define an important characteristic of a *workflow event*. Examples of workflow specifications for the collect event include the *sample specification* and the *background specification*.

workflow tree A hierarchy of individual *workflow events* or groups of workflow events. The workflow tree can be used to view the general instructions or an associated *specification* for any event in the open *workflow*.

Workflow wizard A software wizard that steps you through the process of creating a functional *workflow* with collect, measure, report and archive *events*.

workstation The local computer that runs *RESULT software* and *Windows* operating system.

Z

Zero Filling A feature available in some *sample specifications* in RESULT Integration, such as the gas cell sample specification for the *Antaris IGS*. Zero Filling improves the line shape of a spectrum by adding interpolated data points. The Zero Filling setting affects the length of time required to process (i.e., Fourier transform) each interferogram to a spectrum.

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