# Antaris MX and Antaris EX Process Analyzers User Guide

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# Contents

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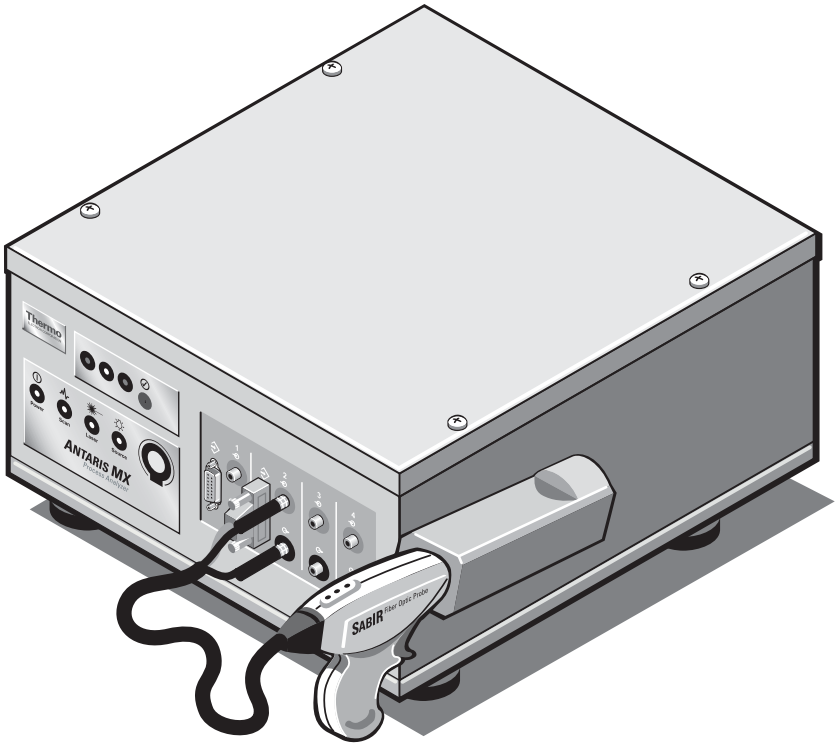
# Introduction

Congratulations on your purchase of an Antaris™ MX Process Analyzer from Thermo Fisher Scientific. The Antaris MX is a dedicated Fourier-transform near-infrared (FT-NIR) analyzer designed for use in the industrial environments of the pharmaceutical, chemical, polymer, food, and beverage industries. The analyzer allows continuous process monitoring at multiple sampling locations simultaneously. When combined with the Thermo Scientific RESULT™ software for routine sample analysis, the Antaris MX is a powerful yet simple tool for production applications that require remote sampling.




Antaris MX Process Analyzer

## How to use this manual

This manual explains how to use your analyzer to collect and analyze FT-NIR spectra after Thermo Fisher Scientific installs the system. Included is information on using RESULT software to run the analyzer, as well as chapters on how to maintain and service the system and a glossary.

After you read this chapter to become acquainted with the parts of the analyzer and its safe use, set up the system for data collection as explained in the "Preparing the System" chapter. Then read the "Your First Experiment" chapter to learn how to collect data.

Setup, maintenance, and service information is also 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 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. ▲

To learn more about the software that runs your analyzer, see your *RESULT User's Guide*.

## Conventions

The following conventions are used in this manual to draw your attention to the on-line documentation and other important information.

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. 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 analyzer 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, you can contact our sales or service representative in your area or use the information at the beginning of this document to contact us.

## Safety

Each person who operates the Antaris MX should first read the safety information in the *Site and Safety Information Guide*. The guide is in your manual set and is also available as a PDF file in your Thermo Scientific software. The guide is available in several languages; contact your local Thermo Fisher Scientific office for more information.

Before using the analyzer, read "Operating precautions" in the "Preparing the System" chapter to avoid damaging components or causing injury. Additional safety precautions are included where appropriate throughout this manual.

**⚠ Warning** To prevent personal injury and damage to equipment, always follow the safety precautions in this manual and in the *Site and Safety Information Guide* that came with your system whenever you use the analyzer. ▲

## Hardware components

This section describes the Antaris MX analyzer's major internal and external hardware components. You can replace key parts of the analyzer, such as the laser, light source, and power supply. See the "Service" chapter for instructions.

Instructions for replacing components are also available on-line. Choose Servicing The Antaris Analyzer from the Service menu in RESULT Operation to access ordering information and step-by-step instructions.

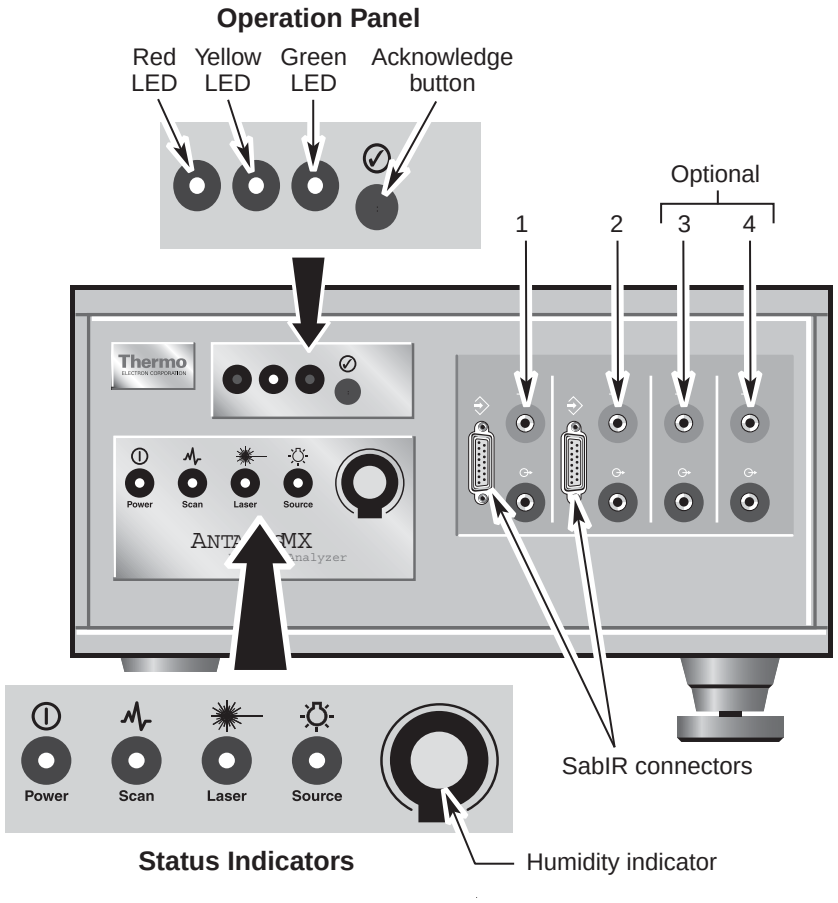
Your analyzer is sealed and desiccated to prevent damage to optical components from environmental humidity and corrosive solvents. An optional purge kit is available if your analyzer environment is excessively humid (above 95% non-condensing) or contaminated by routine use of potentially corrosive solvents or other agents. Purging (forcing dried air or nitrogen through the analyzer to eliminate water vapor and other airborne contaminants) better protects the system's internal components under those conditions. Instructions for selecting a purge gas and installing the purge source and connectors are in the *Site and Safety Information Guide* included with your system. See "Setting optional purge" in the "Preparing the System" 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 a combustible 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. ▲

**Note** The analyzer is also available with an environmentally controlled enclosure. See the *Process Installation and Maintenance Guide* for more information. ▲

## Front panel

The following illustration identifies the major components visible on the front of the analyzer.




Components on front panel

**Humidity indicator.** This shows when there is too much moisture inside the analyzer. 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 “Replacing the desiccant” in the “Maintenance” chapter for instructions.

**Status indicators.** These illuminate to show the status of the analyzer operation:

| Indicator | Description |
|---|---|
|  | Lights when the analyzer power is on and the power supply voltages are within specifications. |
|  | Flashes with each scan of the interferometer. |
|  | Lights when power is supplied to the laser and it is operating within specifications. |
|  | Lights when the source is illuminated and is operating within specifications. |

**Operation panel.** This contains indicators that tell you to take an action. The following tables list the meaning of each indicator and indicator state:

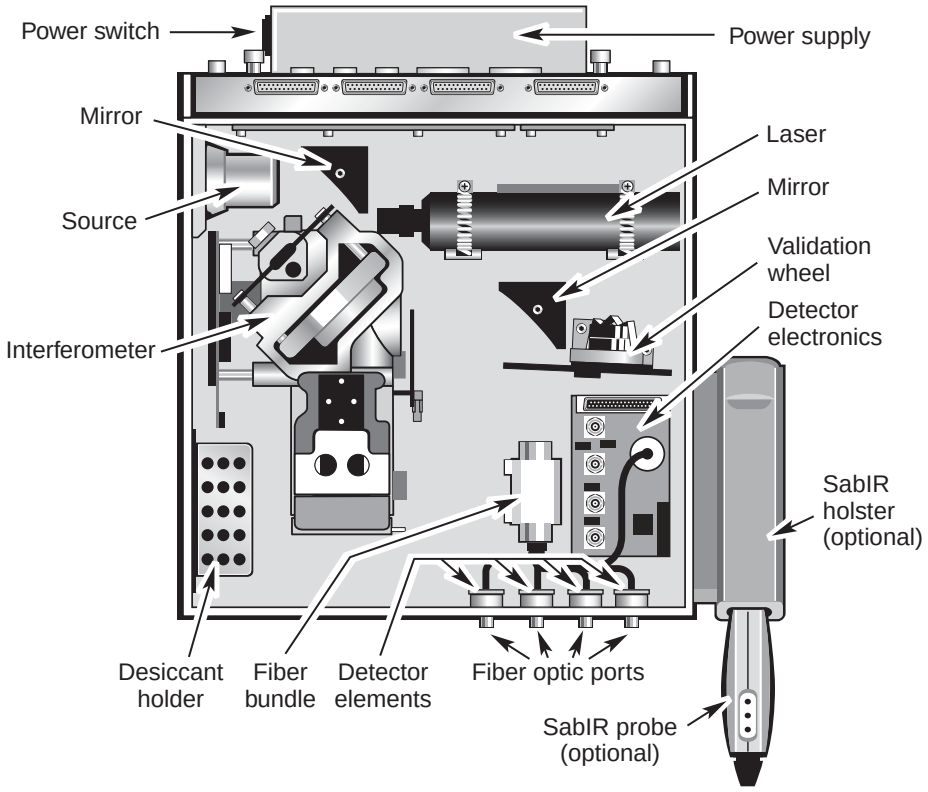
| Indicator | Meaning |
|---|---|
| Green | The system is waiting for a response from the operator. |
| Yellow | The system is collecting data. The fiber optic accessory should remain in the same position until the yellow light goes off. |
| Red | A QC failure occurred while the system ran a workflow or other process. |

| Indicator State | Meaning |
|---|---|
| Steady | The operator can respond by pressing the green Acknowledge button on the operation panel or by choosing a button in a prompt. |
| Flashing | The operator is required to respond by choosing a button in a prompt. |

The green Acknowledge button lets you initiate an action, such as starting data collection. The LED indicators let you see the status of the collection without being directly in front of the computer screen.

## Internal components

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




Internal components

The internal components include:

**Source.** The halogen, near-infrared source emits a beam of white light, which travels through the analyzer 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.

**Laser.** This 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 is a helium-neon (HeNe) laser head, with a neutral-density filter to help reduce power and reflections. The analyzer collects data at precise laser-calibrated points.

**Mirrors.** Precision mirrors focus and direct the near-infrared beam for optimum performance.

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

The analyzer uses two or four indium gallium arsenide (InGaAs) detectors that provide usable data from 12,000 $cm^{-1}$ to 3,800 $cm^{-1}$ (833 nm to 2,630 nm). The detectors and their associated optical components make up the “fiber optic module.”

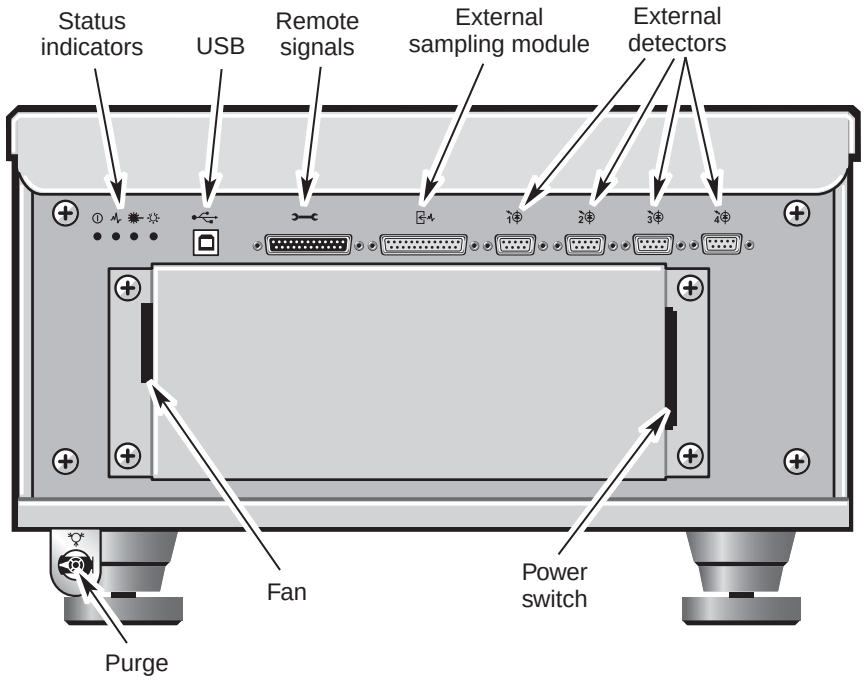
**Note** Detectors can become saturated or produce a distorted signal if too much light reaches them. Light attenuators that attach to the SMA connectors on the front of the analyzer are available. ▲

**Desiccant holder.** This contains a bag of desiccant that keeps the internal humidity level low and constant for improved accuracy in certain spectral regions.

**Validation wheel.** This optional wheel holds six samples, including five glass transmission standards and a polystyrene sample. The glass standards are calibrated to transmit approximately 2%, 10%, 20%, 40%, and 80% of the incident light beam. Use them for instrument qualification with 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 and is used for background and sample collections.

## Rear panel

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




Rear panel

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

The status indicators illuminate to show the status of the analyzer operation. See the descriptions in "Front panel" earlier in this chapter.

The data cable from the computer connects to this USB 2.0 port (USB 1.1 is not supported by this port). To avoid data loss, use only the Thermo Scientific data cables to connect the computer to your analyzer.

Use this connector to install a source of purge gas if the analyzer is purged. Instructions for selecting a purge gas and installing the purge source and connectors are in the *Site and Safety Information Guide*. Instructions for setting purge pressure and flow are in "Setting optional purge" in the "Preparing the System" chapter of this manual.

**⚠ Danger** *Never* use a flammable gas or argon 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. ▲

The remote signals connector is used by Thermo Fisher Scientific Technical Support for diagnostic purposes.

This connector is used for running an external Antaris sampling module.

These four connectors can carry the signal from an external detector or communication from an external accessory.

The power supply includes an IEC 320 receptacle for connecting the AC power cord and a power switch.

Be sure to use an appropriate power cord for your electrical service. The supplied cord 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. ▲

## Sampling channels

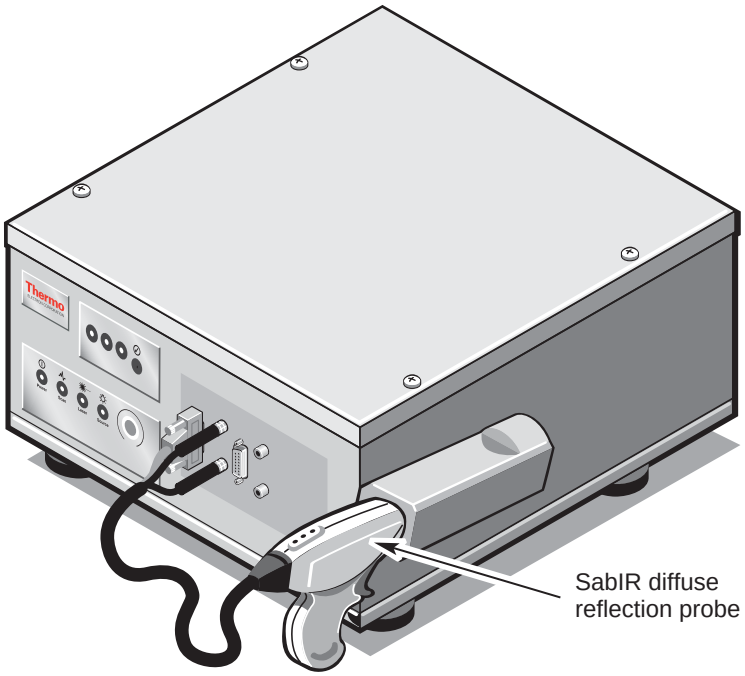
You can simultaneously collect data from multiple channels for continuous, remote sampling for quality measurements and sample component analysis. The analyzer is available in two configurations, with two or four channels for attaching fiber optic accessories. Each channel has industry-standard SMA connectors that accommodate a wide range of optical fibers and probes.

**Note** The output connectors are designed for 1.8 mm diameter fiber bundles. Using mismatched fibers or probes may reduce light throughput. ▲

The SMA connectors let you analyze powders, solids and other opaque materials using appropriate sampling probes. You can sample materials directly or indirectly through packaging materials.

Many compatible probes are available from Thermo Fisher Scientific. The analyzer is also compatible with other commercially available fiber optic accessories that use standard SMA connectors.

Channels 1 and 2 support the SabIR™ fiber optic probe for diffuse-reflection sampling of powders, solids, and other opaque materials. (You can use one or two SabIR probes.) You can sample materials directly or indirectly through packaging materials.




Antaris MX with SabIR probe

The probe holster contains a Spectralon® reference for collecting backgrounds. Automatic background collections using the Spectralon reference help to ensure consistent sampling and repeatable results. For more information about the SabIR probe, see the “Using the Optional SabIR Probe” chapter.

## RESULT software

RESULT is a dedicated analysis software package that includes the following applications:

**RESULT Operation** has an easy-to-use graphical interface for routine sample analysis. The software 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.

**RESULT Integration** lets you set up controlled operating environments for routine sample analysis. You can integrate quantitative, qualitative, and spectral measurement methods with simple data collection, archiving, and reporting routines to create custom analyses without the use of complicated programming or macro coding.

**RESULT Data View** is a tool for viewing sequence data files collected from time-based experiments. Use this application to display sequence spectra as well as measured concentration values or other analysis results.

RESULT works with the Thermo Scientific TQ Analyst™ method development software for seamless method creation and design. TQ Analyst lets you develop analytical methods for mid-infrared, near-infrared and other spectroscopic applications.

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 Fisher Scientific.
- The Unscrambler® version 7.6, or version 9.5 or higher 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.

## On-line help

The Service menu of RESULT Operation provides access to an on-line help system. It includes maintenance and service procedures, warranty information, and a list of part numbers for optional and customer-replaceable parts. See "Section 3 RESULT Operation Software" in your *RESULT User's Guide* for more information.

## For more information

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

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

*RESULT User's Guide* – For basic information about RESULT Integration, read "Section 2 RESULT Integration Software." For information about RESULT Operation, read "Section 3 RESULT Operation Software." For information about RESULT Data View, see "Section 4 RESULT Data View Software." 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 3 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 since the *RESULT User's Guide* was last revised.

*Servicing Antaris* – Choose Servicing the Antaris Analyzer from the Service menu in RESULT Operation to access a detailed parts list, ordering information, and part replacement procedures.

*Release Notes* – Release notes for your software applications 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 Technical Support representative for more information.

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# Preparing the System

This chapter explains how to prepare your analyzer for operation and data collection. Be sure to heed the operating precautions in the next sections whenever you use the system.

## Operating precautions

Before operating the analyzer and sampling accessories, read the following operating precautions to avoid damaging components or causing injury.

### Laser safety

The analyzer is a Class I laser product. This means the accessible radiation levels are below Class I limits defined by the United States Department of Health and Human Services and the International Electrotechnical Commission (IEC).

**⚠ Warning** 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 analyzer fiber optic connectors. To avoid exposure to this energy, never stare into the end of a fiber optic cable or the tip of a fiber optic accessory that is connected to the analyzer. ▲

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

### Handling 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, reducing performance.

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

- 10 cm for the test fiber.
- 30 cm for the cable attached to the SabIR probe.

For the minimum diameter for other fiber optic cables and probes, see the manufacturer's documentation.

Do not touch the tips of the cables or test fiber with your fingers. If you must clean the tips, place a drop of alcohol on them and wipe with lens paper. Do not use other solvents for cleaning.

To avoid damaging the cables, connectors or ports, do not use tools to tighten connectors.

To avoid damaging the connectors, the test fiber or the fiber optic ports, do not over tighten the connectors when attaching the cables or test fiber to the ports.

Always keep the protective caps on the ends of the cables, fiber optic ports, and test fiber when they are not in use. This helps prevent damage to the connectors and protects the detectors from contaminants and moisture.

## Using fiber optic sampling accessories

This section explains how to use the analyzer with fiber optic sampling accessories, including connecting the accessories, collecting data, and specifying workflow events. Because the analyzer 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.

If you use the analyzer with the optional SabIR probe, see the "Using the Optional SabIR Probe" chapter for specific instructions about connecting the probe, compatible sample types, typical spectra, collecting backgrounds and sample data, developing workflows, and maintaining the probe.

## Connecting fiber optic accessories

The analyzer is compatible with fiber optic accessories that have standard SMA connectors. You can connect these accessories using the fiber optic ports on the front of the analyzer. When connecting accessories, please note the following:

- The two electrical connectors on the analyzer (for channels 1 and 2) are for use with the SabIR probe only. Other sampling accessories requiring SMA connectors can also be used with fiber optic channels 1 and 2 without connecting the SabIR electrical connector.

- If the analyzer power is off while you install a fiber optic accessory and has been off for more than 20 minutes, after you turn on the analyzer, let it stabilize for about one hour before collecting data. Each time you turn the analyzer power on and off, be sure to log off and then log back in to RESULT.

- Do not discard the protective caps from any fiber optic accessories or the analyzer. Put the caps back on the fiber optic connectors when the accessory and/or analyzer are not in use.

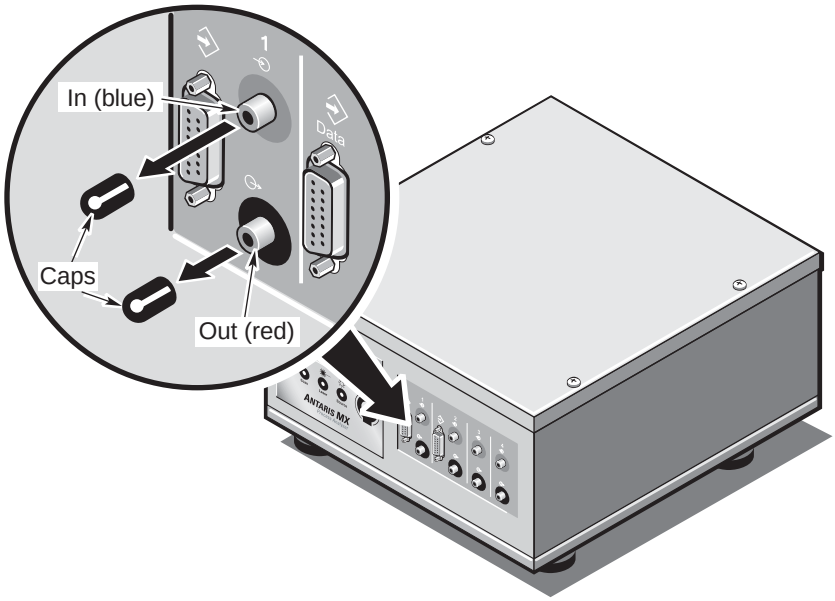
- Fibers with a diameter larger than 235 µm and some fiber bundles may require additional attenuation for some applications. Consult an application specialist if you need assistance.

To connect a sampling accessory to the analyzer:

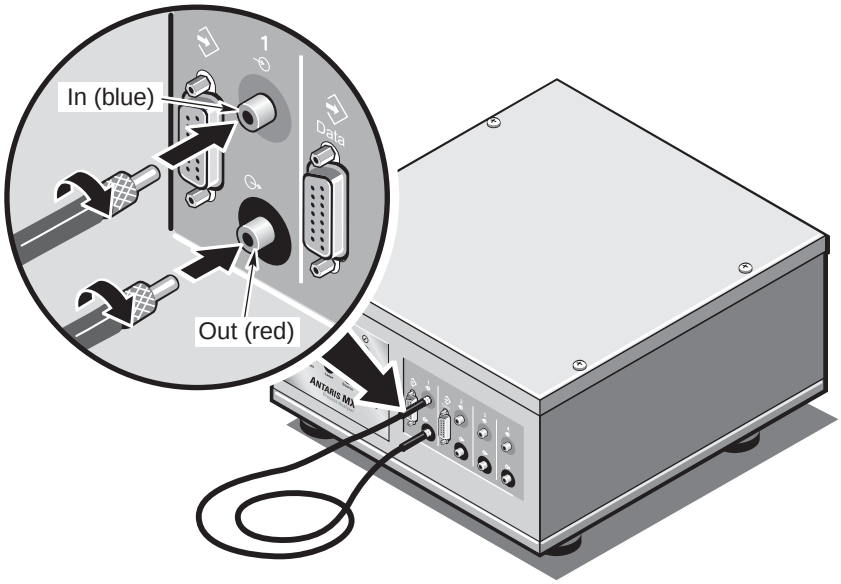
1. **Remove any protective caps from the sampling accessory connectors.**

   Save the caps so they can be put back on the accessory for storage.

2. **Remove the protective caps from the In and Out fiber optic ports you wish to use.**



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 analyzer through the blue In port. The connectors are color-coded for compatibility with the SabIR probe. You can also use the color coding to consistently connect the cables on your sampling accessory to the same ports on the analyzer.

**Notice** Be consistent when attaching fiber optic cables to the ports. If the cables are different and not always attached to the same ports, your data may be affected. ▲

Hand-tighten the connectors until you begin to feel a small amount of resistance; that is, until they are finger-tight.

**Notice** To prevent damage to connectors on the probe or analyzer, do not over tighten the connectors or use tools to tighten them. ▲

4. **Turn on the analyzer power and log in to the software.**

If the analyzer power has been off for more than 20 minutes, let the analyzer stabilize for about one hour before collecting data.

## Connecting the strain relief mechanism

The strain relief mechanism holds the fiber optic cables of the SabIR or other fiber optic accessories and helps prevent damage to the cables caused by bending.

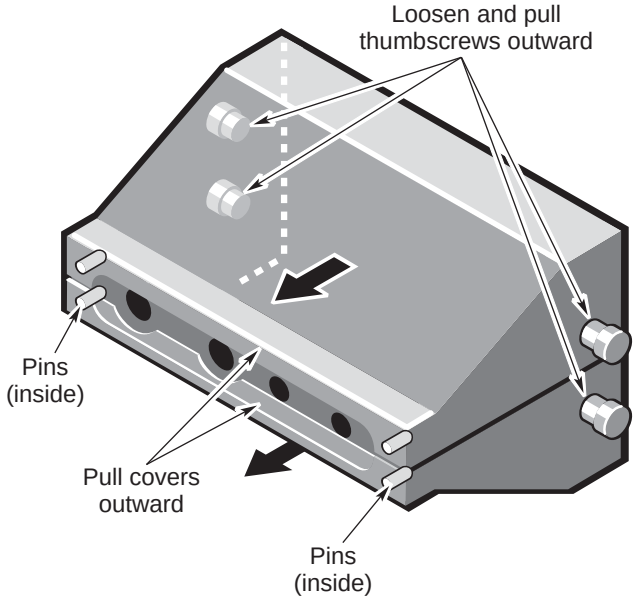
**Notice** Keep the front bar of the mechanism, where the slots for the cables are located, under the fiber optic cables during installation. ▲

**Note** If you are using a SabIR probe, connect it to either channel 1 or 2. The cable slots on either end of the strain relief mechanism are sized to accommodate the SabIR fiber optic and electrical cables. ▲

To attach the strain relief mechanism:

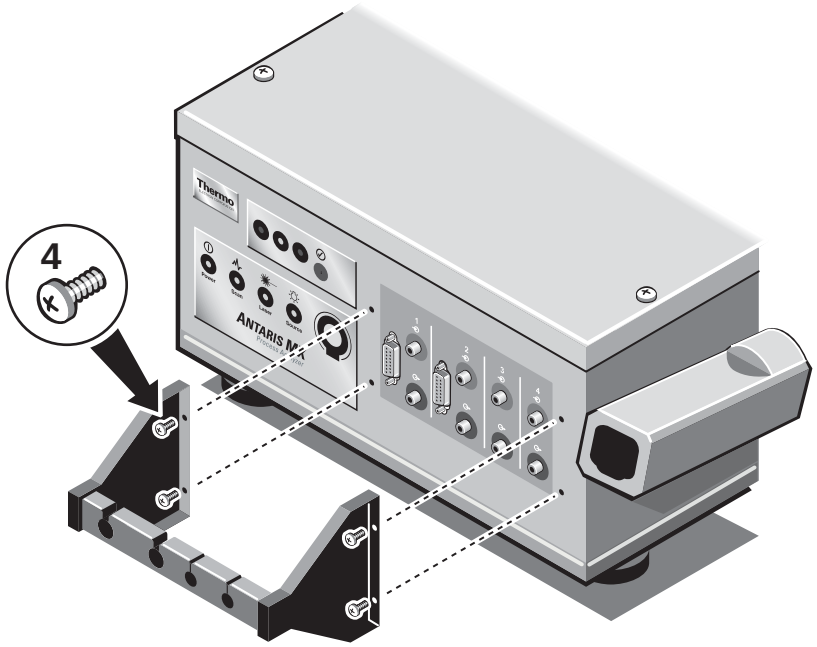
1. **Loosen the thumbscrews on the strain relief covers, and then remove the covers.**

   You must slide the pins in the front of the cover out of their holes in the front of the strain relief bar.



2. **Insert the provided screws into the four corners of the strain relief base.**

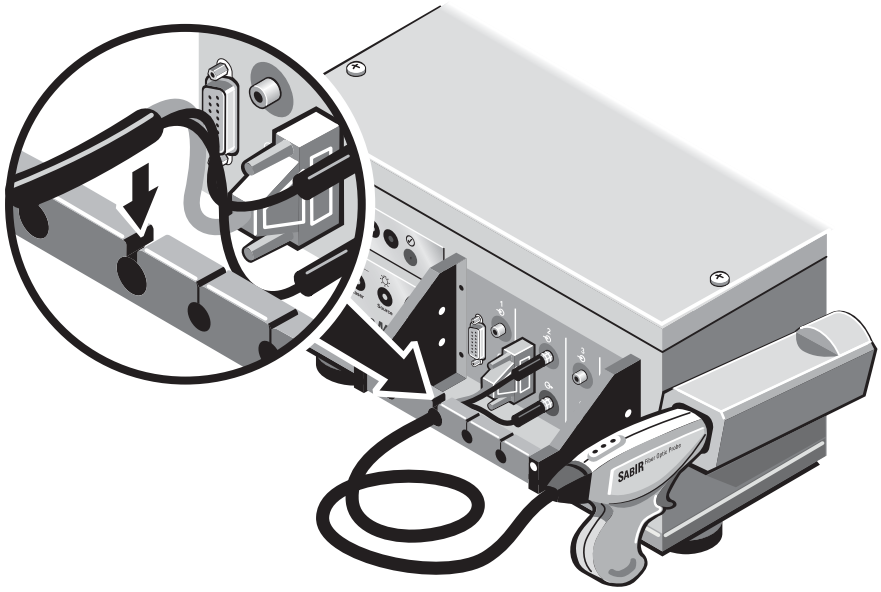
   Use a No. 2 Phillips screwdriver to tighten the screws.




**Notice** Every fiber optic cable has a bend radius that should not be exceeded. To help avoid damaging the cables, never bend them any more than necessary to work with them. Spread the material around the cable slot in the strain relief mechanism apart when you fit the cable into it. ▲

3. **Gently fit the fiber optic cables into the cable slot.**

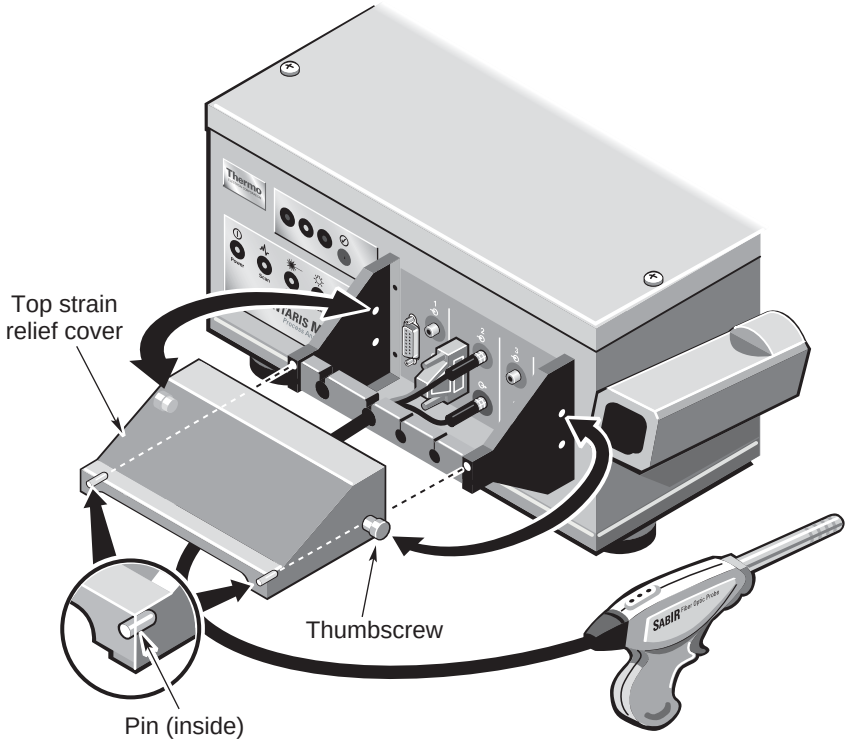
   If you are using a SabIR probe, fit both the fiber optic and electrical cables into the cable slot.




**Notice** Make sure the cables are in their slots before placing the cable cover on the strain relief base. Also make sure the covers do not compress the cables. ▲

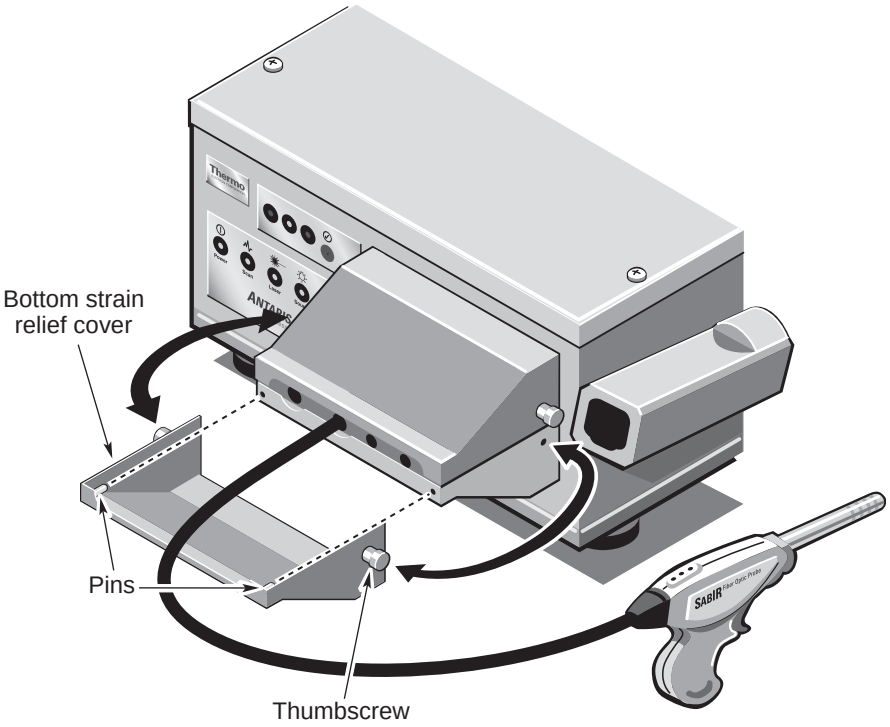
4. **Hold the cables in place with one hand and gently install the top strain relief cover.**

   Slide the pins in the front of the cover into their holes in the front of the strain relief bar, and then tighten the thumbscrews.



**5. Install the bottom strain relief cover.**

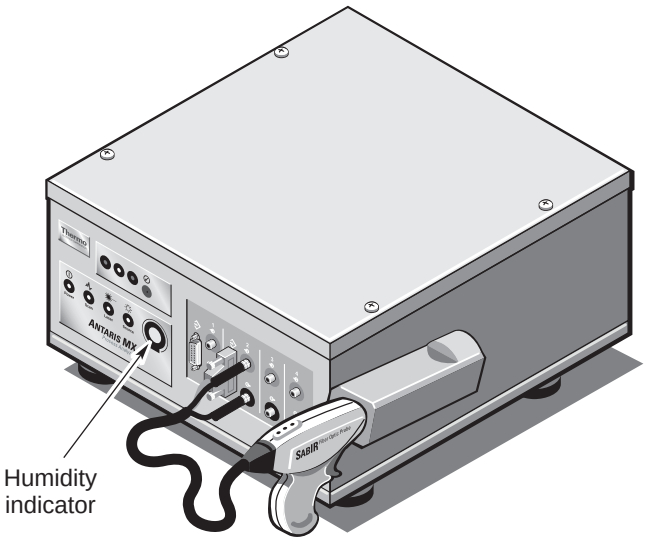
Slide the pins in the front of the cover into their holes in the front of the strain relief bar, and then tighten the thumbscrews.



## Checking the desiccant

A bag of desiccant is inside the analyzer, near the front-left corner. The desiccant reduces the water vapor inside the analyzer.

Keep all covers closed tightly and check the humidity indicator on the front of the analyzer monthly (or every two months if the analyzer is not used regularly).




Change the desiccant if the indicator is pink. See “Checking and changing the desiccant” in the “Maintenance” chapter for instructions.

To view this information, start RESULT Operation and choose Servicing The Antaris Analyzer from the Service menu. Then view “Maintaining your analyzer” and read the “Checking and changing the desiccant” topic. See “Ordering parts” to find the part number for ordering desiccant bags.

**⚠ Warning** Avoid burn and fire hazard. Do not attempt to regenerate desiccant packs. ▲

## Turning on the system components

We recommend keeping 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 the most consistent results. If you must turn the analyzer off, let it stabilize for at least one hour after it is turned on before collecting spectra.

Follow these steps to turn on the system components:

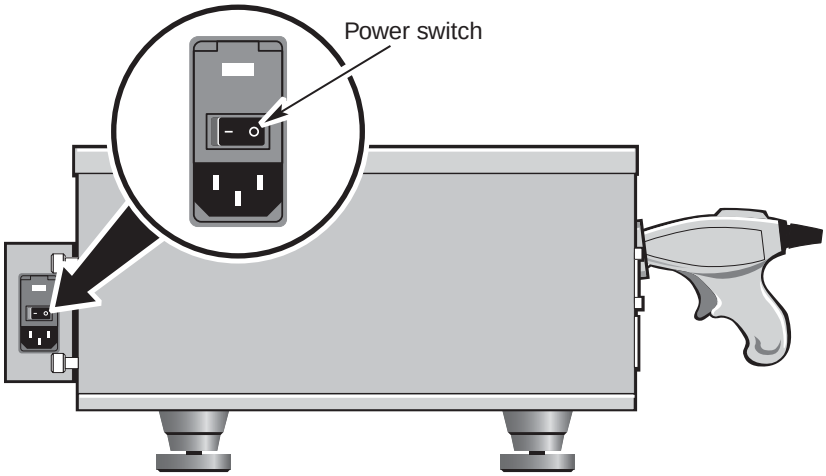
1. **Install any sampling accessories you plan to use.**

   See the documentation that came with the accessory for more information.

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

2. **Turn on the analyzer by pressing the power switch on the rear.**

   I = On
   O = Off




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 turning on the analyzer, let it stabilize for at least one hour before collecting spectra.

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

   See the documentation that came with those components for instructions.

**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 Operation

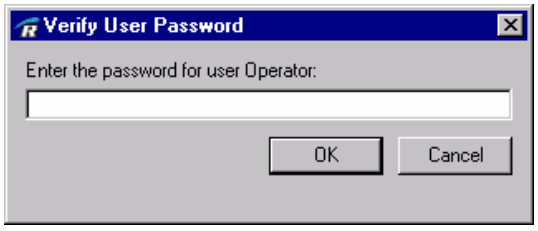
Before starting RESULT Operation, you must log on to the computer workstation. Before doing this, you must receive a Windows user name and password from your Windows administrator. If you are not a RESULT administrator, the RESULT software administrator must also add your logon information to the RESULT user list.

Depending on how your workstation has been configured, RESULT Operation may start automatically when you log on to the workstation. If it does not, double-click the RESULT Operation shortcut on your workstation desktop:

If the shortcut is not present, click the Start button on the Windows taskbar, point to Programs, point to Thermo (or Thermo Nicolet), and choose RESULT Operation.


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

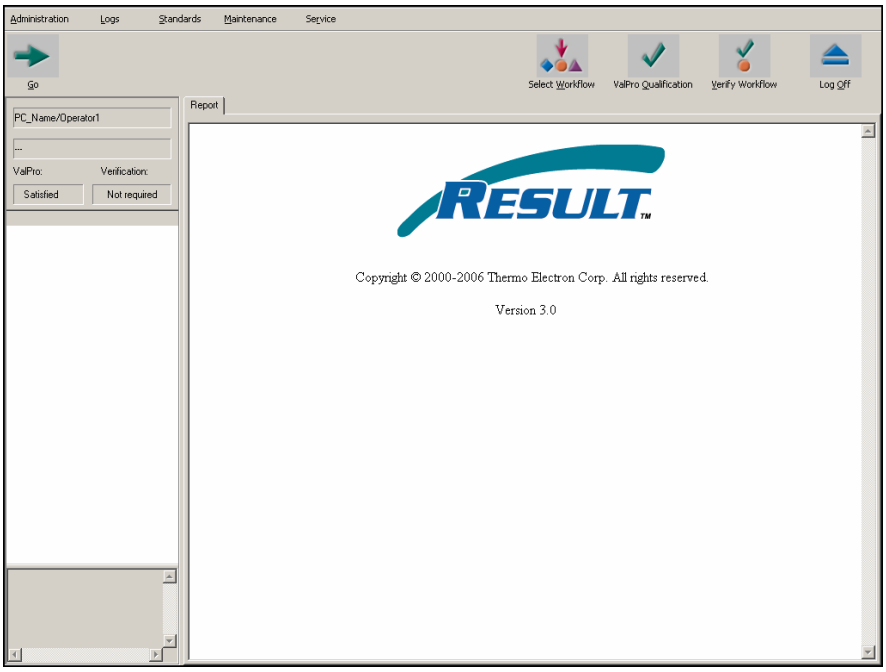
The password you entered must match your Windows password exactly, including the letter case.




Enter your Windows password, and then choose OK.

**Note** You are allowed three attempts to enter your Windows password correctly. See your RESULT software administrator if you are unable to start the software. ▲

When the software starts, the RESULT Operation main window appears:




RESULT Operation main window

## Setting optional purge

If your analyzer has an optional purge kit, set the pressure regulator between 10 psi and 20 psi (pounds per square inch). The flowmeter should read approximately 20 SCFH (standard cubic feet per hour). If you need to adjust the flow rate, or if your application requires a different flow rate, follow the instructions in "Setting the purge gas controls" in the "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 gases such as argon (Ar), can damage the analyzer. ▲

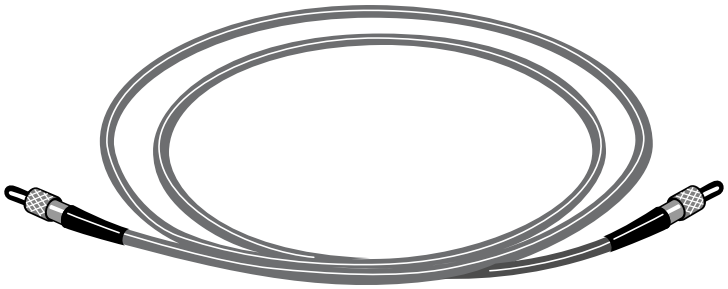
We recommend leaving the purge on at all times (even when the analyzer power is off). This keeps the analyzer free of undesirable gases, protects the optics, and improves thermal stability.

For information about installing purge equipment, see "Installing purge gas controls" in the "Service" chapter. Instructions for inspecting and changing the purge gas filter are in the "Maintenance" chapter.

To view this information from your computer, choose Servicing The Antaris Analyzer from the Service menu of RESULT Operation. Then view "Maintaining your analyzer" and look for the appropriate topics.

## Testing the analyzer

The analyzer includes a 235 µm, multimode, optical test fiber for performing operation troubleshooting tests without attaching a fiber optic sampling accessory.



Optical test fiber

Use the test fiber along with Instrument Check in RESULT Operation to test the optics and detectors or to collect a background.

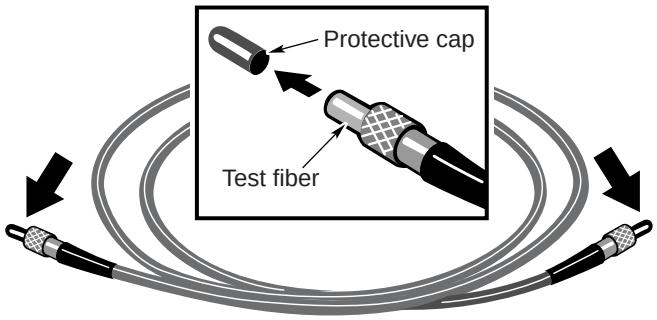
## Connecting the test fiber

Follow the steps below to connect the test fiber to the analyzer. It is not necessary to turn off the analyzer.

**Notice** Do not discard the protective caps from the test fiber or the analyzer. Put the caps back on the fiber optic connectors when the test fiber and/or analyzer are not in use to protect the fiber optic and to maintain the purged or desiccated environment of the analyzer. ▲

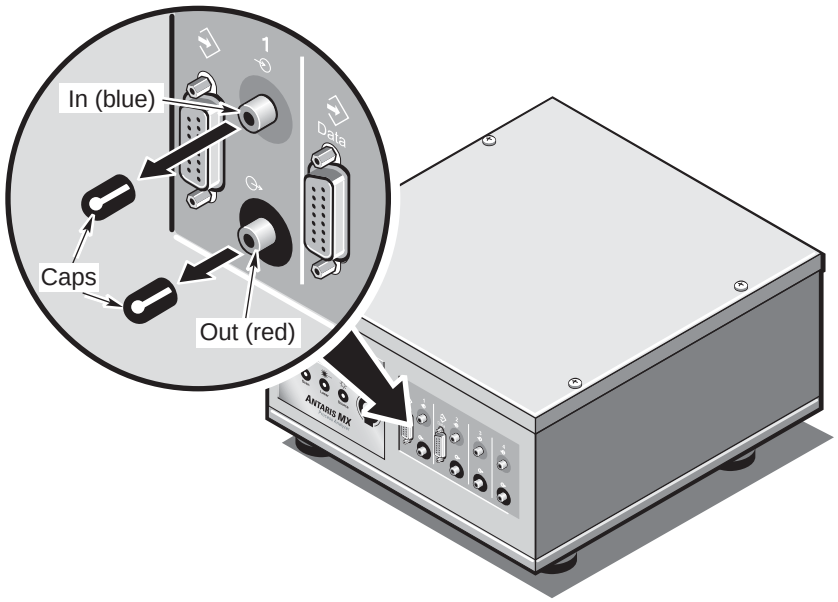
1. **Remove the protective caps from the ends of the test fiber.**

You can connect the test fiber to any channel. You will be prompted during the test to specify the channel.

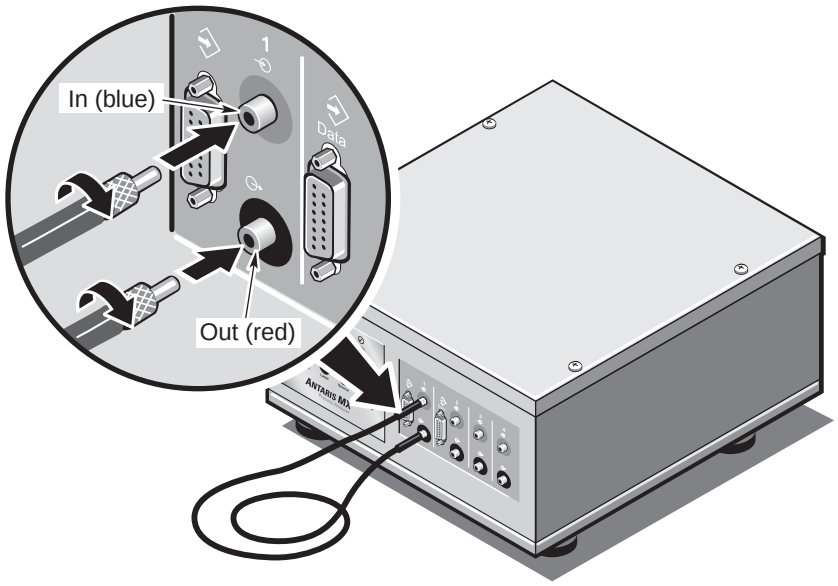


**2. Remove the protective caps from the In and Out fiber optic ports.**

You can connect either end of the test fiber to either of the ports.




**3. Connect both ends of the test fiber to the In and Out ports on the analyzer, and hand-tighten the thumbscrews on the test fiber connectors until they are finger-tight.**




**Notice** To prevent damage to the ends of the test fiber or the connectors on the analyzer, do not over tighten the thumbscrews or use tools to tighten them. ▲

**⚠ Caution** Do not stare into the fiber optic connectors or into the non-terminated end of the test fiber when the analyzer is turned on. ▲

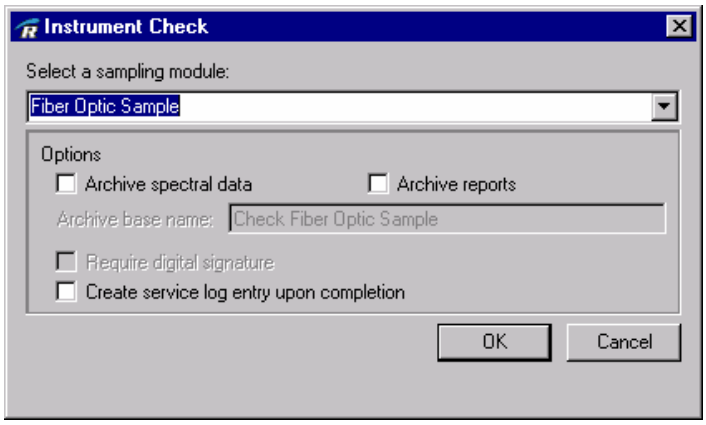
## Performing an instrument check

Use Instrument Check in RESULT Operation to run an operation test as explained below. Before running the test, attach the test fiber and turn on the analyzer power as explained in the preceding section. If the power has been off for more than 20 minutes, wait at least one hour before running the test.

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

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

   The Instrument Check dialog box appears:




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

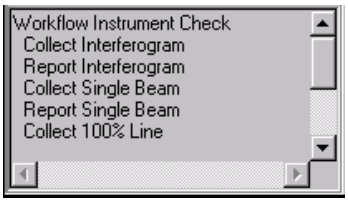
3. **Make sure Select A Sampling Module is set to Fiber Optic Sample.**

4. **Choose OK.**

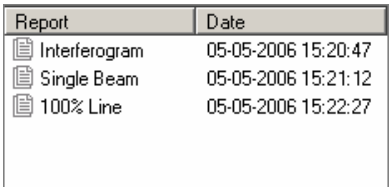
   The Select Channel dialog box appears:


5. **Select the channel you are using from the drop-down list box, and then choose OK to start the test.**

   The status indicator on the lower-left side of the RESULT Operation main window indicates the status of the instrument check:




   As each spectrum is created, the software creates a report. The report titles are listed in the report navigation frame:




   To view a report in the display area, click its title in the Report column. See "Chapter 5 System Maintenance" in "Section 3 RESULT Operation Software" of 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. "Chapter 5 System Maintenance" also contains sample spectra generated from an instrument check and information about each type of spectrum produced.

# Your First Experiment

This chapter takes you through a basic experiment using a simple workflow provided with RESULT. Before you begin, prepare the system as explained in the preceding chapter, using the provided test fiber.

**Note** The following procedure describes a single-channel collection. Multi-channel collections use the full capabilities of the system. See your *RESULT User's Guide* for complete information about performing multi-channel data collections. Also see the "Developing Workflows for the Antaris MX" chapter in this manual. ▲

Follow these steps:

1. **Start RESULT Integration.**

   You can do this by double-clicking the RESULT Integration shortcut on your workstation desktop:

If the shortcut is not present, click the Start button on the Windows taskbar, point to Programs, point to Thermo (or Thermo Nicolet), and choose RESULT Integration.

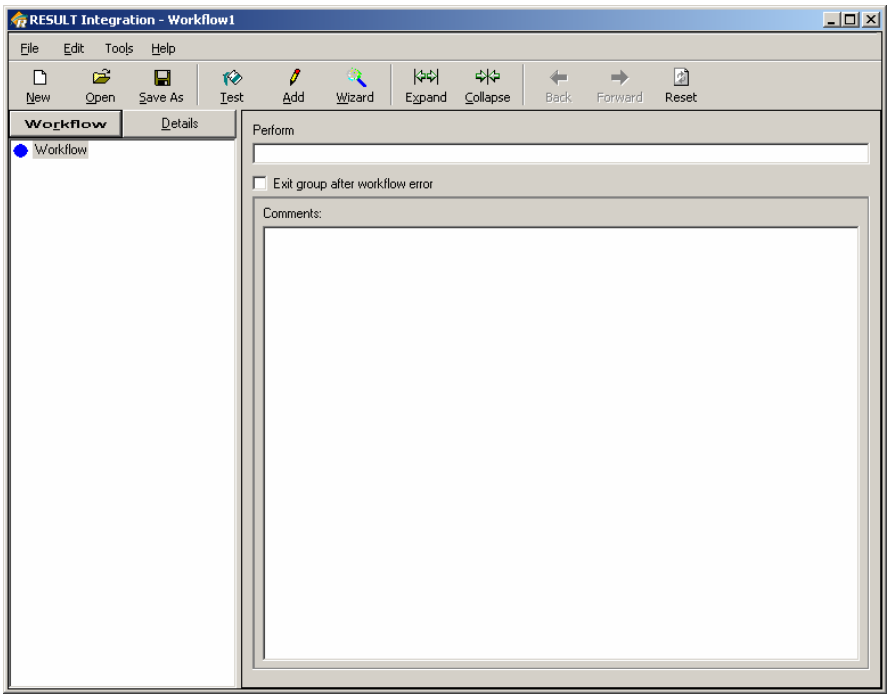

   Depending on how the software has been configured, RESULT may open a dialog box asking for your password, as shown below.

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


   Enter your Windows password, and then choose OK.

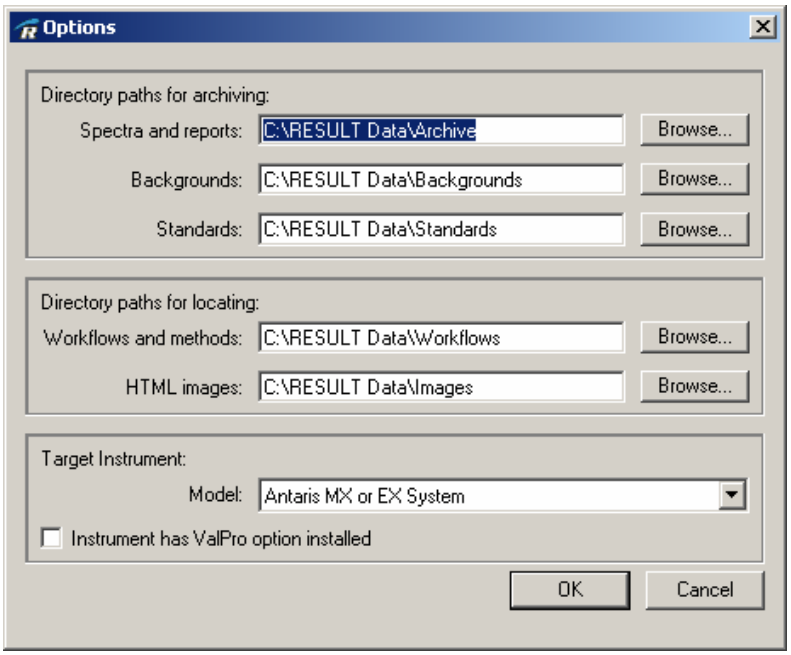
**Note** You are allowed three attempts to enter your Windows password correctly. See your RESULT software administrator if you are unable to start the software. ▲

   The software starts and the RESULT Integration main window appears:




2. **Make sure RESULT Integration is set to use the Antaris MX analyzer.**

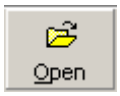
   To do this, choose Options from the Edit menu. The Options dialog box appears:



Make sure Model in the Target Instrument group is set to Antaris MX Or EX System and then choose OK.

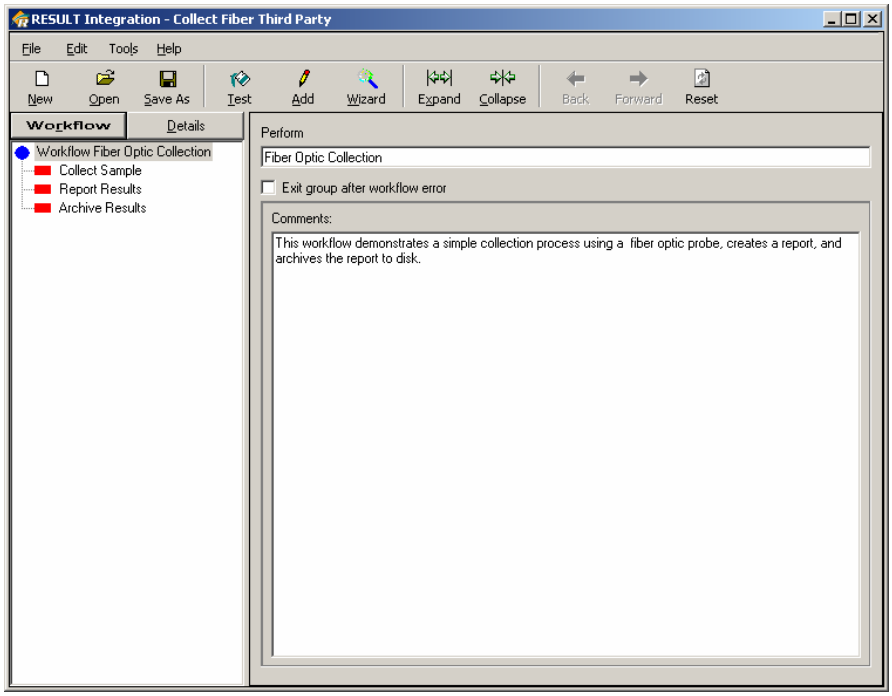
### 3. Open the workflow for our experiment.

To do this, click the Open button on the toolbar near the top of the RESULT Integration main window.




The Open dialog box appears listing the existing workflows. Select the workflow file named Collect Fiber Third Party.wfl; it is specially designed for performing a basic data collection using a fiber optic sampling accessory.

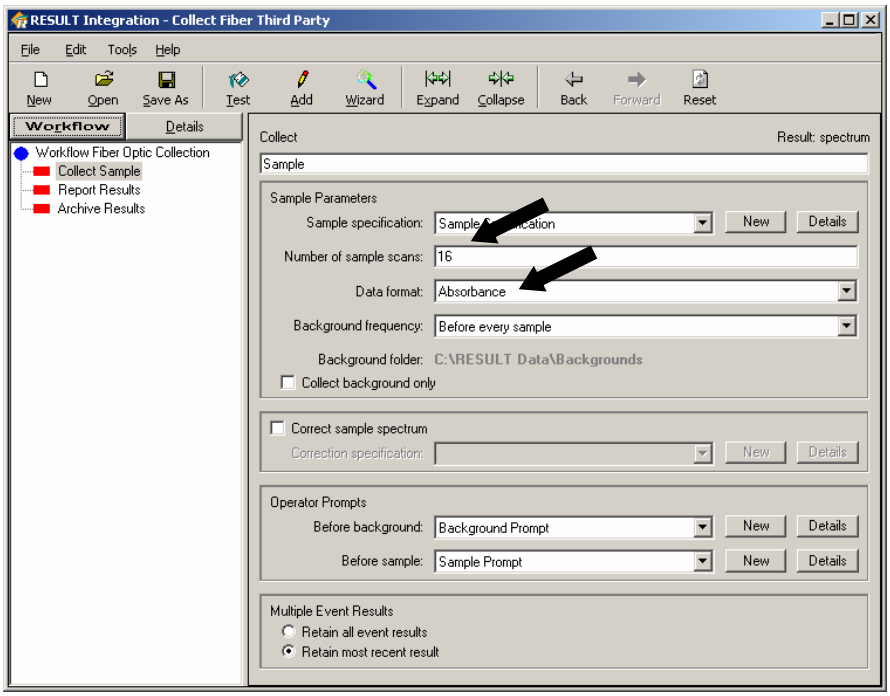
Choose Open to open the selected workflow. Information about the opened workflow appears in the RESULT Integration main window:



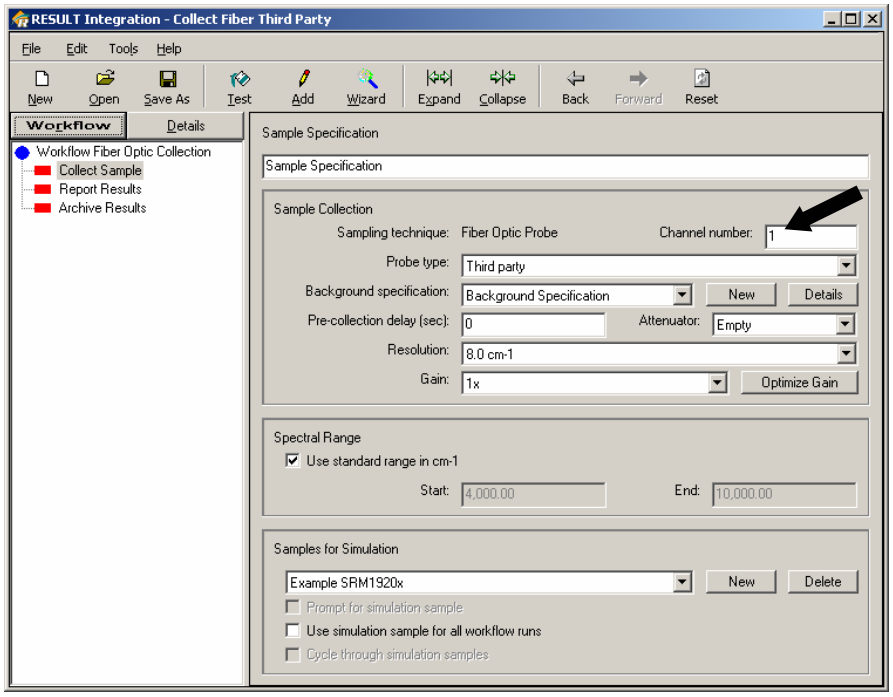

The workflow navigation frame at the left side of the window is used to create, add to or simply display the contents of the open workflow. A typical workflow consists of a sequence of events that collect, measure, report, and archive spectral data.

An event may have specifications that define how it will be performed. To see the specifications for the first event in our workflow, click the Collect Sample event in the workflow tree. Collection event parameters appear in the large display area of the window:

Notice that 16 sample scans will be collected by this event and that the collected data will be displayed in absorbance units.



If you click the Details button in the Sample Parameters group, the sample specifications appear:



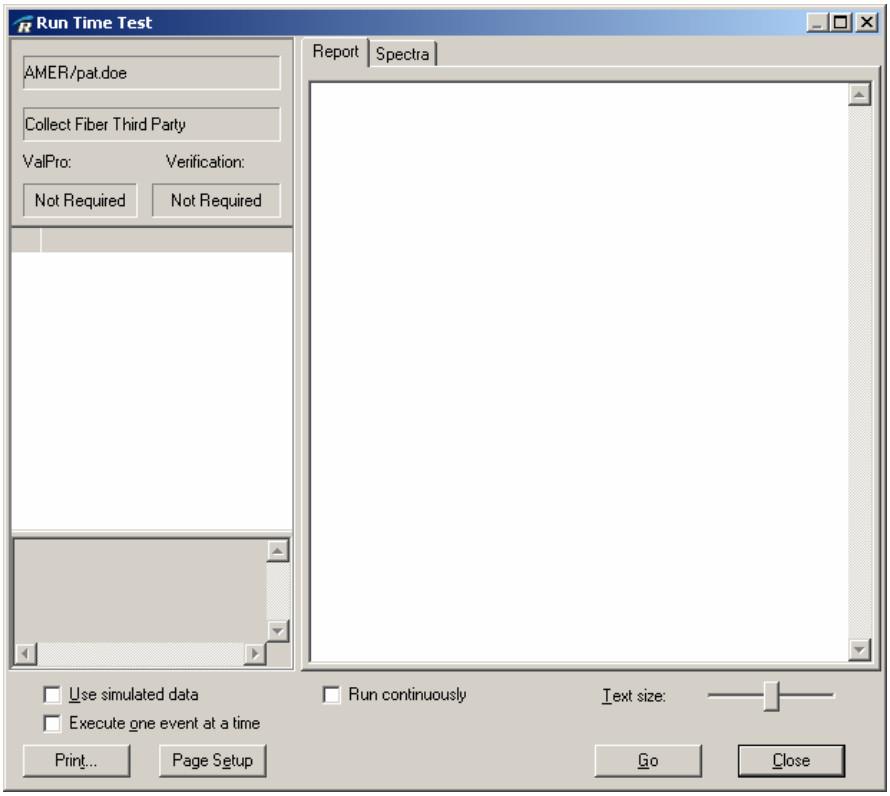

Notice that this workflow is set to use channel 1 for collecting data. If your test fiber is connected to another channel, type its number in the Channel Number text box. (Note: Channel 0 is the internal reference.)

You can return to the previously displayed information by clicking the Back button on the toolbar above the display area.

If you make changes to a workflow, you can save them by using Save Workflow in the File menu or by clicking the Save button on the toolbar.

**4. Start the workflow by clicking the Test button on the toolbar.**

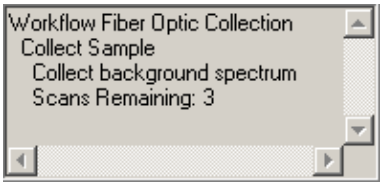
The Run Time Test window appears:




This window mimics the RESULT Operation main screen. In the upper-left corner is logon information for the current user and the name of the workflow. The ValPro and Verification indicators always show that these processes are not required for workflows run in RESULT Integration.

**5. Click the Go button to start data collection.**

The status of the workflow progress appears in the status box near the lower-left corner of the window:

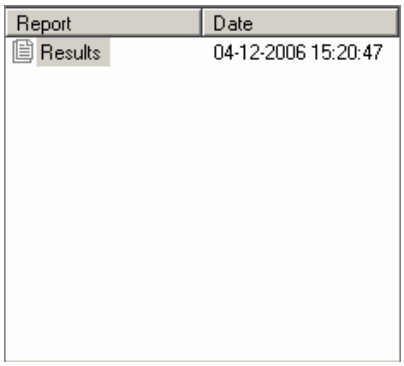



Any operator prompts that were set up in the workflow—for example, instructing the operator to prepare for background or sample collection—appear at the appropriate time. Follow the instructions in these prompts when they appear.

If you want to view the spectral data during collection, click the Spectra tab at the top of the Run Time Test window. The first spectrum is displayed as it is collected. As new spectra are added to the spectral window, they are overlaid. The most recent spectrum appears in red.

RESULT provides a variety of options for viewing and manipulating the spectral data. See "Chapter 2 Running Workflows" in "Section 3 RESULT Operation Software" of your *RESULT User's Guide* for more information about using these features.

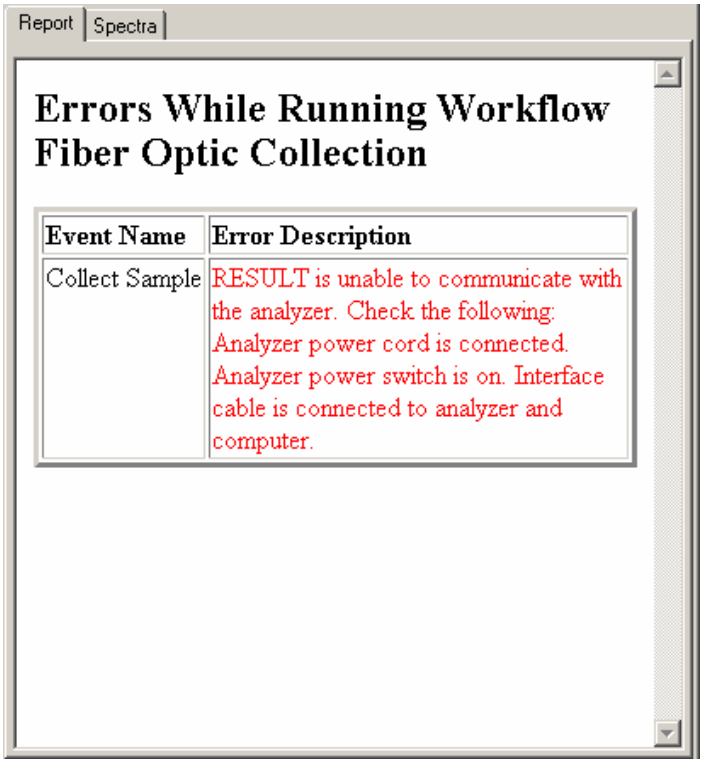
A report appears on the Report tab when the workflow is completed. The name of the report and when it was created appear in the report navigation frame to the left of the report:




You can print the report with the Print button at the bottom of the window or by right-clicking the report and choosing Print from the shortcut menu. You can set up the page before printing by using the Page Setup button.

The software adds a disclaimer to the end of the report to indicate whether it was generated in diagnostic mode with simulated data or in normal off-line production mode. This lets you easily distinguish reports that are created by workflows run in RESULT Integration from reports created by workflows run in production mode in RESULT Operation.

If workflow errors occurred, they are listed in a table. Here is an example:

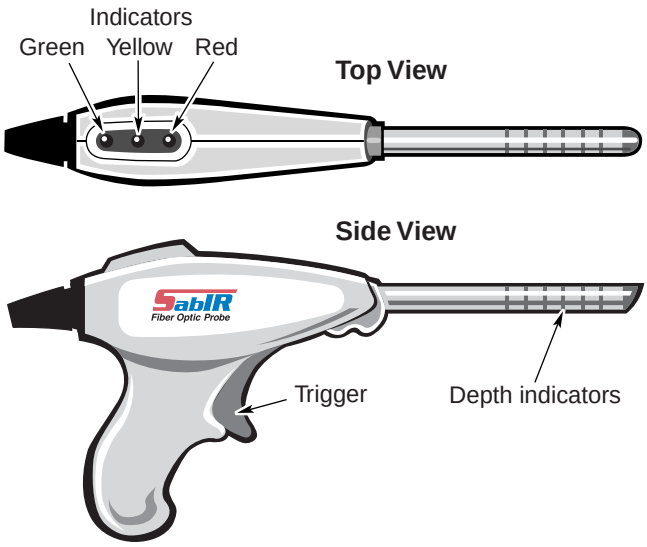



Read the error descriptions and suggestions for resolving the errors. See "Chapter 7 Troubleshooting RESULT Operation Software" in "Section 3 RESULT Operation Software" of your *RESULT User's Guide* for more information about errors that may occur when testing workflows.

6. **When you are finished running the workflow and reviewing the report, click the Close button to close the Run Time Test window.**

# Using the Optional SabIR Probe

You can use the analyzer with the SabIR probe for remote diffuse-reflection sampling of solids and powders. This chapter contains information about SabIR features and instructions for attaching, using, specifying workflow settings for, and maintaining the SabIR.




SabIR probe

The following important features are included with the SabIR:

**Probe holster.** The analyzer has a holster on the left or right side (or both sides, if you have two probes). Keep the probe in the holster whenever it is connected to the analyzer but not in use. The holster contains a Spectralon reference for collecting background data. It also contains a magnet that works with a sensor in the probe that detects whether the probe is in the holster during the background collection. (See "Collecting a background spectrum with the SabIR probe" later in this chapter for more information about the sensor and magnet.)

**Probe fiber optic cables.** These are available in two- and three-meter lengths. The cables are color-coded to match the In and Out ports on the analyzer. To prevent damage to the cables, keep the protective caps on the ends of the cables whenever they are not connected to the analyzer.

**Probe electrical connector.** This attaches to the electrical port on the analyzer and is the power source for the SabIR probe.

**Note** The strain relief mechanism holds the SabIR fiber optic and electrical cables and accessory fiber optic cables and helps prevent damage from bending and stress. ▲

**Probe handle.** This contains the following items:

- **LED indicators.** These have the same function as the indicators on the analyzer. They let you see the status of the collection without being in front of the analyzer or computer screen.

- **Trigger.** This lets you activate sample collection from a remote location and can be used in place of the Acknowledge button on the instrument. Do not use the trigger to collect background spectra with an external reference.

- **Sensor.** A sensor on top of the probe handle, near the probe shaft, works with a magnet in the holster to detect when the probe is properly inserted in the holster during background collection using the probe's internal Spectralon reference.

**Probe shaft.** The near-infrared (NIR) beam travels through the probe shaft to the probe tip. The stainless-steel shaft is 15.8 cm long, with a diameter of 1.6 cm. Graduated rings around the shaft help you insert the probe into substances at consistent depths.

**Probe tip.** This contains a sapphire window that can analyze samples directly or indirectly through packaging materials. The tip is angled to minimize specular reflection from highly reflective surfaces. This means that more light diffuses, producing a more accurate, detailed spectrum. Leave the protective cap on the probe tip whenever the SabIR is not connected to the analyzer.

## Samples compatible with the SabIR probe

The SabIR probe lets you remotely sample 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. Some examples of sample types include:

**Liquids** – Use the SabIR probe to sample liquids with the SabIR Transflectance Adapter available from Thermo Fisher Scientific.

**Solids** – Use the SabIR probe to analyze any solid with a rough or diffuse surface, such as paper, wood, plastics (especially those with a milky, opaque appearance), coated textiles, polymers, and pharmaceutical tablets.

**Powders** – The SabIR probe works well with large quantities of powder samples. You can insert the probe directly into the sample. If you are concerned about the sample leaving a residue on the probe, you can put the sample into a glass container and sample it indirectly through the glass.

When using the SabIR probe, take into consideration the sample thickness or the amount of sample. 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” chapter for more information.

## Operating precautions

Observe the following precautions when handling the SabIR 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 press the probe trigger prematurely, stop and restart the experiment.
- Do not use the probe for extended periods in temperatures under 0 °C or over 95 °C. Do not use the probe in temperatures under -25 °C or over 120 °C. Avoid rapid changes in temperature extremes (for example, from 0 °C to 100 °C), as thermal shock may weaken or damage the window or seal.
- To prevent damage to the probe tip, do not use it to sample harsh chemicals, such as amyl alcohol, acetone, chromic acid, fluorine, and oleum unless you are using the transflectance probe.
- Avoid getting substances onto or into the probe housing.
- Always follow appropriate safety precautions when working with explosive or other hazardous samples.

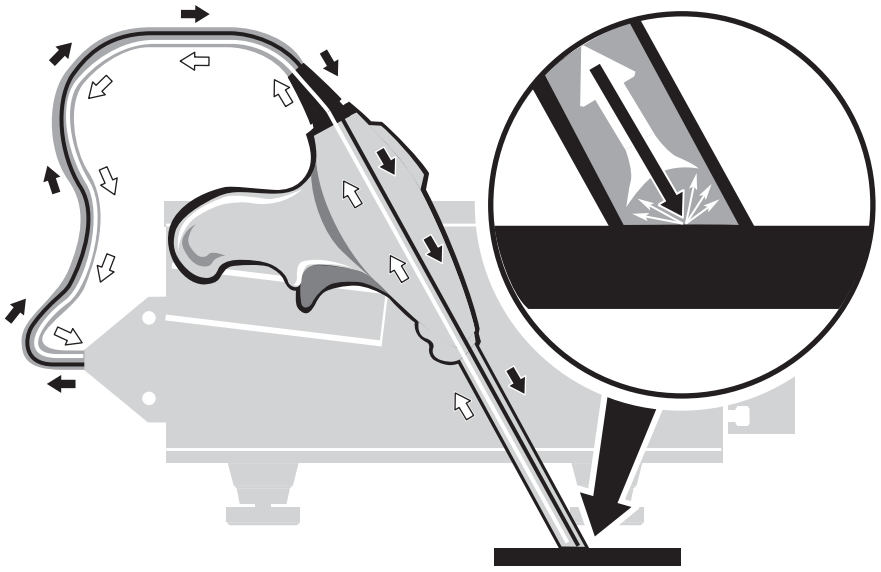
## Understanding diffuse-reflection sampling

The SabIR probe produces diffuse-reflectance 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 (for example, lactose, cellulose, polymers, or talc). Sampling is fast and easy because little or no sample preparation is required.

Diffuse-reflection fiber optic accessories measure changes in a light beam when it interacts with a sample of finely ground particles. The beam alternately passes through the particles and reflects from their surfaces. This causes the light to scatter, or "diffuse."

Diffuse-reflection fiber optic accessories often provide excellent results from powders and crystalline materials, which scatter much of the energy from the beam. The more scattering that occurs within the sample matrix, the more absorption information you can obtain and the higher the sensitivity of the measurement.

When you are using the SabIR probe, the light beam leaves the analyzer through the fiber optic Out port, and optical fibers carry the light through the probe. When the beam reaches the sample, the scattered (reflected) light travels back through the optical fibers and into the analyzer through the In port (as shown below) and then to a detector.



## Connecting a SabIR probe

The SabIR probe is easy to connect to the analyzer. Before you begin, however, be aware of the following:

- Make sure the analyzer power is off before connecting the probe to avoid damaging the analyzer electronics. Each time you turn off the analyzer power, be sure to log off any software applications.

- The strain relief mechanism holds and protects fiber optic cables, helping to prevent damage to the cables due to bending.

- If you are going to install both the strain relief mechanism and a SabIR probe, we recommend attaching the strain relief mechanism first to avoid bending the fiber optic cables excessively. If you install the SabIR probe first, be sure to keep the front bar of the strain relief mechanism, where the slots for the cables are located, under the SabIR cables while installing the mechanism. (For more information, see “Connecting the strain relief mechanism” in the “Preparing the System” chapter.) If a strain relief mechanism is already connected to the analyzer, remove the top strain relief cover, connect the probe to the analyzer, insert the fiber optic cables into the strain relief mechanism, and then replace the strain relief cover.

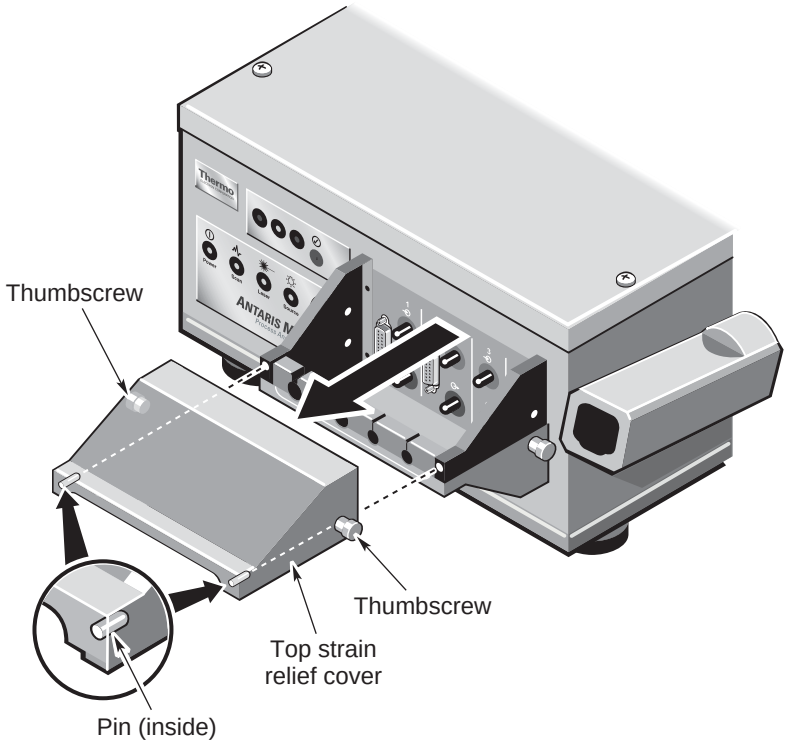
- Connect the SabIR probe to either channel 1 or 2. The cable slots on either end of the strain relief mechanism are sized to accommodate the SabIR fiber optic and electrical cables.

- Save the protective caps from the SabIR probe cables and tip and the analyzer so they can be put back on when these items are not being used.

To connect the SabIR to the analyzer:

1. **If the strain relief mechanism is installed, remove its top cover.**

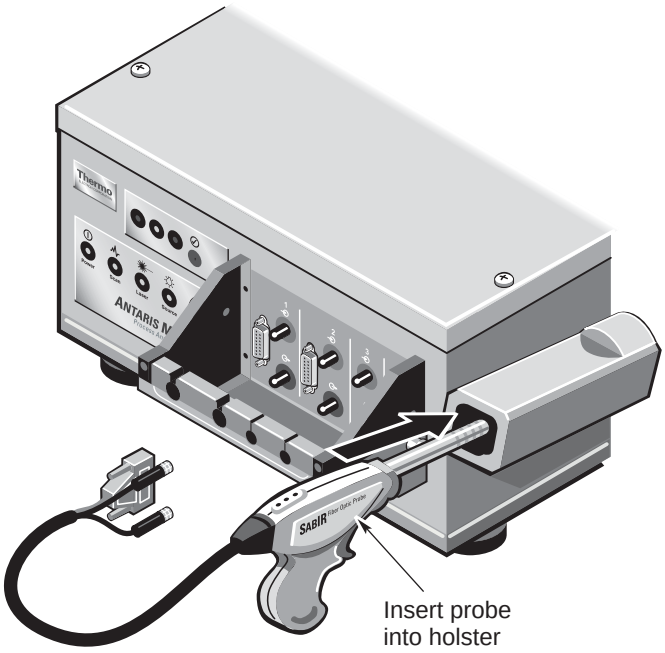
   Loosen the thumbscrews on the cover, slide the cover toward you, and lift the cover off.



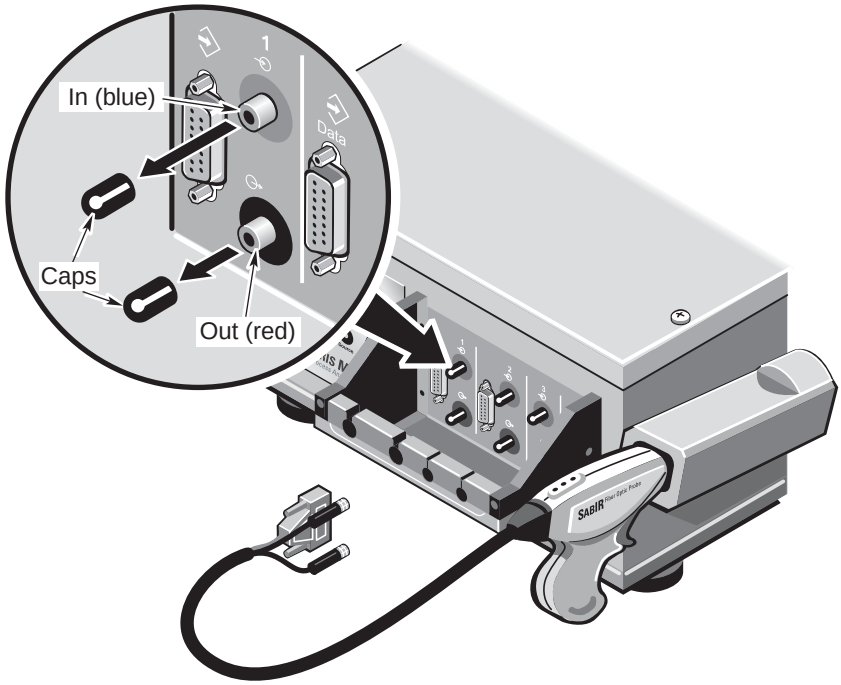

2. **Remove the protective cap from the probe tip.**

3. **Insert the probe into the holster.**

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




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



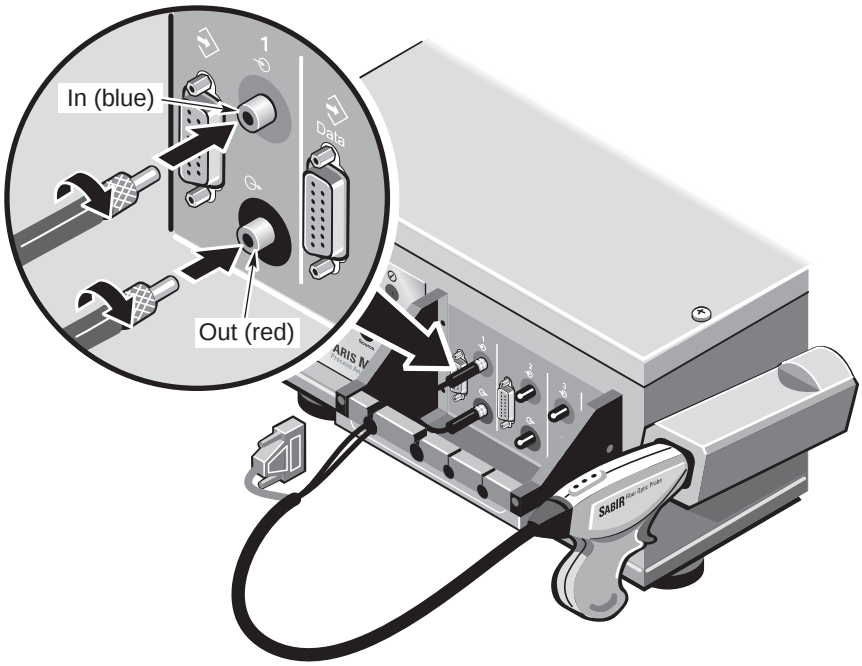
5. **Remove the protective caps from the fiber optic cables.**

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

   Attach the cables 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.

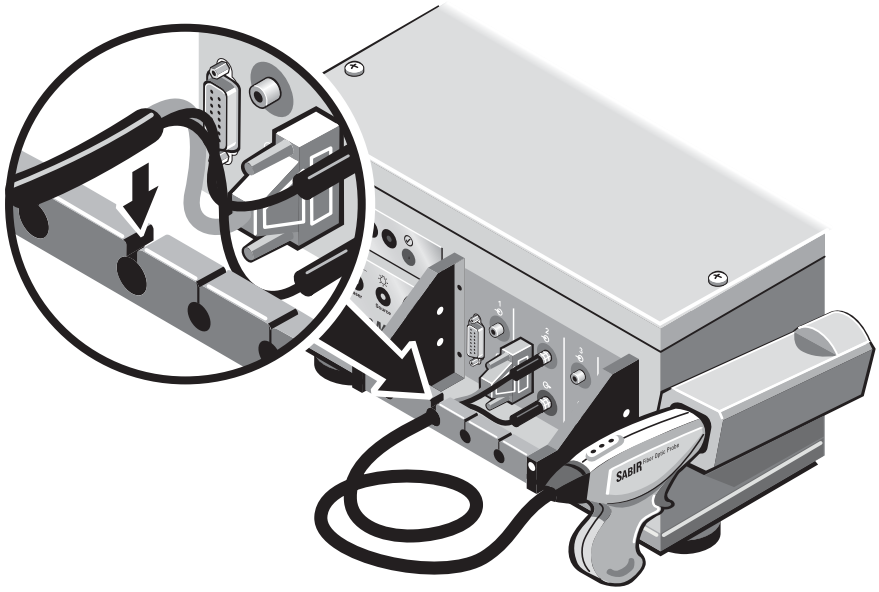
   Hand-tighten the connectors until you begin to feel a small amount of resistance; that is, until they are finger-tight.

**Notice** To prevent damage to connectors on the probe or analyzer, do not over tighten the connectors or use tools to tighten them. ▲



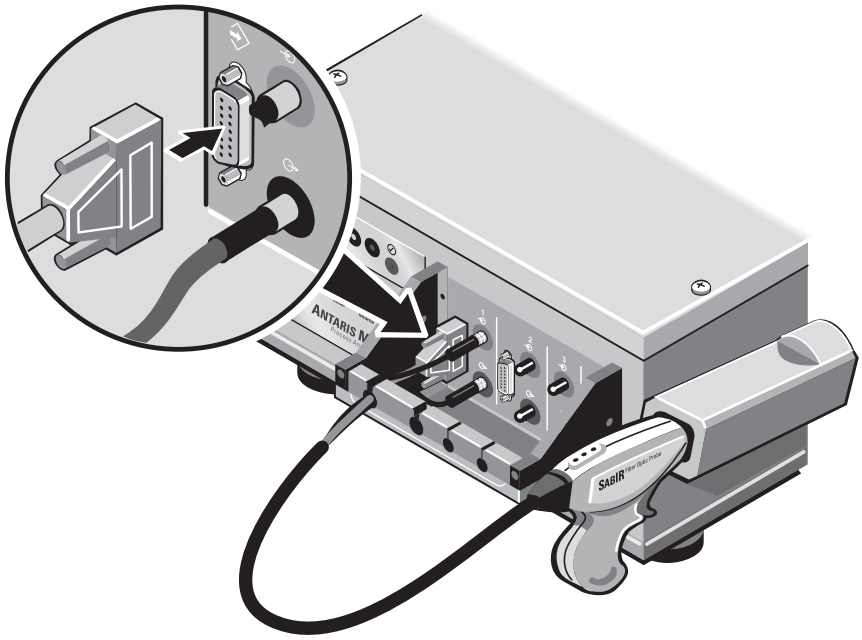

**Notice** If the cables are attached to the incorrect ports, the SabIR will function, but spectral quality or repeatability may be affected. ▲

7. **If you are using the strain relief mechanism, gently fit the fiber optic cables and electrical cable into the cable slots.**



8. **Connect the electrical connector to the electrical port on the analyzer.**

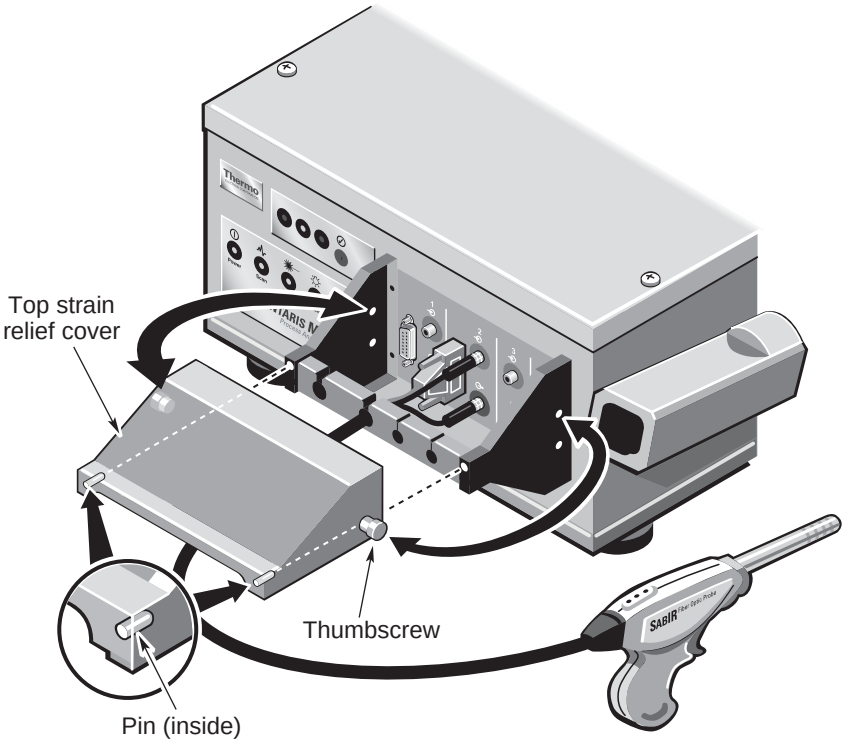
   Fit the connector into the port and then tighten the screws on either side of the connector. You may use a flat-blade screwdriver to tighten the screws, if necessary, but do not over tighten them.



9. **If you are using the strain relief mechanism, hold the cables in place with one hand and gently install the top strain relief cover.**

**Notice** Make sure the cables are in their slots before placing the cable cover on the strain relief base. Also make sure the covers do not compress the cables. ▲

Slide the pins in the front of the cover into their holes in the front of the strain relief bar, and then tighten the thumbscrews. (Do not over tighten the thumbscrews.)

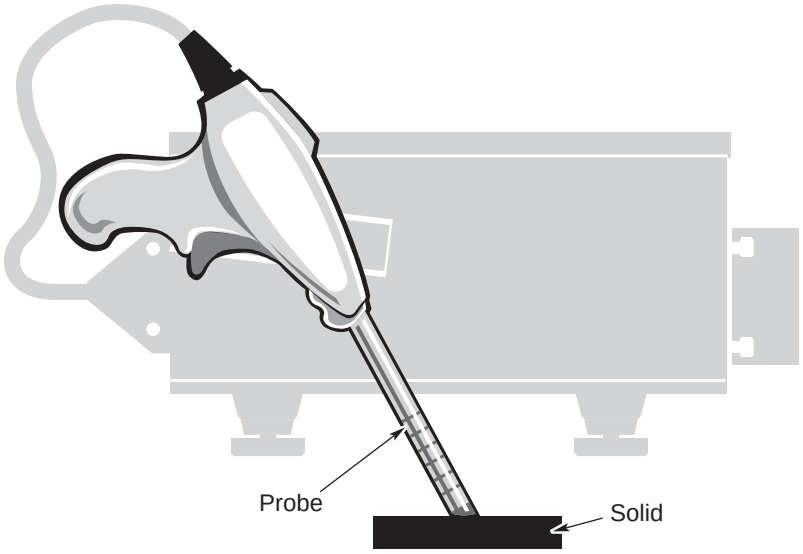



**10. Turn on the analyzer power.**

If the analyzer has been off for more than 20 minutes, let it stabilize for about one hour before collecting data.

## Sampling solids and powders with the SabIR probe

When sampling solids, hold the tip of the probe flush against the solid surface:




Sampling a solid with the SabIR probe

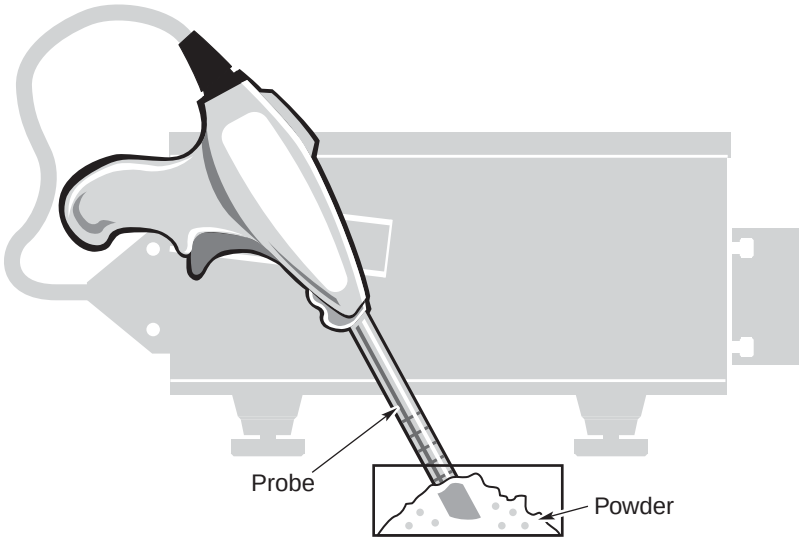
You can also sample solids through clear packaging materials, such as plastic bags, plastic wrap, or glass. Polymeric packaging materials such as plastics, however, have spectral features that may affect analysis results when you sample through them. Sampling through colored packaging materials may also affect spectral data.

As with solids, you can sample powders directly or through clear packaging materials such as glass or plastic. When sampling a powder through these materials, press the probe tip against the material, making sure the powder fully covers the area of packaging material that is between the sample and the probe tip. Here is an example showing how to sample a powder through a clear plastic drum liner:

Sampling a powder through packaging material

When sampling powders directly, make sure the sample is thick enough to fully cover the probe window while leaving enough material underneath the probe window to obtain an accurate reading:

The depth indicator rings on the probe shaft can help you maintain a consistent insertion depth when collecting multiple samples.




Sampling a powder with the SabIR probe

**Note** It is not always necessary to insert the probe into the sample powder. For many samples, you can just hold the probe against the powder surface. ▲

**Note** If the sample is likely to leave a residue on the probe, place the sample in a clear plastic bag or glass container to prevent residue from accumulating on the probe tip. If residue gets on the tip, follow the cleaning instructions in "Cleaning the SabIR probe" later in this chapter. ▲

See the next section and "Collecting sample data with the SabIR probe" later in this chapter for step-by-step instructions for using the SabIR to collect background and sample data.

## Collecting a background spectrum with the SabIR probe

This section explains how to collect a background using the SabIR probe and the internal Spectralon reference or an external reference. A background is a reference spectrum that accounts for the unique optics of the sampling accessory and the analyzer. Each sample spectrum is ratioed against a background so that the final spectrum is free of these features.

The SabIR probe holster contains a Spectralon reference 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 cleaning instructions.

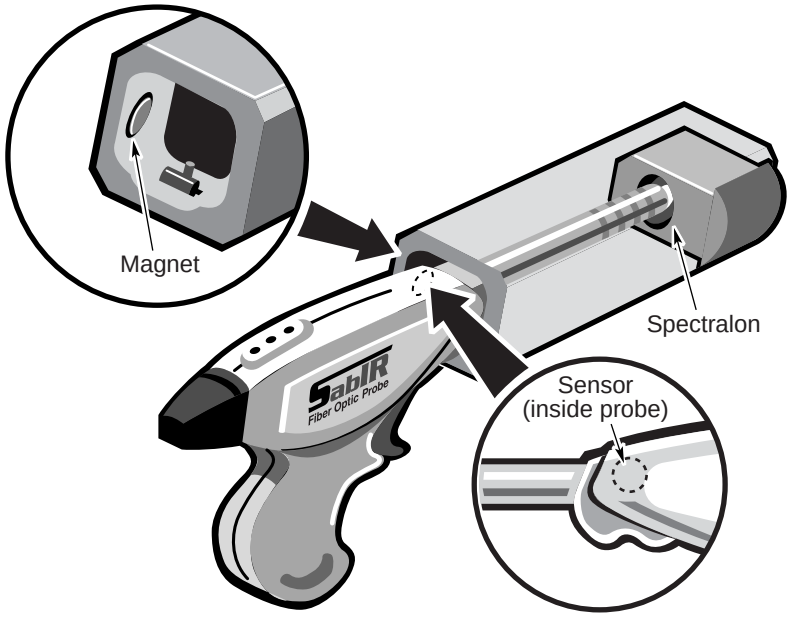
**Note** Be sure to set the appropriate parameters in RESULT Integration to use the internal Spectralon reference. For Collect events, set Position in the Background Collection group to Fiber Optic Probe and clear the Use Sample Position, Gain And Attenuation Settings check box. For Collect Multi-Channel events, set Probe Type in the Multi-Channel Background Collection group to Antaris SabIR and clear the Use Sample Position, Gain And Attenuation Settings check box. ▲

To collect a background using the internal Spectralon reference:

1. **Insert the probe into the holster if it is not already inserted.**

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

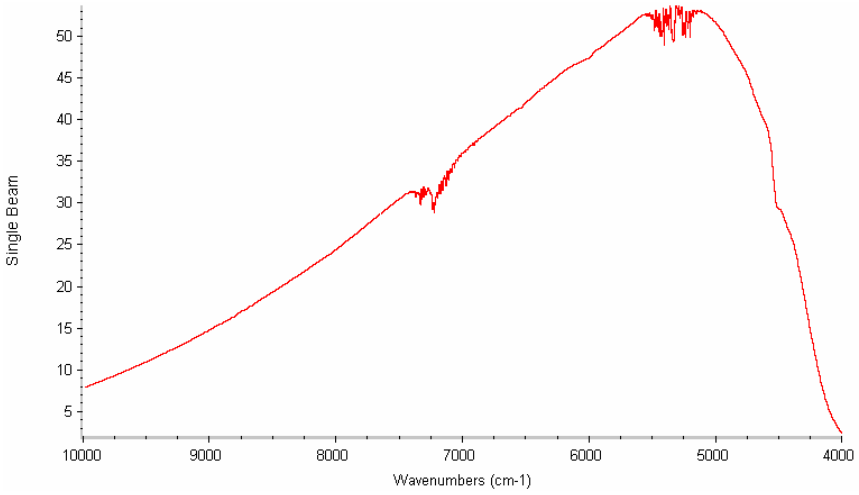
The analyzer can automatically detect probe insertion and collect a background without any operator prompts. A sensor inside the probe responds to a magnet inside the holster:




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

   The system begins collecting the background spectrum. You can view the status of the background scans in the status indicator box in the software. During data collection the yellow indicator light is on. Do not remove the probe from the holster until the light is off.

A typical 8 $cm^{-1}$ background spectrum collected using the Spectralon reference should resemble the following:




See the "Common Problems With Spectral Data" chapter if your background spectrum is not similar to the above or if a background spectrum you collected is very different from previous background spectra.

After you collect the background, the background remains active and is used to process all sample data in this experiment.

Follow the steps below to collect a background using an external reference.

**Note** Be sure to set the appropriate parameters in RESULT Integration to use an external reference. For Collect events, clear the Use Sample Position, Gain And Attenuation Settings check box in the Background Collection group. For Collect Multi-Channel events, clear the Use Sample Position, Gain And Attenuation Settings check box in the Sample Parameters group. ▲

1. **Hold the probe to the reference material.**

   See the preceding section for instructions on how to position the probe.

   The green indicators on the probe and analyzer are on when the analyzer is ready.

2. **If the green indicator on the probe is steady, press and release the probe trigger, press the Acknowledge button, or choose a response**

**to a prompt to begin collecting data. If the green indicator is flashing, begin by responding to a prompt.**

The system begins collecting the background spectrum (see step 2 in the preceding procedure). You can view the status of the background scans in the status indicator box in the software. During data collection the yellow indicator light is on. Do not remove the probe from the holster until the light is off.

## Collecting sample data with the SabIR probe

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

**Notice** Do not press the trigger while removing the probe from the holster, since that would start data collection prematurely and could affect your results. If the probe starts collecting data prematurely, redo the experiment. ▲

To collect the sample data:

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

   The steady green indicator on the probe should be on, indicating 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 probe" section in 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; the collected spectrum may have problems if there is not enough sample material under the window.

3. **If the green indicator on the probe is steady, press and release the probe trigger, press the Acknowledge button, or choose a response to a prompt to begin collecting data. If the green indicator is flashing, begin by responding to a prompt.**

   You can view the progress of the collection in the status indicator of the software main window. While the probe is collecting data, the yellow indicator light is on. Do not move the probe until the light is off.

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

**Note** Check the probe tip to make sure there is no residue before repeating the collection. If there is residue on the probe tip, follow the cleaning instructions in "Cleaning the SabIR probe" later in this chapter. ▲

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

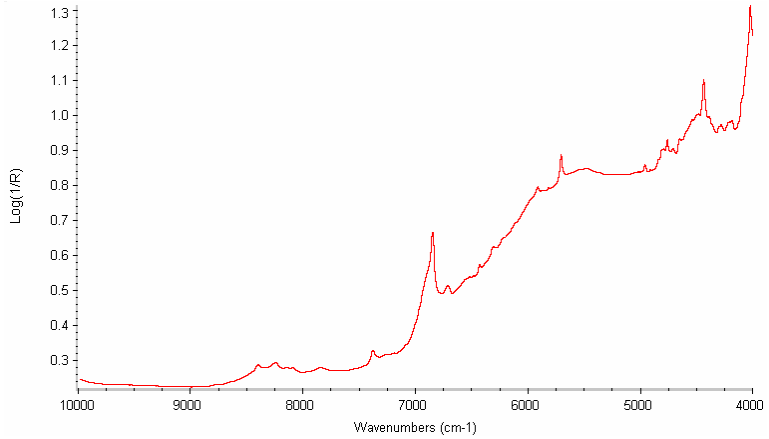
   The software prompts you each time to begin collection. If collecting data from a large sample, you may want to place the probe on a different area of the sample. Continue repeating steps 2, 3, and 4 until the software stops prompting you to begin collection.

**Note** If the probe tip became dirty, clean it properly before inserting the probe into the holster. ▲

6. **Place the probe in the holster when all collections are finished.**

   After you have finished the experiment, each spectrum is listed in the report navigation frame. Select a listed spectrum to view it.

   FT-NIR spectra produced by diffuse reflection have unique characteristics. These were taken into consideration by us when recommending collection parameter settings for the SabIR probe. The following spectrum of ascorbic acid powder is representative of a typical near-infrared spectrum taken using the SabIR probe.




Spectrum of ascorbic acid powder

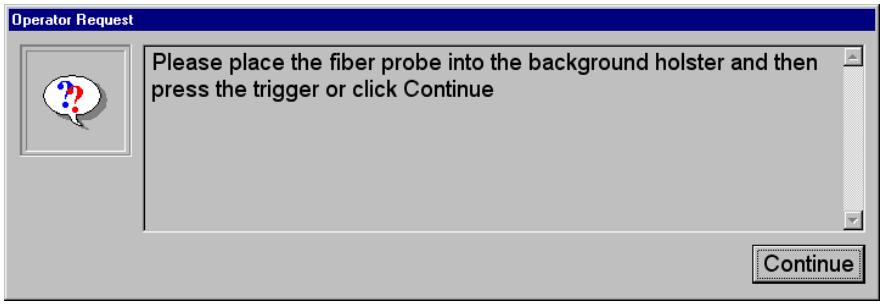
The typical spectral range for a diffuse-reflection sample with the SabIR is 10,000 $cm^{-1}$ to 4,200 $cm^{-1}$. Solids typically exhibit a broad upward slope in absorbance toward smaller wavenumbers (longer wavelengths). See the "Common Problems With Spectral Data" chapter for information about some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

## Using workflows with the SabIR probe

Consider the following information when using the SabIR probe to collect data with workflows developed in RESULT Integration.

- Remote sampling with the SabIR probe requires little or no sample preparation. However, collecting sample spectra in production is controlled by the workflow you are running. Pay close attention to the prompts and any instructions that appear.

- The workflow should indicate whether you are to use the internal Spectralon reference or an external reference for background collection. A workflow developed for use with the SabIR probe enables the probe sensor to detect when the probe is properly inserted into the holster, allowing background collection using the internal Spectralon reference. If you attempt to collect a background when the probe is not properly inserted, the following message appears:




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

- If the workflow dictates that an external background reference be collected, the workflow or any attached instructions should indicate how to prepare and collect the background reference. The software prompts you to begin background collection.

- The workflow dictates how often to collect a background. (See the "Developing Workflows for the Antaris MX" chapter for more information.) The most recent background spectrum remains active and is compared with sample data until a new background is collected. The "Common Problems With Spectral Data" chapter contains suggestions if a background spectrum is very different from previously collected background spectra.

## Disconnecting the SabIR probe

It is not necessary to disconnect the SabIR after each use. However, you can disconnect it if you are not going to use it for a long time, or if you need to remove it to attach a different accessory. Disconnection of the SabIR is essentially a reversal of the connection process described in "Connecting a SabIR probe" earlier in this chapter.

**Notice** When you disconnect the SabIR probe, heed the following precautions:

- First turn off the analyzer power to avoid a possible electric charge that may damage the electronics. Each time you turn off the analyzer, log off any software applications.
- Insert the probe into the holster before disconnecting it. This prevents strain on the fiber optic cables from the weight of the SabIR.
- Do not bend the fiber optic cables any more than necessary. Excessively bending the cables can damage the optical fibers.
- Do not use tools to loosen the connectors from the fiber optic ports on the analyzer.
- Do not over tighten the thumbscrews on the strain relief mechanism. ▲

## Cleaning the SabIR probe

If the tip of the SabIR probe is dirty or contaminated with sample or other material, take the following steps to clean the tip:

1. **Mix one part isopropyl alcohol with nine parts water in a clean container.**

2. **Using an eye-dropper, place a small amount of the mixture on a fresh piece of lens paper.**

3. **Gently rub the lens paper on the optical window for 10 to 20 seconds.**

4. **Allow the window to dry for at least two minutes.**

To clean the probe shaft:

1. **Prepare a cleaning solution of one part isopropyl alcohol with nine parts water in a clean container.**

2. **Pour a small amount of the mixture onto a soft cloth.**

3. **Gently rub the cloth on the probe shaft for 10 to 20 seconds.**

4. **Let the shaft air-dry.**

## Storing the SabIR probe

Store the SabIR probe in a dust-free environment, such as a cabinet or box. If coiling the cables, make sure they 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.

# Collecting Backgrounds

A background is a reference spectrum that accounts for the unique optics of the sampling accessory and the analyzer. Each sample spectrum is ratioed against a background so that the final spectrum is free of these features. 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" chapter contains suggestions you can use if a background spectrum is not typical of previously collected background spectra.

Backgrounds are normally collected along with the sample data using a collection event in a workflow. For diagnostic purposes, you can also collect a background using RESULT Operation's Test Background feature 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. Quick Collect is helpful if you want to test background collection independent of a workflow. Quick Collect is also available in RESULT Integration.

There are many options for collecting backgrounds for fiber optic experiments. You can collect backgrounds using internal or external references and use the same channel as the sample collection or a different channel. We recommend measuring the background at the same channel as the sample measurement to automatically remove from the final spectrum the characteristics of the instrument, fiber and sampling accessory. If that is inconvenient, use a different channel with the same type of fiber and sampling accessory for the background or the instrument's internal background reference (channel 0) and apply a transfer correction to compensate for any differences between the two beam paths. See "Transfer corrections" later in this chapter for more information. For experiments that require a high degree of photometric accuracy, use a dark background correction for the sample and/or background to eliminate the effects of any back reflections in the beam path. See "Dark background corrections" later in this chapter for more information.

The next sections discuss using internal and external references for background collections.

## Using the internal reference

The internal reference (available only for Collect Multi-Channel events) is a channel that sends the near-infrared beam to the reference detector. You can use the internal reference to quickly collect backgrounds for use in any type of fiber optic experiment. You can collect a background at the same time as a sample spectrum. Because the reference is internal, it is always accessible, requires no maintenance and always produces the same spectrum, ensuring consistent sample processing. The internal reference is also useful for diagnostics and tracking changes in the analyzer over time.

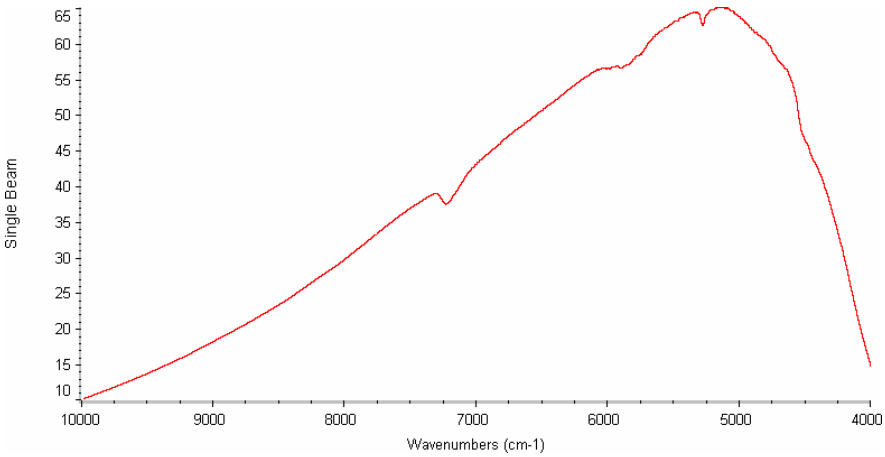
Background spectra collected with the internal reference include the characteristics of the system, letting you remove those features from the final spectrum. Since the background and sample spectra in this case are collected using different detectors and fiber optics, you may use a transfer correction in RESULT to compensate for any resulting differences.

**Tip** If your sample spectrum includes significant features that are due to the optical cable and sampling accessory, consider using an external reference sample, the test fiber, or another fiber shunt for collecting backgrounds instead of the internal reference. Alternatively, these features can be accounted for in the chemometric model or corrected using a transfer correction. ▲

If you are prompted to begin a background collection, the green LED indicator on the analyzer lights when it is time to begin collection. If the indicator is steady, you can begin collecting data by pressing the Acknowledge button or responding to a prompt. If the indicator is flashing, you must begin data collection by responding to a prompt and cannot use the Acknowledge button.

The status indicator in the software shows the status of the collection.

A typical 8 $cm^{-1}$ background spectrum collected using the internal reference channel should resemble the following.




Typical internal reference background spectrum

See the “Common Problems With Spectral Data” chapter if your background spectrum is not similar to the above spectrum or if it is not similar to previous background spectra.

## Using an external reference

An external reference can be any material that mimics spectral characteristics you want to minimize in your sample spectra, including the optical fiber used in the experiment and compounds contained in the air. Examples of configurations and materials used as external references include:

- **External reference sample.** Some materials that can be used as an external reference for reflection experiments include:

  - Ceramic or sintered Teflon® plate
  - Barium sulfate, Teflon (powders)
  - Spectralon (used to collect backgrounds for reference spectra)
  - Diffuse gold (used to collect backgrounds for reference spectra)

  Your sampling accessory documentation may suggest additional materials for background measurements.

- **Fiber optic shunt.** You can use the Antaris test fiber or another fiber with SMA connectors on both ends. We recommend using a 235 µm fiber that contains a minimal amount of O-H compounds to help prevent interfering peaks. Connect the test fiber to the In and Out ports of the channel designated for background collections. (Shunts are available from Thermo Fisher Scientific.)

- **Empty liquid transmission cell or transflectance probe.** If you are using a transmission cell or transflectance probe attached to the fiber, use the same type of cell used to collect the sample data, but make sure the cell is empty and clean before measuring the background.

Your sampling accessory documentation should contain information about appropriate background materials and how to prepare and position the background material for data collection.

You can take background measurements with an external reference from the same channel and fiber optic sampling accessory used to collect the sample data, or through a separate channel. See the next section for information about applying a transfer correction to compensate for differences between beam paths when using different channels for collecting sample data and background data using an external reference.

During data collection the status indicator in the main window displays the status of the collection. Do not move the reference material or sampling accessory until collection is complete.

## Transfer corrections

You can use a transfer correction to correct background spectra taken with a channel that is different from that used for taking sample data. This 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 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.

## Dark background corrections

Dark background corrections can be used to improve the photometric accuracy of reflection measurements by removing undesirable back reflections from the sample spectra. These reflections can be from the face of a glass vial or other container or from unwanted material clinging to the surface of a sample window, or even from the window itself. They are the sum of any reflections that cannot be attributed to the sample material.

If the background is measured with the same conditions as the sample and the sample and background materials are both highly reflective, back reflections are not important to the analysis and a dark background correction is not needed. The correction is most useful when the reflectivities of the sample and background are significantly different, because the back reflections account for a greater portion of the total reflection.

The correction requires a dark background spectrum, which is a single-beam spectrum of the surfaces causing the unwanted back reflections (everything but the sample). The term “dark background” refers to the fact that a small amount of illumination still reaches the reflection detector when there is no sample in the beam path. The dark background spectrum can be subtracted from the single-beam spectrum of the sample before that spectrum is ratioed to the background to produce the final sample spectrum. If the background measurement also contains unwanted back reflections, you can subtract a dark background spectrum from the background single-beam spectrum before it is ratioed against the sample spectrum. Removing these inherent back reflections from the sample spectra can improve the photometric accuracy and resulting linearity of the NIR measurement.

# Developing Workflows for the Antaris MX

You can operate the Antaris MX analyzer using RESULT Integration or RESULT Operation with workflows developed in RESULT Integration. You can set up workflows to collect and analyze data from any fiber optic accessory installed on the analyzer and in any sequence.

This chapter provides information about using workflow features to optimize background and sample data collection. It also describes the workflow events and specifications that are specific to the Antaris MX analyzer. We will assume that you have some familiarity with creating workflows.

Some example workflows are available in C:\RESULT Data\Workflows. You used the Collect Fiber Third Party workflow to perform a basic data collection in the "Your First Experiment" chapter. When setting up a custom workflow for your application, you may save time by modifying an appropriate example workflow and saving it with a new name.

For more detailed information about using workflows to collect data, see "Chapter 2 Running Workflows" in "Section 3 RESULT Operation Software" of your *RESULT User's Guide*.

## Sample data collection

This section provides information about creating workflows to collect sample spectra with the Antaris MX. For more information, see "Chapter 2 Creating and Editing Workflows" in "Section 2 RESULT Integration Software" of your *RESULT User's Guide*. See the "Common Problems With Spectral Data" chapter in this manual if your sample spectrum is not similar to prior sample spectra. Your sampling accessory documentation may contain more specific information about sample collection problems.

A collection event in RESULT Integration instructs the instrument to collect a spectrum of a sample. Depending on the requirements for data collection, a workflow may contain one collection event, a collection event contained in a repeat loop, multiple collection events set in sequence and/or in a loop, or multi-channel data collection.

Repeat loops are useful for collecting data continuously over a span of time from either single or multiple samples. The spectra produced can be used to measure concentrations, check homogeneity or produce a representative spectrum of a non-homogenous sample. See "Section 5 Workflow Events and Specifications" in your *RESULT User's Guide* for information about adding collection events and repeat loops to a workflow.

Tips for setting up collection events to run the analyzer are below. For general information about collection event parameters and the placement of collection events in a workflow, see "Section 5 Workflow Events and Specifications" in your *RESULT User's Guide*.

Use sample specifications in RESULT Integration to set parameters for data collection. Sample specifications are linked to collection events in workflows and are customizable by sampling accessory, sample types and level of interest in different spectral characteristics. Refer to your sampling accessory documentation for information about a good starting point for the resolution and the spectral range when developing sample specifications for workflows designed to run the analyzer.

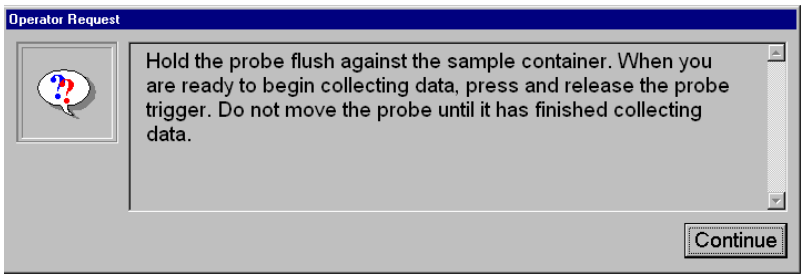
Consider the following when setting parameters for collection events and sample specifications.

- **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 an acceptable signal-to-noise ratio (determined by error of prediction or a predefined limit) if sampling time is at a premium. If you are 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.

  Keep in mind that diffuse-reflection experiments require a longer collection time (more scans) than transmission experiments. If sampling time is at a premium, consider the ratio between the number of scans and resolution. See the table in the "Sample specifications" section of "Section 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.

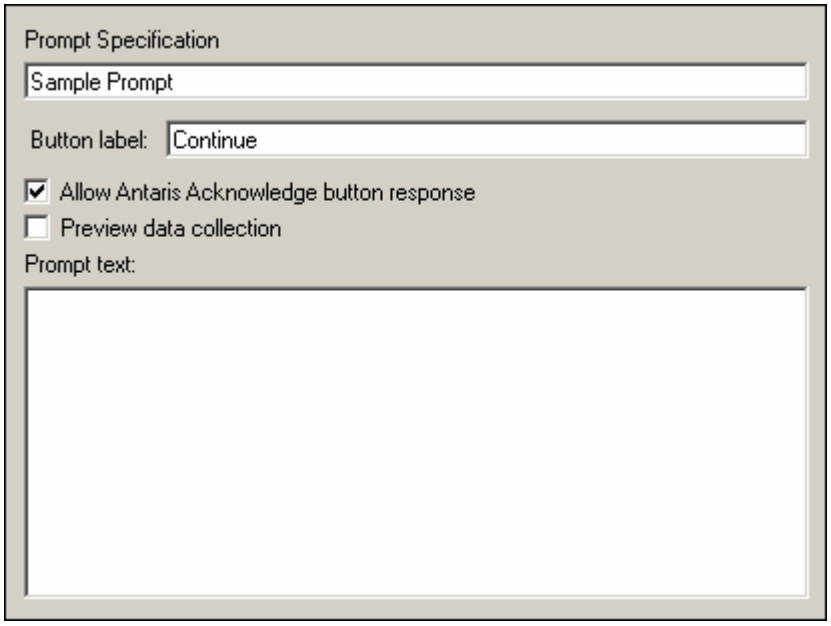
- **Background Frequency.** If you are only collecting samples periodically, collecting a background before every sample is recommended. If you are collecting many samples at a time, collecting a background every hour should be sufficient.

- **Operator Prompts.** The collection event lets you include operator prompts for sample and background collections in a workflow. For continuous, remote sampling with automatic background measurements, the workflow initiates sample and background collections, and operator prompts are not needed. If sampling must be initiated manually, you can configure the workflow to display a message to the operator before collecting data. Here is an example:

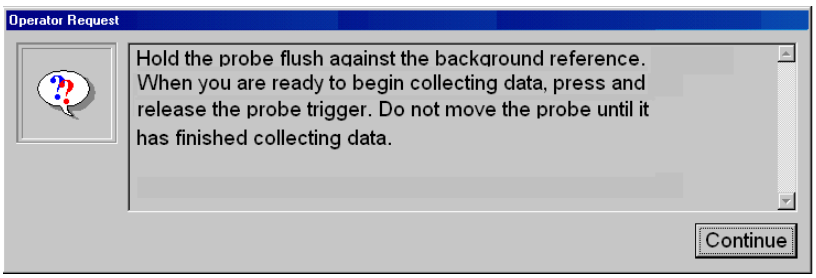



- When creating sample collection prompts, make sure they include specific information about how to prepare and position the sample. If the operator must reposition the sampling accessory—for example, if you've created a repeat loop in a workflow to collect multiple samples of a substance in a large bin—you could set up the workflow to prompt the operator each time the accessory requires repositioning.

- If the operator will perform sampling remotely and sampling time is at a premium, you can let the operator respond to prompts with the Acknowledge button. To do this, leave Allow Antaris Acknowledge Button Response selected in the user prompt specification in the software, as shown below.




If you are using a SabIR probe and the Spectralon reference in the holster, a background prompt is not necessary. The computer detects whether the SabIR is inserted. If the SabIR is not inserted into the holster properly, the software prompts the operator to insert the probe. However, if you are using an external reference for background collection, we recommend including a detailed operator prompt, like the following, to ensure that the background data is collected properly.



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

- **Probe Type.** Set this to Antaris SabIR if you are using the SabIR probe, or to Third Party if you are using another fiber optic accessory.

- **Attenuator.** Since the Antaris MX does not have an automated attenuator, this parameter is not available.

- **Gain.** We recommend starting with a Gain setting of 1x for the sample data and increasing the gain if necessary to achieve a sufficient interferogram peak intensity (typically at least one volt). If too much light reaches the detector and causes signal saturation, you can use a light attenuator (available from Thermo Fisher Scientific) that attaches to the SMA connectors on the front of the analyzer.

- **Sample Position.** This parameter is for Collect Multi-Channel events and is available only for instruments that include the optional validation wheel (see "Using the validation wheel" later in this chapter). Set Sample Position to Empty for sample data collections that do not use the validation wheel.

- **Background Position.** This parameter is for Collect Multi-Channel events and is available only for instruments that include the optional validation wheel (see "Using the validation wheel" later in this chapter). Set Background Position to Empty for sample data collections that do not use the validation wheel.

- **Sample Channel.** This parameter is for Collect Multi-Channel events and specifies the channel to use for sample data collection.

- **Channel Number.** This parameter is for Collect events and specifies the channel to use for sample data collection. (The parameter appears on the fiber optic sample specification.)

## Background collection

A background specification in RESULT Integration defines data collection for background spectra generated by a workflow. When setting up background collection, take the items in the next sections into consideration. The available parameters and recommended settings vary depending on whether you are setting up a Collect Multi-Channel event or Collect event.

**Note** When setting up a Collect Multi-Channel or Collect event, be sure to complete both the sample specification and background specification; they are used in conjunction to collect data. ▲

## Background collection for Collect Multi-Channel events

When setting up background collection for a Collect Multi-Channel event, consider the following items:

- **Gain.** Use this option in the background specification to set the gain for the background measurement. We recommend starting with a Gain setting of 1x and increasing the gain if necessary to achieve a sufficient interferogram peak intensity (typically at least one volt). If too much light reaches the detector and causes signal saturation at a gain of 1, you can use a light attenuator that attaches to the SMA connectors on the front of the analyzer.

- **Probe Type.** Set this option in the background specification to Antaris SabIR or Third Party depending on the type of probe you are using.

- **Background Channel.** Use this column in Channel Setup in the Collect Multi-Channel event to specify the channel for background collections. To collect a background using an external reference, set this to the channel to be used for background collection and set Probe Type as explained above. Set Background Channel to 0 (zero) to collect a background from the instrument's internal background reference.

- **Use Sample Channel For Background Measurements.** Select this option in the Collect Multi-Channel event to collect background data from an external reference sample measured at the same channel used to measure the sample. Selecting this option overrides the setting of Background Channel (described above).

## Background collection for Collect events

Consider the items below when you set up background collection for a Collect event.

- **Position.** Set this parameter to Fiber Optic Probe. The other available settings do not apply to the Antaris MX.

- **Number Of Background Scans.** The available options let you collect the same number of background scans as sample scans (default setting) or twice as many (to reduce noise). For recommendations related to this parameter you can consult an application specialist, refer to your sampling accessory documentation, or contact the accessory (probe) manufacturer.

  If you are using a SabIR probe, the setting is affected by whether you use the probe's internal Spectralon reference or an external reference for background collections. In either case, a good starting point for the parameter is Same Number Of Scans As For Sample.

- **Use Sample Position, Gain And Attenuation Settings.**

  - If you are using the SabIR probe, the setting of this option has the following effects:

    - If this option is selected, the background is measured at the sample location using the sample Gain setting for the external reference. Some materials that can be used as an external reference for SabIR probe sampling include:

      Ceramic or sintered Teflon plate (solids)

      Barium sulfate, Teflon (powders)

      Reference materials related to the sample of interest (a pure solvent, for example)

      Spectralon (used to collect backgrounds for reference spectra)

      Diffuse gold (used to collect backgrounds for reference spectra)

    - If this option is cleared, you must use the SabIR probe's internal Spectralon reference for background collection. The software automatically controls this portion of the collection.

- If you are using a third-party probe, the setting has the following effects:

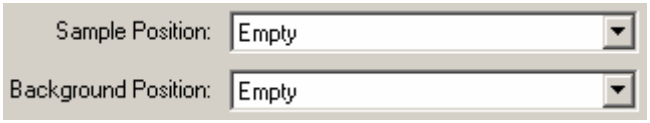
    - If this option is selected, the background is measured at the sample location using the sample Gain setting for the external reference.

    - If this option is cleared, the background is measured at the sample location using a Gain setting of 1x.

## Using the validation wheel

The optional validation wheel contains standard samples that can be used for diagnostic purposes and for running qualification tests with the Thermo Scientific optional ValPro System Qualification package. (See "Setting RESULT Integration options" in "Section 2 RESULT Integration" of the *RESULT User's Guide* for instructions for configuring the validation wheel.)

When the validation wheel is properly configured, the Sample Position and Background Position parameters (shown below) become available in the Collect Multi-Channel event. You can then set these parameters to the desired wheel positions.




The wheel 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 are intended for running ValPro instrument qualification tests. The polystyrene sample is calibrated to a thickness of 0.0325 inch and can be used to run instrument performance and diagnostic tests.

The seventh position in the wheel is empty. RESULT uses the empty position to take background measurements for the instrument qualification and performance tests. For sample measurements set Sample Position to the desired wheel position (such as 10% Filter or Polystyrene), and set Background Position to Empty.

**Notice** The validation wheel is positioned in the NIR beam before the beam is sent to the individual fiber optic channels. As a result, the wheel setting affects all channels. When collecting data from samples using fiber optic accessories connected to the instrument, set both Sample Position and Background Position to Empty. ▲

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# 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. Spectra may also be influenced by 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," check the following items:

- Make sure the fiber optic accessory is properly attached to the fiber optic ports on the analyzer and that the cables on the accessory have been consistently attached to the same In and Out ports.
- Make sure the fiber optic accessory connections to the fiber optic ports are finger-tight. You may want to remove and reattach the accessory before attempting to re-collect the sample.

**Notice** To avoid damage to connectors, do not over tighten the connections or use tools to tighten them. ▲

## Software diagnostics

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

**Quick Collect.** Quick Collect, available in both RESULT Operation and RESULT Integration, lets you scan and collect a background and/or sample without relating it to a workflow. See "Chapter 5 System Maintenance" in "Section 3 RESULT Operation Software" of your *RESULT User's Guide* for more information.

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

**Running a workflow off-line.** This feature, available in RESULT Operation, lets you run an entire workflow off-line, so the results do not affect production data. See "Chapter 5 Managing Workflows" and "Chapter 6 Managing Users" in "Section 6 Software Administration" of your *RESULT User's Guide* for more information.

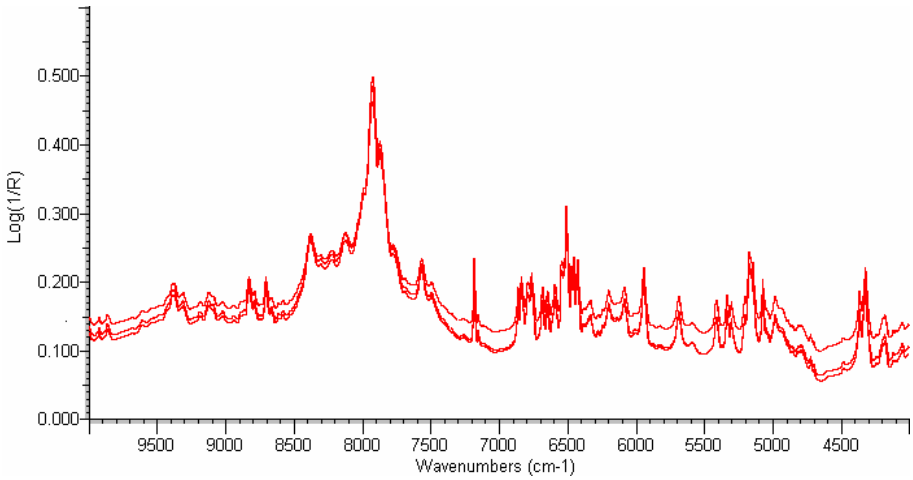
**Running a workflow in test mode.** This feature, available in RESULT Integration, lets you test a workflow while it is in development. See "Testing a workflow" in "Chapter 2 Creating and Editing Workflows" in "Section 2 RESULT Integration Software" of your *RESULT User's Guide* for more information.

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

## Problems with optical fibers

If the signal-to-noise ratio or predictive ability of your method is failing, inspect the fibers in the fiber optic cables. Optical fibers are delicate and damage to them can create subtle differences in your results.

Moving or bending fiber optic cables during data collection may also affect 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. Collect data with the fiber optic cables in the same position each time.

## Problems with background spectra

If a background spectrum is different from previously collected backgrounds or from the typical spectrum described in "Using the internal reference" in the "Developing Workflows for the Antaris MX" chapter, the problem may be one of the following:

If you are using the internal reference (available only for Collect Multi-Channel events), the attenuation and optical properties of the fiber may be very different from those of the reference. Try using an external reference, the test fiber, or another fiber optic shunt.

If you use an external reference and the same type of accessory used to collect the sample data, one of the following may be true if you use a channel other than the one used to collect sample data.

- The optical fiber used for the background is not attached properly or is damaged.
- The fiber was moved during collection.

**Note** You may be able to solve problems with external-reference backgrounds by using the transfer correction in RESULT. See "Transfer corrections" in the "Developing Workflows for the Antaris MX" chapter for more information. ▲

If you are using a SabIR probe for sample collections and the Spectralon sample in the probe holster for background collections, it is possible that:

- The Spectralon sample needs cleaning. Follow the instructions in "Maintaining the Spectralon reference" in the "Maintenance" chapter.
- The probe window is dirty. Follow the instructions in "Cleaning the SabIR probe" in the "Using the Optional SabIR Probe" chapter.
- The SabIR was not properly inserted into the holster. Make sure the SabIR is properly inserted (you should hear it "click" in place) and re-collect the background.

If you were using a SabIR probe or another fiber optic sampling accessory to take a background using a method other than those mentioned above, it is possible that:

- The sample material was run as the background.
- The fiber optic accessory was not held flush against the background material.
- The fiber optic accessory was moved during collection.

For all the problems above, we recommend taking test backgrounds using either Quick Collect (not associated with a workflow) or Test Background (following the steps for background collection in a workflow) in RESULT Operation 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.

## 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 Test Sample, or by using Quick Collect in RESULT Operation.

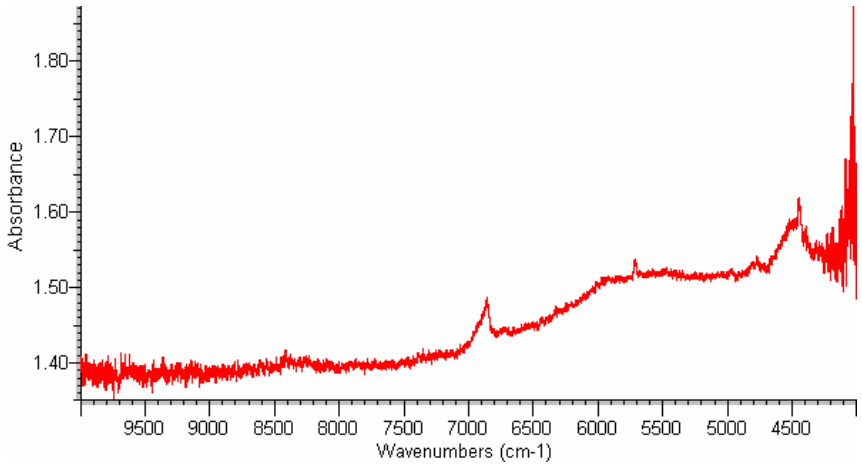
While you are using the diagnostic features, make sure none of the following occur:

- When using the SabIR probe, do not press the trigger prematurely. Keep your fingers alongside the probe and away from the trigger until you are ready to start collecting data.
- Do not move the sampling accessory while it is collecting data. Hold it 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. If you are using a sampling accessory other than the SabIR probe, also refer to your accessory documentation for other suggestions.

## High noise

A spectrum that contains high noise can resemble the following.




Ascorbic acid spectrum with high noise using SabIR

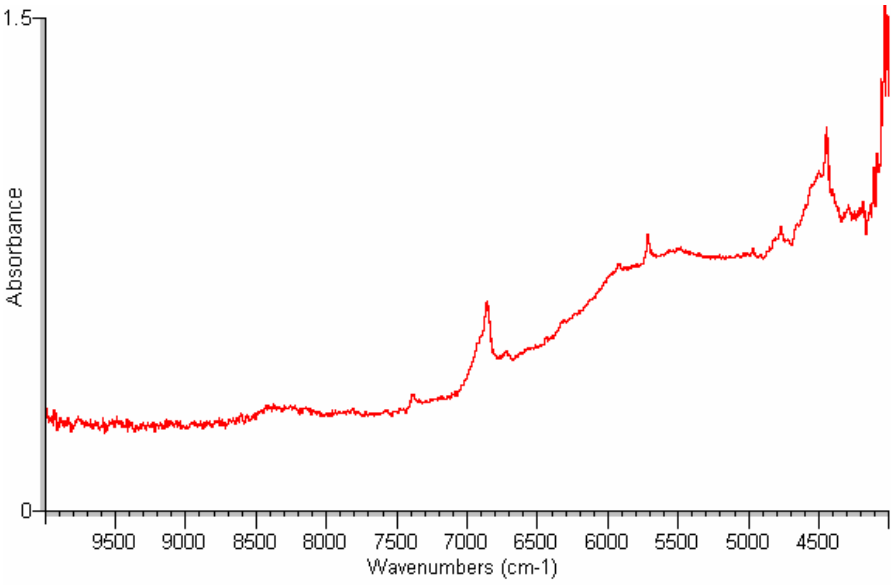
The high noise level appears as sharp peaks above and below the baseline. This may be caused by not holding the accessory or probe close enough to the sample to make good sample contact. If the problem persists after you repeat the experiment with the accessory held closer, make sure you are using the proper gain setting.

High noise can also be caused by broken or dirty fibers, so inspect the fiber optic cable for these conditions.

It is also possible that the sample density or reflectivity is too low for a diffuse-reflection measurement.

## 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 zero absorbance units. However, this baseline is shifted upward and the relative intensities of the peaks are smaller. If you experience this problem, one of the following may have occurred:

- Good sample contact was not made.
- The sample density or reflectivity is too low.

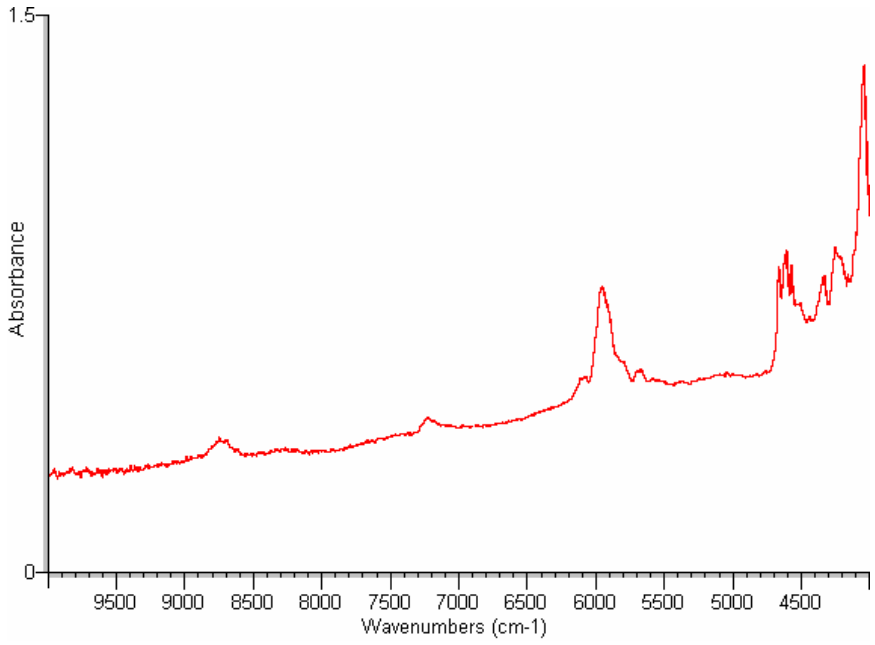
- A solid sample is too thin.
- There is not enough of a powder sample, or a sampling accessory was inserted too far into the powder so not enough of the powder was underneath the probe tip.

Attempt the scan again in a diagnostic mode. If you are using the SabIR probe, make sure the accessory tip is against the sample and at the proper angle (flush with the sample if you are using the SabIR). Do not move the accessory until data collection is finished.

**Tip** If you collect a background using Spectralon, the internal reference or an external reference sample, the intensity of the background spectrum may be different from that of your sample. In this case, the baseline of the sample spectrum may be shifted. To prevent this, include a baseline correction in the analysis method. (See the documentation that came with TQ Analyst or other method development software for more information.) ▲

## Samples not appropriate for the sampling accessory

Some solid samples may not be diffuse enough to use with the SabIR probe or some other sampling accessories. Samples that are diffuse typically have a rough surface. An example spectrum of a smooth sample may resemble the following.




Spectrum of thin polystyrene film using SabIR

Note that 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 can 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 affect the effective pathlength, causing differences in band intensity.

Spectral quality is most affected by extreme differences in particle size; for example, a sample containing particles smaller than 3 µm and larger than 500 µm.

Sample homogeneity can affect reproducibility. To achieve a representative sample spectrum, consider the degree of homogeneity when setting the number of collection event repetitions. The spectral data will probably be of good quality, but individual spectra may not be representative of the sample as a whole.

Concentration can affect the signal-to-noise ratio, especially at lower sample concentrations.

To minimize these problems, consider adding repeat loops in workflows to collect data from different areas of the sample. The collected spectra can be measured to check homogeneity or averaged to produce a representative spectrum. See “Section 5 Workflow Events and Specifications” in your *RESULT User’s Guide* for more information about using these features.

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# Maintenance

This chapter describes general maintenance routines for the Antaris MX analyzer. We define "maintenance" as an occasional procedure you perform to keep the analyzer running efficiently.

**⚠ Warning** Perform *only* those procedures described in this chapter. If there are other problems with the system, contact Thermo Fisher Scientific technical support. ▲

**⚠ Caution** 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. ▲

If you need help with a maintenance or service procedure, see "Questions or concerns" in the "Introduction" chapter for information for contacting Thermo Fisher Scientific.

Maintenance procedures are performed periodically, as a part of normal operations, to ensure optimal performance. They include:

- Powering the analyzer on and off
- Cleaning the analyzer
- Removing and replacing the main cover
- Maintaining the Spectralon reference
- Checking and changing the desiccant
- Checking and changing purge gas filters

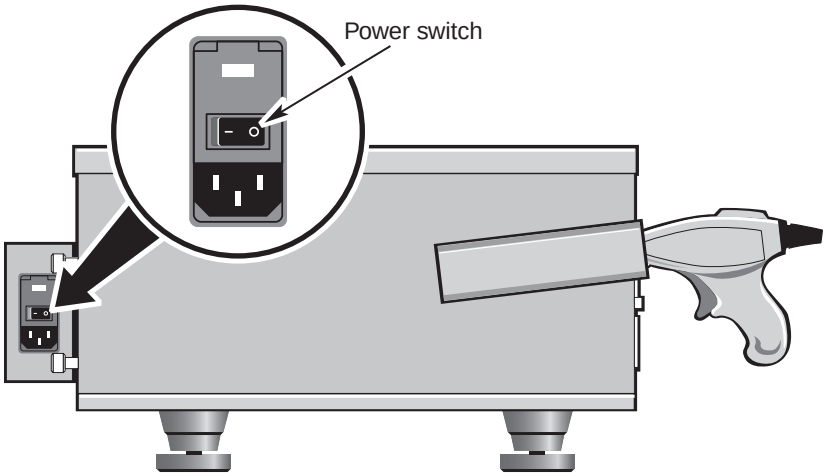
## Powering on and off

To prevent shock hazard, many maintenance procedures require that you turn off the power before you work on the analyzer.

To turn on or off the analyzer:

Press the power switch on the rear of the analyzer.

**I** = ON
**O** = OFF



## 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 and the analyzer. Then use a damp (not wet), soft cloth and a mild soap to clean the outside of the of the analyzer.

**⚠ Warning** Avoid shock hazard. Do not allow liquid to run into the instrument. ▲

**⚠ 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. ▲

**Notice** Do not use harsh detergents, solvents, chemicals or abrasives; 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. ▲

# Removing and replacing the main cover

Some maintenance and service procedures require that you remove the main cover of the analyzer. Be sure to replace and secure the cover upon completion of the procedure.

**Notice** Although the main cover can be removed and replaced easily by the system operator, we recommend that only Thermo-certified service engineers or Thermo-trained on-site maintenance personnel perform this operation. Whenever the main cover is removed, there is a potential for damage to sensitive components. Damage to components inside the analyzer affects the performance of the system. ▲

Tool needed: No. 2 Phillips screwdriver

## Removing the main cover

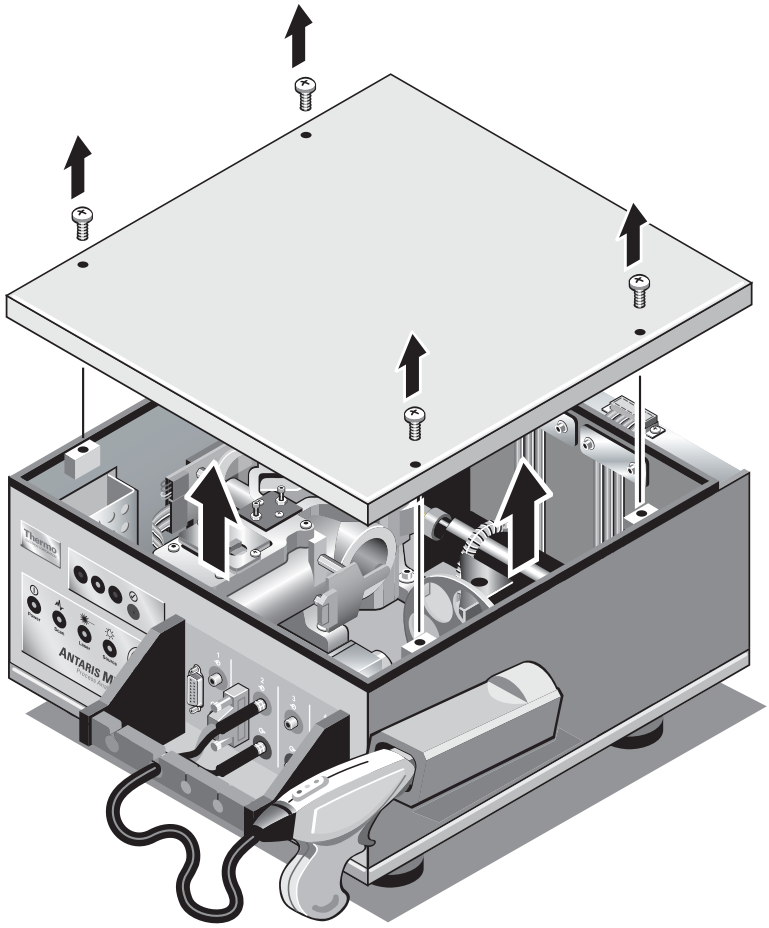
Follow the steps below to remove the main cover.

**⚠ Warning** Before removing the main cover, turn off the analyzer power and disconnect the power supply. ▲

**Notice** Although the main cover can be easily removed by the system operator, it is recommended that only Thermo Fisher Scientific-certified service engineers or our-trained 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. ▲

1. **Make sure you have open access to the top of the analyzer. Remove any sample materials or other items from the top of the analyzer, and if it is in a rack, slide the analyzer out.**

2. **Use a No. 2 Phillips screwdriver to remove 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. ▲

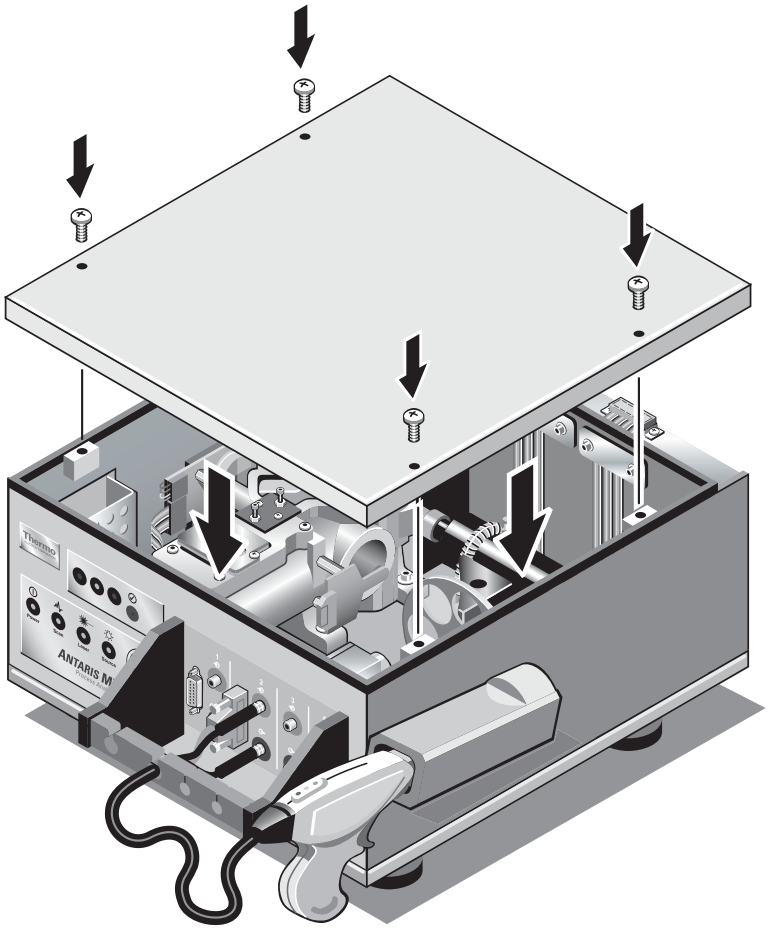
**Notice** Make sure you keep the screws you remove from the main cover. You will need them when you replace the main cover. ▲

3. **Lift the cover off the analyzer and set the cover and screws in a safe place.**

## Replacing the main cover

To replace the main cover:

1. **Place the cover on the analyzer, and use the screwdriver to secure the cover with the screws you removed earlier.**



2. **Reconnect the power cord and any cables you disconnected when you opened the analyzer.**

   You may notice increased levels of water in spectra collected immediately after you have had the cover open. If this interferes with your data, wait until equilibrium is re-established.

## 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 durable, take care to prevent contaminants such as finger oils from contacting its surface. It is a good idea to wear clean, powder-free gloves when handling the material.

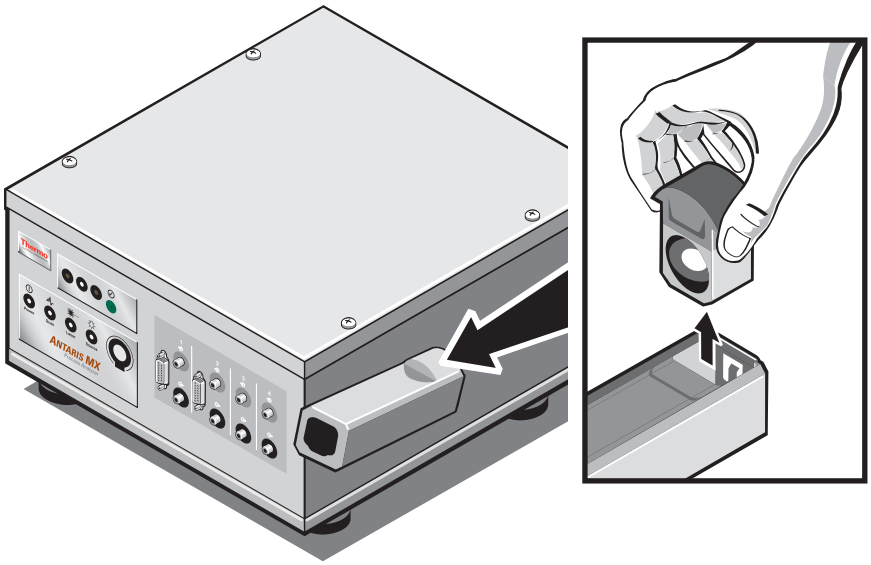
## Removing the Spectralon reference from the holster

Keep the Spectralon reference in the holster at all times, unless you need to clean it or replace it.

**Notice** Avoid touching the surface of the Spectralon reference with your fingers. Dirt and oils from your fingers can leave residue on the sample. ▲

**Notice** Make sure the SabIR probe is removed from the holster before removing the Spectralon reference. ▲

To remove the reference from the holster, use your thumb to pull the lip of the reference holder out of the groove in the holster. Then, while your thumb is still holding the lip of the reference holder, use the thumb and forefinger of your other hand to remove the cartridge, as shown below.



## Cleaning the Spectralon reference

Follow the steps below to clean the Spectralon reference after removing it as explained in the preceding section:

**Notice** Avoid touching the surface of a Spectralon reference with your fingers. Dirt and oils from your fingers can leave residue on the sample. ▲

1. **Use an air brush to gently blow dust and other particles from the reference with clean, dried air or nitrogen.**

2. **If this does not sufficiently clean the reference, gently sand it with a 220 - 240 grit waterproof emery cloth.**

**Notice** If you are using a low reflectance Spectralon reference (<10% reflectance), skip to step 4. The low reflectance Spectralon reference should not be run under water. ▲

Optional low reflectance Spectralon references are available as part of the reflection standards kit.

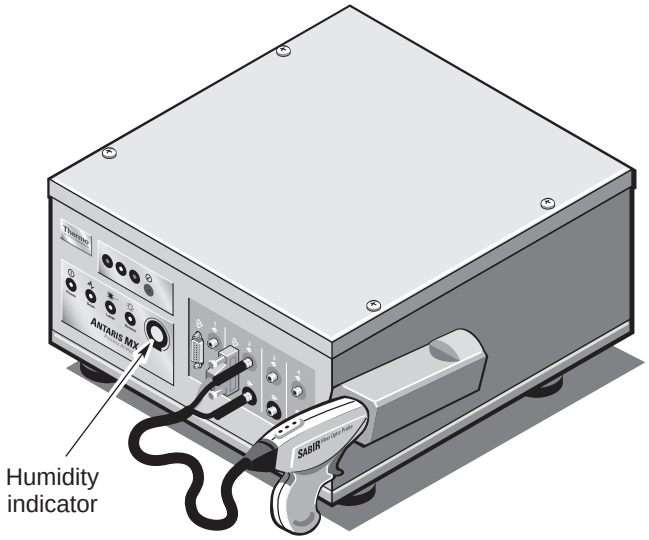
3. **If you are using high reflectance Spectralon reference (>90% reflectance) and the sample is still not sufficiently clean, sand the reference under running water with a 220 - 240 grit waterproof emery cloth until water beads and immediately runs off the surface.**

   Dry the reference sample with a jet of clean, dried air or nitrogen, or allow the material to air dry.

4. **If the background quality does not improve after you have thoroughly cleaned the reference, replace the reference.**

## Checking and changing the desiccant

Antaris analyzers are sealed and desiccated to keep the analyzer internally free of excess moisture. The humidity indicator on the front panel (shown below) lets you check the desiccant; check the indicator monthly, or every two months when the analyzer is not in use. If the indicator is pink, replace the desiccant as explained in the next section.




**⚠ Caution** Avoid burn and fire hazard. Do not attempt to regenerate spent desiccant packs. ▲

## Replacing the desiccant

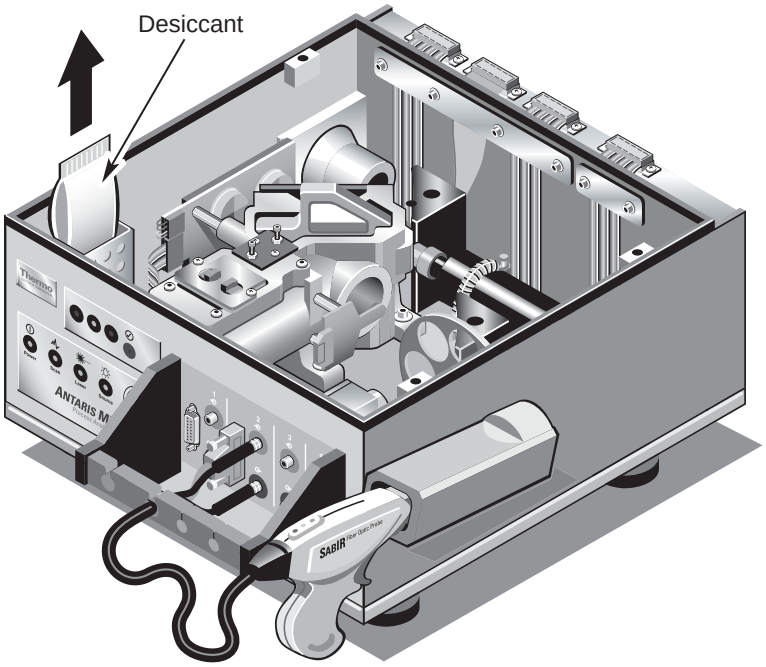
Follow the steps below to change the desiccant:

**Note** Be sure to record the desiccant installation date by using Update Instrument Information in the Service menu of RESULT Operation. ▲

1. **Open the main cover.**

   See "Removing the main cover" earlier in this chapter for instructions.

2. **Lift the desiccant out of the desiccant holder.**




**⚠ Warning** The desiccant is harmful if swallowed. Be sure that you dispose of packets safely. ▲

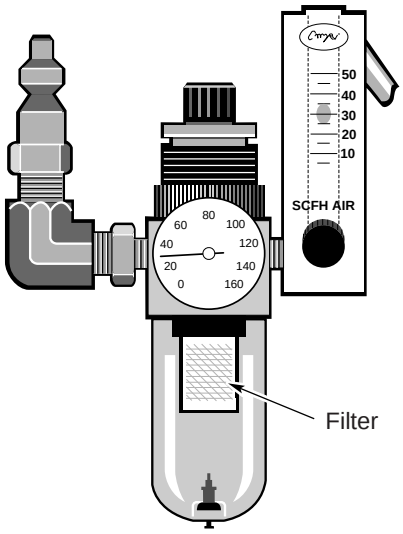
3. **Discard the old packet and put in the new one.**

4. **Close the main cover.**

   See “Replacing the main cover” earlier in this chapter for instructions.

## Checking and changing the purge gas filter

If your analyzer has an optional purge kit, check the purge filter occasionally to make sure it is clean. If the filter is discolored, use the following procedure to replace it.

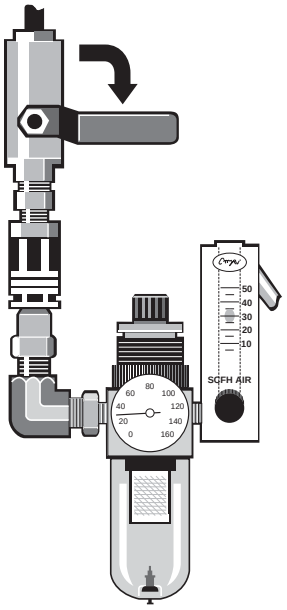



**⚠ Warning** Never use a flammable gas to purge the analyzer. The purge gas must be free of moisture, oil, carbon dioxide and other reactive or infrared-absorbing materials. Use dried air or nitrogen to purge the analyzer. Other gases, even inert gases such as argon (Ar), can damage the analyzer. Never use them to purge the analyzer. ▲

To replace the purge filter:

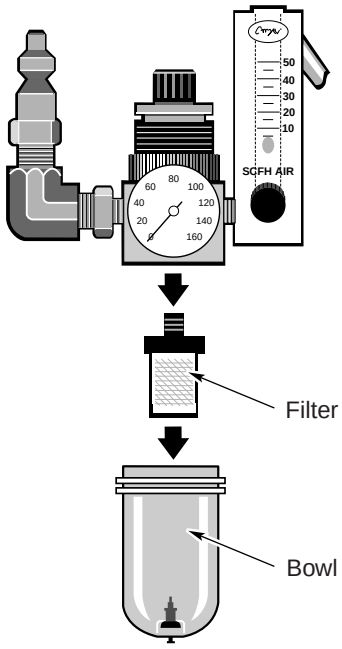
1. **Turn off the purge gas at the shutoff valve.**

   Do not turn down the flowmeter or the pressure regulator.

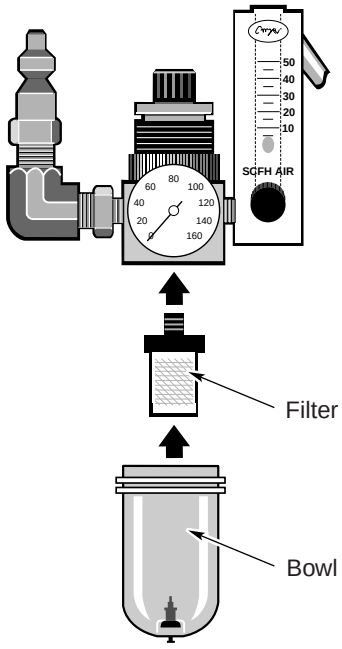


2. **Remove the plastic bowl that houses the filter, and then remove the filter.**

   You can unscrew the bowl and filter by hand.




3. **Install the new filter, and then reinstall the plastic bowl.**



4. **Turn on the purge flow to the analyzer.**

   You may notice increased levels of water in spectra collected immediately after you change the purge filter. If this interferes with your data, wait 3 to 5 minutes until purge is re-established.

# Service

The Antaris analyzer was designed so that you can install optional hardware and replace many of the components yourself. The information that follows describes a variety of hardware service procedures, including:

- Replacing fuses
- Replacing the power supply
- Replacing a source
- Replacing a laser
- Installing an optional purge kit and setting the purge gas controls

**Notice** Although the system operator can perform the service procedures easily, we recommend that only Thermo Fisher Scientific-certified service engineers or on-site maintenance personnel who have been trained by Thermo Fisher Scientific perform these operations. Whenever these procedures are performed, there is a potential for damage to sensitive components. Damage to components inside the analyzer affects system performance. ▲

## Tools

Service procedures generally require special tools. For some procedures you may need one or more of the following tools and/or supplies.

Replacement of the power supply, source or laser:

- No. 2 Phillips screwdriver

Installation of a purge kit:

- ¾-inch open-ended wrench
- ¼-inch male fitting or a ⅜-inch female fitting
- 11/16-inch open-ended wrench
- Shutoff valve

## Replacing fuses

The analyzer is protected by two fuses in the power supply. If you ever need to replace these fuses, read the instructions in the *Site and Safety Information Guide* that came with your analyzer.

## Replacing the power supply

The power supply may need to be replaced if it develops a fault. 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.

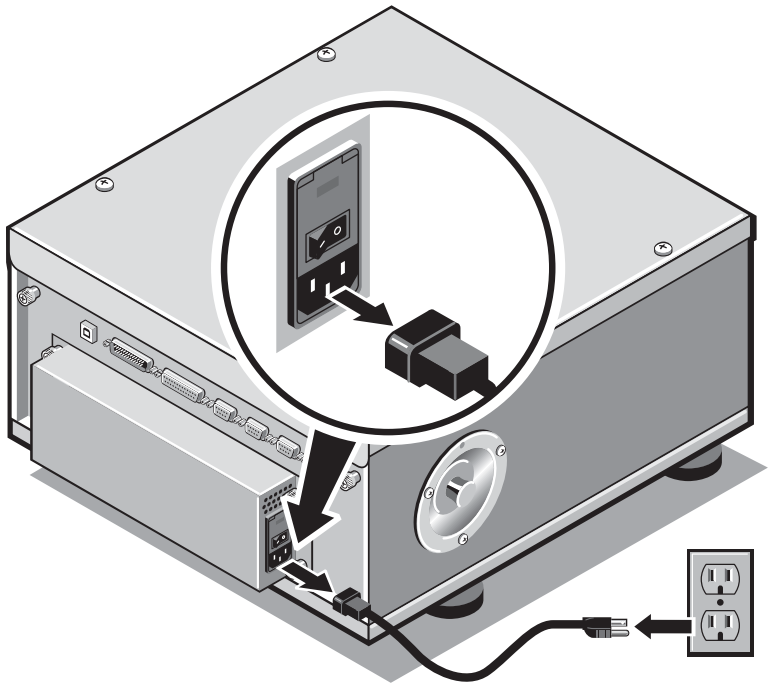
**⚠ Warning** *Do not* attempt to disassemble the power supply. ▲

**⚠ Warning** To avoid shock hazard, always turn off the analyzer and disconnect the power cord from the wall outlet or power strip before you disconnect the supply from the analyzer. ▲

To replace the power supply:

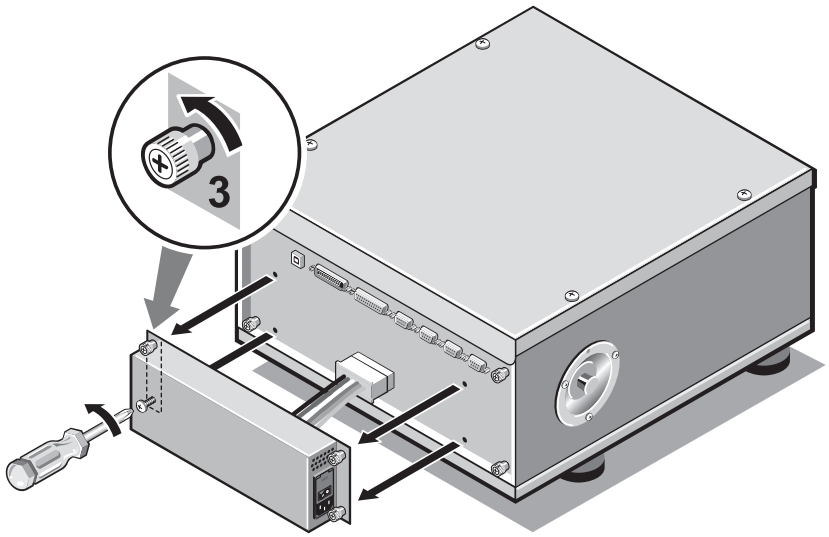
1. **Turn off the analyzer power.**

2. **Disconnect the power cord from the power strip or wall outlet, and then disconnect the power cord from the analyzer.**



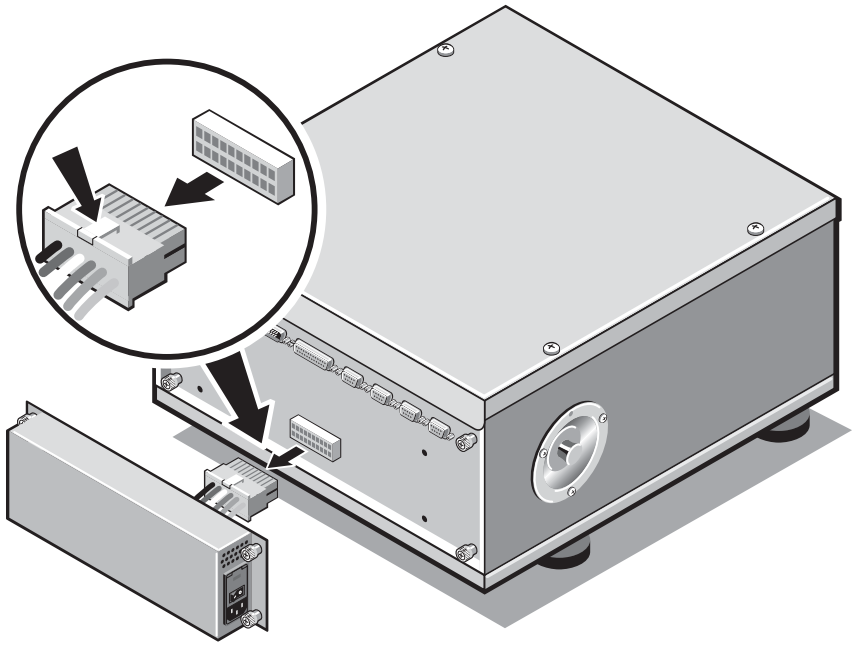
3. **Use a No. 2 Phillips screwdriver to loosen the screws that secure the power supply module to the back of the analyzer, and then remove the power supply.**

**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. ▲



4. **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.

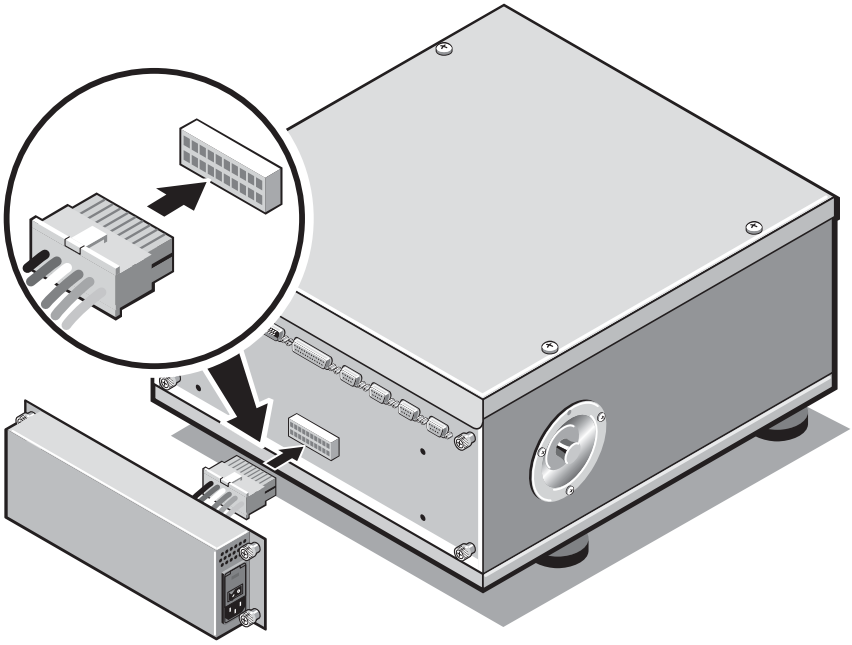


**Note** Be sure to record the installation date and the serial number of the new power supply before you install it. Use Update Instrument Information in the Service menu of RESULT Operation. ▲

**⚠ Warning** Avoid shock hazard! Before you install a new power supply, make sure the analyzer power is turned off. ▲

5. **Connect the cable from the new power supply module to the electronics module.**

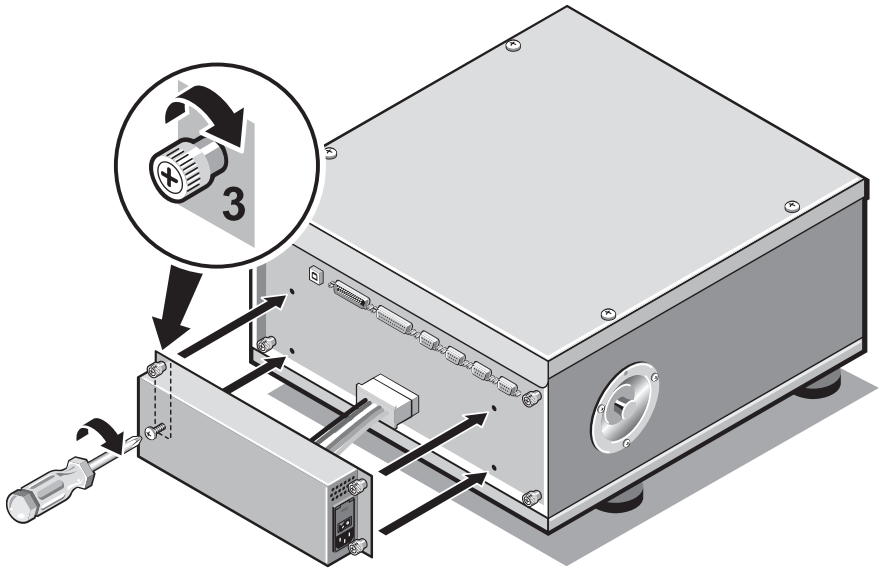
   Make sure the tab on the cable connector snaps into place.



**Notice** Make sure no cables or wires get pinched under the power supply module when you attach it to the analyzer. ▲

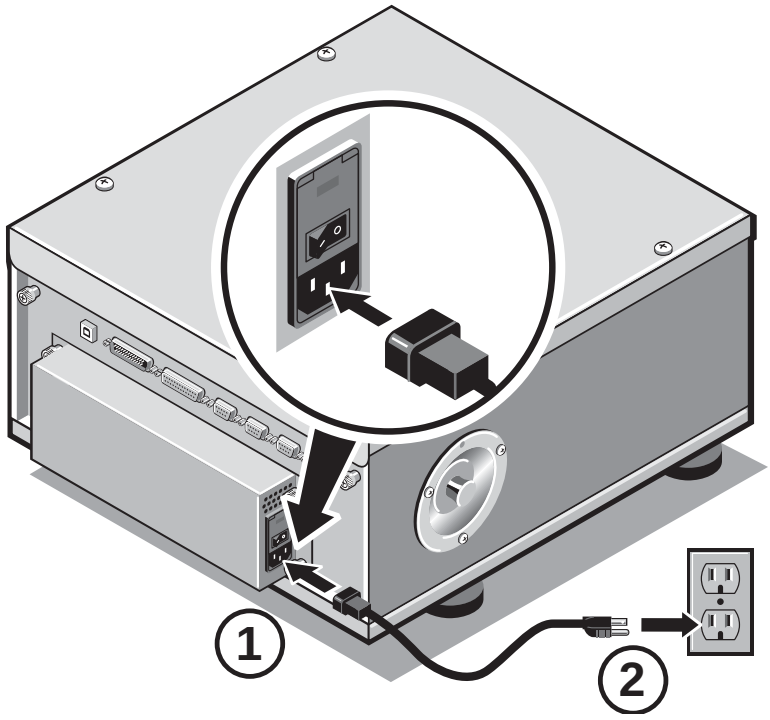
**6. Attach the new power supply module to the analyzer.**

Tighten all of the power supply module screws, but do not over tighten them.




**Note** Three of the screws on the power supply module are thumbscrews that you can tighten without a screwdriver. The fourth screw is a Phillips screw that you will need a No. 2 Phillips screwdriver to tighten. ▲

7. **Connect the power cord to the analyzer, and then connect the power cord to a wall outlet or power strip.**




8. **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 the power back off 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 Technical Support.

## Replacing the source

As with all light sources, the white light source in the analyzer must be replaced occasionally.

**Notice** Never touch the new source bulb with your bare fingers. Skin oils or other deposits on the bulb will shorten its life. ▲

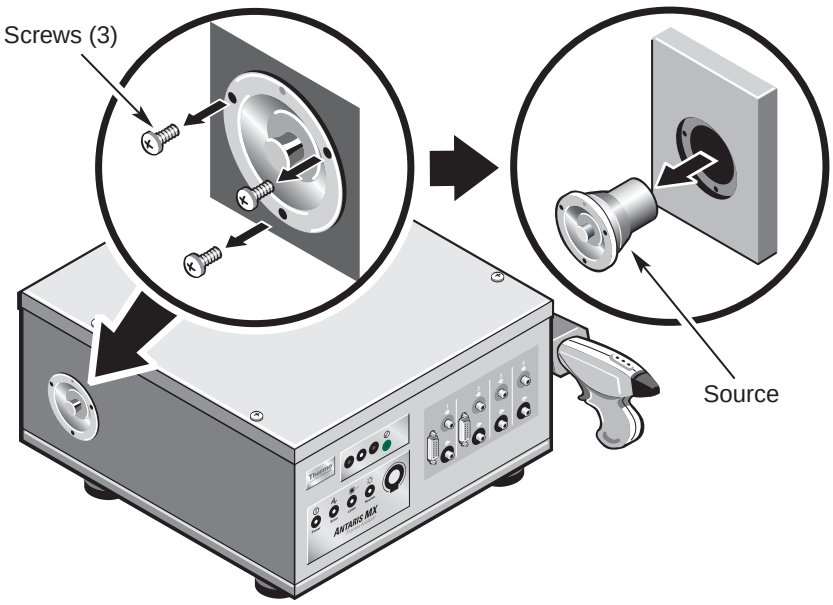
**Note** Be sure to record the installation date and the serial number of the new source before you install it. Use Update Instrument Information in the Service menu of RESULT Operation. ▲

**⚠ Caution** The source becomes extremely hot during normal analyzer operation. Always turn off the analyzer and allow the source to cool for at least 15 minutes before removing it from the analyzer. ▲

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 to reassemble the analyzer.

**⚠ Caution** Avoid burn hazard. Always turn off the analyzer and allow the source to cool for at least 15 minutes before removing it from the analyzer. Always grasp the base of the source when removing it from the analyzer. ▲

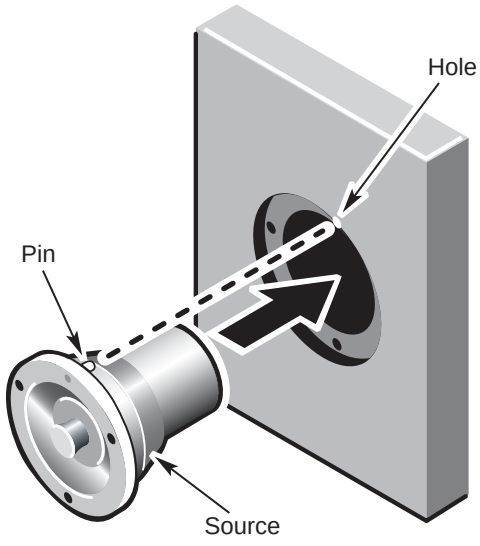
**3. Slide the source module out of the analyzer.**

See the preceding illustration.

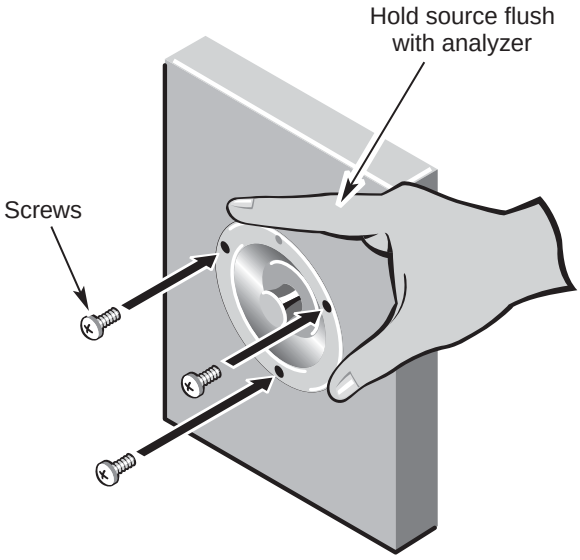
**Notice** Never touch the new source bulb with your bare fingers. Skin oils or other deposits on the bulb shorten its life. ▲

**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 Operation 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 finish.

   If the new source is not working properly, make sure the source module is firmly seated and is flush with the analyzer chassis. If the source still does not work, contact Technical Support.

7. **Wait 15 minutes for the new components to stabilize thermally, and then align the analyzer.**

   See "Chapter 5 System Maintenance" in "Section 3 RESULT Operation Software" of your *RESULT User's Guide* for information about aligning the analyzer.

8. **If the system has optional ValPro software, use it to confirm that the analyzer is performing properly.**

**Note** You may notice increased levels of water in spectra collected immediately after you change the source. If this interferes with your data, wait until equilibrium is re-established. ▲

9. **Use the analyzer qualification procedures and/or run workflows developed for the analyzer, and confirm the results.**

   After confirming the results, you can begin collecting spectra.

## Replacing the laser

The analyzer contains a HeNe laser that is used for timing interferometer scans. If the laser burns out or is otherwise not functioning properly, the analyzer does not scan.

**Notice** Although the laser can be easily replaced by the system operator, it is recommended that only Thermo Fisher Scientific-certified service engineers or our-trained 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. ▲

**Note** Be sure to record the installation date and the serial number of the new laser before you install it. Use Update Instrument Information in the Service menu of RESULT Operation. ▲

**Notice** If your system has the ValPro option, you may need to re-qualify your system before analyzing production samples. ▲

## Removing the laser

Follow the steps below to remove the laser.

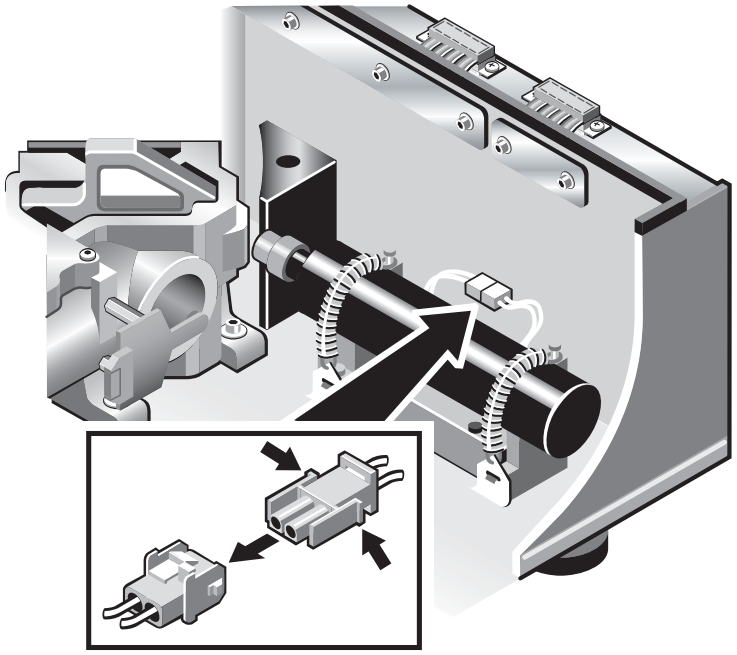
**⚠ Warning** Before removing the burned out laser, make sure you turn off the analyzer power and disconnect the power cord from the wall outlet or power strip. ▲

1. **Turn off the analyzer power and then disconnect the power cord from the wall outlet or power strip.**

2. **Open the main cover.**

   See “Removing the main cover” in the preceding chapter for instructions.

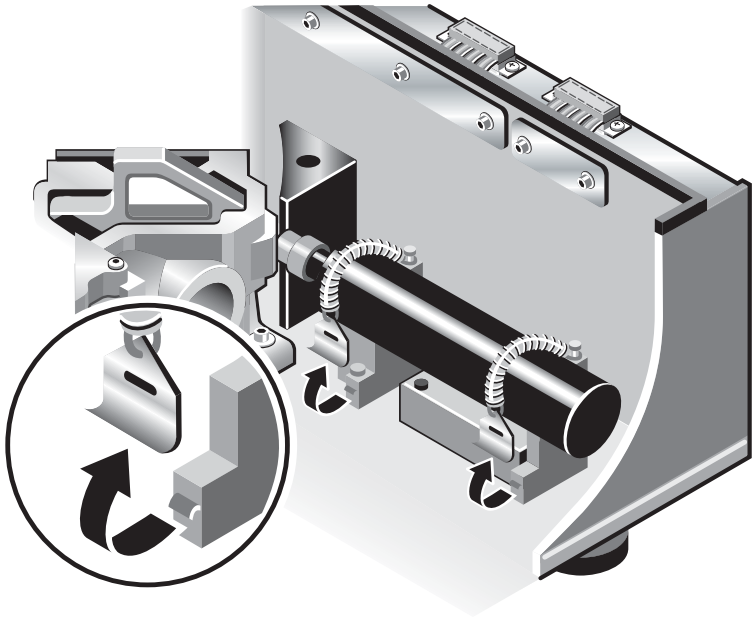
3. **Disconnect the laser power supply cable.**



**Notice** Make sure you hold onto the clip at the end of the spring when you release the spring. Needle-nose pliers may help you hold onto the clip. ▲

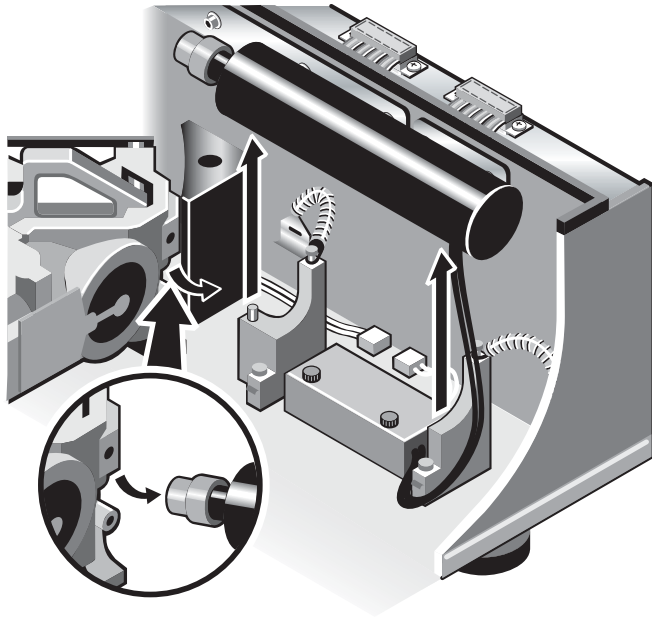
4. **Grasp the clips at the ends of the springs and gently release them.**

   The laser is held in position by two springs and an alignment pin.

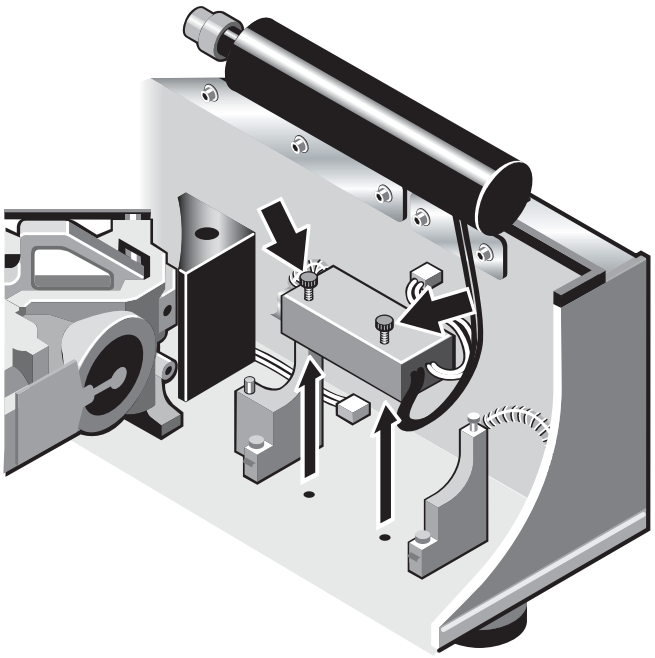


5. **Lift the laser straight up until it clears the alignment pin on the cradle and then angle the laser out from under the metal casting.**

**Notice** Hold the laser while you remove the laser power supply. ▲



6. **Remove the thumbscrews that secure the laser power supply, and then lift the laser power supply out of the analyzer.**



Save the thumbscrews. You will need them to secure the power supply for the new laser.

**Notice** Please return the old laser and power supply to Thermo Fisher Scientific so we can determine why it failed. ▲

## Installing a new laser

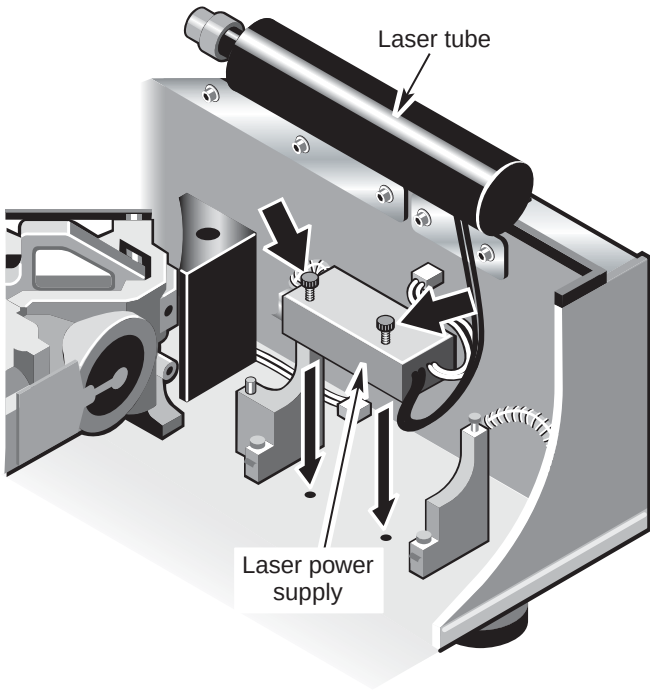
Follow the steps below to install a new laser.

**⚠ Warning** Before installing a new laser, turn off the analyzer power, disconnect the power cord, open the main cover, and remove the old laser as explained in the preceding section. ▲

**Notice** Make sure no wires get caught or pinched under the new laser power supply when you secure it to the analyzer baseplate. ▲

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.

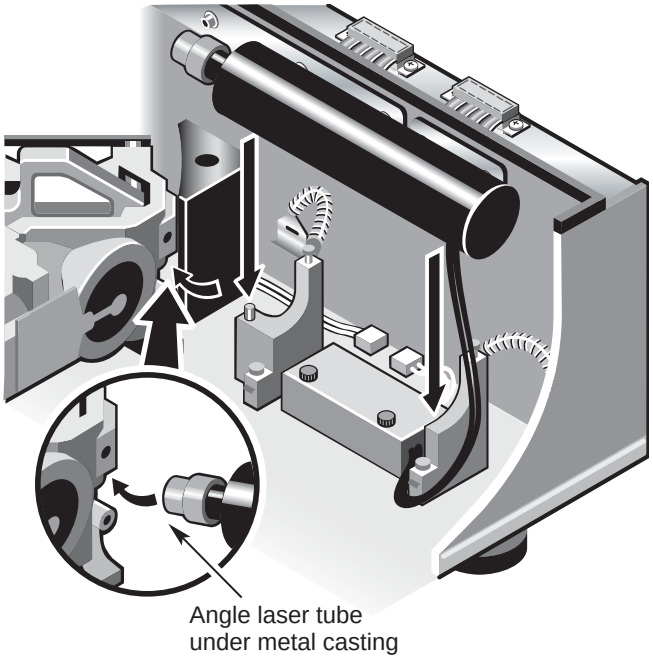



**Notice** Do not attempt to twist or turn the laser once it engages the alignment pin. If the laser is misaligned, the analyzer will not scan. ▲

**Notice** Make sure no wires get caught or pinched under the new laser tube when you lower it onto the cradle. ▲

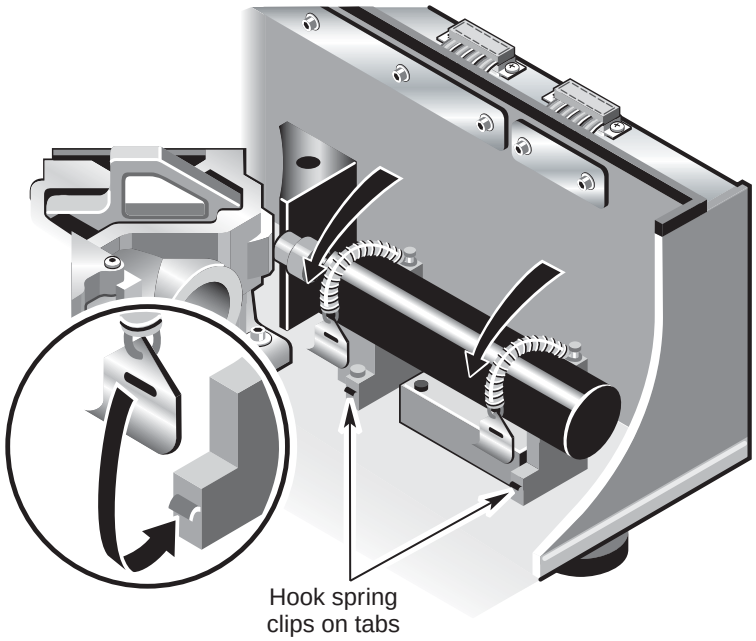
2. **Angle the laser tube under the metal casting and then lower it onto the cradle.**

   Be sure the hole in the laser is aligned with the pin on the cradle.



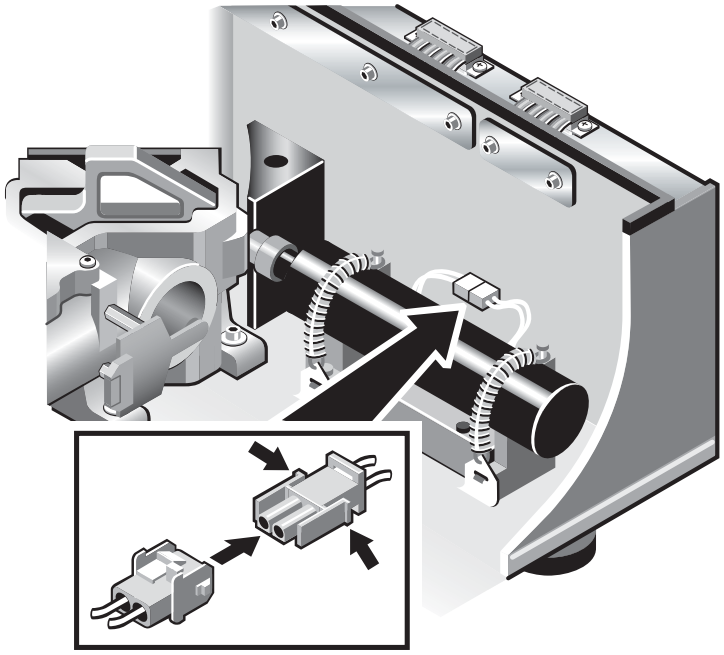
**Notice** Make sure you hold onto the clip at the end of the spring when you release the spring. Needle-nose pliers may help you hold onto the clip. ▲

3. **Grasp the clips at the ends of the springs that hold the laser in position. Gently stretch the springs over the laser tube and hook the clips on their tabs.**



4. **Connect the cable to the laser power supply.**

   The connectors are keyed so that you cannot plug it in backwards.



5. **Close the main cover and secure it with the screws you loosened earlier.**

6. **Reconnect the power cord and any cables you removed earlier, and then turn on the analyzer power.**

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, make sure the laser power cable is properly connected. If it is, and the laser still does not work, contact Technical Support.

8. **Wait 15 minutes for the new components to stabilize thermally and then align the analyzer.**

   See "Chapter 5 System Maintenance" in "Section 3 RESULT Operation Software" of your *RESULT User's Guide* for information about aligning the analyzer.

9. **If the system has optional ValPro software, use it to confirm that the analyzer is performing properly.**

   You may notice increased levels of water in spectra collected immediately after you change the laser. If this interferes with your data, wait until equilibrium is re-established.

## Installing purge gas controls

Antaris MX analyzers are sealed and desiccated. Under normal operating conditions, this provides adequate protection against environmental humidity and corrosive elements that can damage the optical components inside the analyzer.

If you wish to remove water from background spectra, or 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 as explained below. 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. Contact Technical Support for information about air driers and clean air systems. The next section explains how to set the purge gas controls.

**⚠ 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 gases, even inert gases such as argon (Ar), can damage the analyzer. Never use them to purge the analyzer. ▲

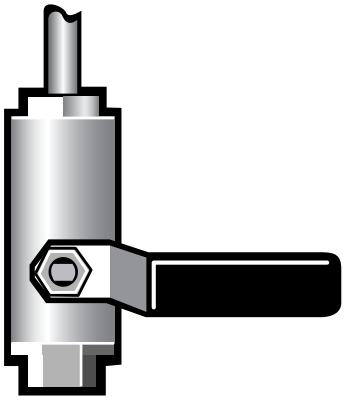
For this procedure you will need the following tools and supplies:

- ¾-inch open-ended wrench
- ¼-inch male fitting or a ⅜-inch female fitting
- $^{11}/_{16}$-inch open-ended wrench
- Shutoff valve
- Optional purge kit

Follow these steps:

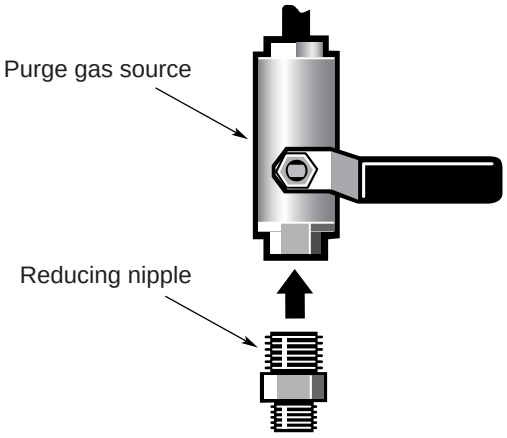
1. **Install a shutoff valve and either a 1/4-inch male fitting or a 3/8-inch female fitting on the purge gas source.**

   Choose a shutoff valve and fittings that are appropriate for the purge gas source.



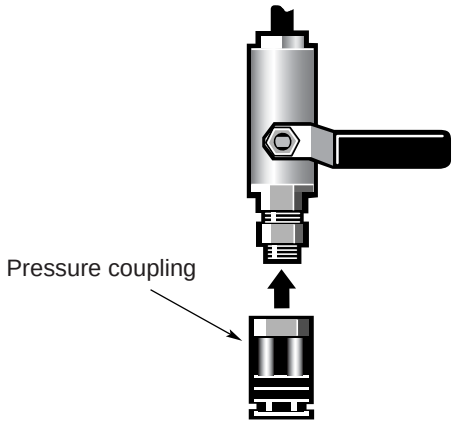
2. **If you used a 1/4-inch male fitting, go on to the next step. If you used a 3/8-inch female fitting on the purge gas source, install the 3/8-inch to 1/4-inch reducing nipple that was included with the pre-installation kit.**

   Use an 11/16-inch open-ended wrench to tighten the connection.



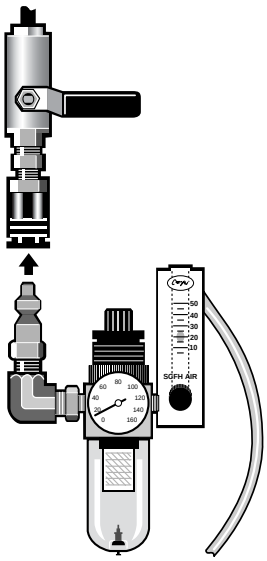
3. **Install the pressure coupling.**

   Use a 3/4-inch open-ended wrench to tighten the connection.



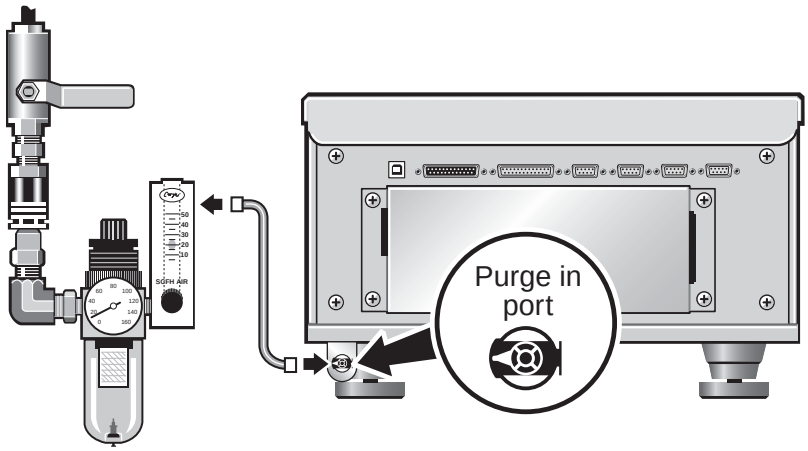

4. **Install the purge filter, pressure regulator, and flowmeter.**

   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.

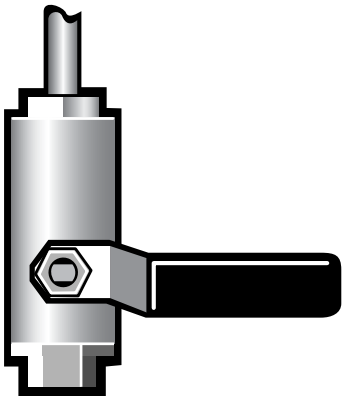



The next section explains how to set the purge gas controls.

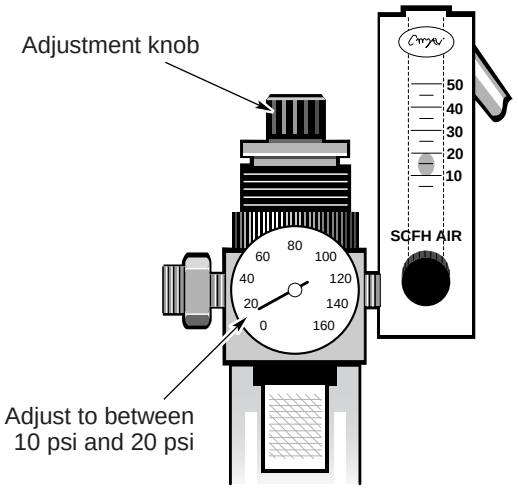
## Setting the purge gas controls

After you have installed the purge gas controls as explained in the preceding section, follow these steps to set the controls:

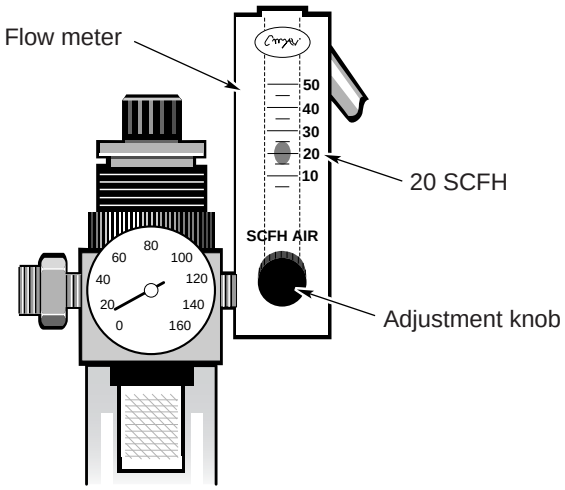
1. **Turn on the shutoff valve.**



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.**



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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 x $10^{-6}$ 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 s**ee *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** 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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