Glossary for RESULT Software and Antaris Systems

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 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*.

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 year, month, day and local time and 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 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* 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*.

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 software.

M

MCT detector Mercury cadmium telluride detector. See also *detector.*

Measure event A workflow event in *RESULT Integration* that instructs the software to measure the spectrum from a specified *collect event, collect sequence event,* or *collect multi-channel event* using the indicated settings for the measurement parameters and a *measurement specification*. Each measurement event produces a measurement result, such as a spectral peak height, concentration value, or class.

measured value The concentration value or spectral measurement produced by the *calibrated* method for each spectrum. Measured values are produced by a *measure event* or *a compare event* in *RESULT Integration*.

Measurement Only A *spectral measurement method* in *TQ Analyst* that measures attributes of an unknown sample spectrum, such as a peak height or area, and reports the measured value(s).

Measurement specification A workflow *specification* in *RESULT Integration* that contains advanced measurement parameters that are optimized for a given method development software package and measurement type.

Memo Item specification A *workflow specification* in *RESULT Integration* that defines a line or lines of text in a sample report and the specific text that will be included. A memo item specification can be used to add comments, descriptions, or other information to a *sample report*.

MEMS Microelectromechanical Systems (MEMS) is the technology of the very small, with devices measured in micrometers. In the *Antaris Target Blend* analyzer, the heart of the micro-spectrometer is a MEMS microelectronics board. The board houses the *Fabry Perot interferometer* and the *laser* source.

menu A list of *commands* that you can choose to carry out an action or see information.

menu bar The horizontal list of *menu names*, typically near the top of a software application window.

menu name The name of a *menu* that appears in the *menu bar*. You can see the *commands* available in a menu by selecting the menu name.

message-response dialog box A *dialog box* developed using a *request event* in *RESULT Integration* that can contain up to 10 messages requiring responses from an operator when running the *workflow*. The dialog box generates a result containing messages and their corresponding responses.

method A set of parameters and *spectra* that can be used to create a *method model*.

method file A file that specifies the parameter settings and spectra for an analytical *method*.

method model A mathematical relationship that describes how the spectral data for the *calibration standards* correlate with the concentration or classification data.

Michelson interferometer A device that uses a fixed mirror and a moving mirror to split and then recombine the *infrared beam* in a Fourier-transform infrared (FT-IR) or near-infrared (FT-NIR) *spectrometer* or *analyzer*. The process causes constructive and destructive interference across all wavelengths of the infrared light. The output signal is an *interferogram*. A *Fourier transform* is applied to the interferogram to determine the energy at each wavelength. The final output is a *single beam spectrum*.

micrometer The X-axis unit used for *wavelength*. One micrometer equals 1×10^{-6} meter. A micrometer is also known as a micron.

micron see *micrometer*

mid-infrared (mid-IR) The region of *infrared* radiation extending from approximately 4,000 cm^{-1} to 400 cm^{-1}.

model see *method model*

moving mirror The mirror in the *Michelson interferometer* that reflects the infrared *beam* back to the *beamsplitter* while moving toward and away from the beamsplitter in a repeating cycle.

multi-lens optics A system of lenses for efficiently delivering the modulated infrared radiation to the sample.

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 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. We offer 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. Our factory technicians confirm the cleaning with a visual inspection of the component under a polarized light.

P

parameter A property whose value determines the characteristics or behavior of a software application.

Partial Least Squares (PLS) A *quantitative method* in *TQ Analyst* that uses a partial least squares statistical analysis to find relationships between the absorbance spectra and the component concentrations of the corresponding samples.

Paste A *command* that uses *RESULT Integration's* memory features to place information being stored on the application's *clipboard* into another *workflow* file.

path The route followed by an application or operating system to find, *archive*, or retrieve files on a disk.

pathlength The distance a beam of incident energy travels within a *sample*. A longer pathlength increases the absorption of infrared energy by the sample. If the pathlength is too great, totally absorbing bands will result. Since the absorption depends on the pathlength (as well as on concentration), if the pathlengths of the *samples* and the *standards* used to quantify them are not the same, the quantitative method must account for the differences in pathlength. If the pathlength values are known, they can be entered in the quantitative method or specified at run time. A quantitative method can also be configured to predict or calculate the pathlength values if the spectra contain a peak or region that varies with pathlength.

PCR see *Principal Component Regression*

PDF see *portable document format*

peak A region of a *spectrum* where the sample absorbs radiation.

peak area The intensity of a spectral region, determined by finding the sum of the intensity values in the specified X-axis range.

peak height The intensity (Y value) of a spectrum at a given X value.

Perform event A *structural workflow event* in *RESULT Integration* that performs a group of events in sequence. The perform event *parameters* allow you to add comments to the group, check the group for errors, and stop executing the events in the group if errors are found.

performance index A measure of how accurately a *calibrated method* can quantify or classify the *validation standards*.

performance qualification The routine process of verifying that an instrument is performing according to requirements for the instrument's intended use.

Perform-If event A *structural workflow event* in *RESULT Integration* that performs a group of events in sequence. The perform-if event parameters allow you to specify the conditions for when the events in the group should be performed or skipped, based on a *logical test specification* and *conditional test*.

Perform-While event A *structural workflow event* in *RESULT Integration* that performs a group of events in sequence. The perform-while event parameters allow you to specify the conditions for how long the events in the group should be performed, based on a *logical test specification* and *conditional test*.

permissions Rules that govern access to a resource associated with a *workstation* or network, such as a printer or shared folder.

phase see *data collection phase*

Pirouette® A method development software package from InfoMetrix®, Inc. that is compatible with *RESULT software*.

PLS see *Partial Least Squares*

PLSplus/IQ™ A method development software package from Thermo Scientific 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 software 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* software 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 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*. 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 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. We produce *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*. 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 AS 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 software.

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 software 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.